

Simulating organization of convective cloud fields and interactions with the surface

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Somewhere, Dreaming (V) 01.01.13 at 14:55

Jess Sutton

30cm x 30cm

Oil paint on Canvas

Declaration

This dissertation is the result of my own work and contains nothing which is the outcome of work done in collaboration with others, except where specifically indicated in the text and acknowledgements. It describes work undertaken at the University of Cambridge under the supervision of Professor Hans-Friederich Graf. This dissertation has not been submitted in whole or in part for any other degree, diploma, or other qualification at this or any other university.

This dissertation does not exceed the regulation length of 80 000 words, excluding appendices and the bibliography.

Alex Hoffmann

Summary

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The mesoscale organization and structure of convective clouds is thought to be rooted in the thermodynamic properties of the atmosphere and in the turbulent to mesoscale dynamics of the flow. Such structure may contribute to the transition between shallow and deep convection. The thermodynamic state of the boundary layer is forced by the amount of surface fluxes from below. Conversely, landscape patterns and land-cover heterogeneity may equally give rise to focused regions for deep convection triggering, in particular when patch sizes exceed 10 km. Since the convective boundary layer has a mediating function between the surface and deep storm clouds, the connection between surface and upper atmosphere is not straightforward. It is generally believed to involve local erosion of the capping inversion layer, the build-up of a moist energy supply, gradual humidification of the lower-free troposphere that reduces dry air entrainment into burgeoning deeper clouds, and thermal mesoscale circulations that can generate moisture convergence and locally forced ascent. To what extent microscale realistic surface heterogeneity and an interactive surface response matter to shallow and deep convection and its organization remains an open question.

In this dissertation, we describe the coupling of a physiology-based vegetation model (HYBRID) and of a sea surface flux algorithm (COARE) to the cloud-resolving Active Tracer High-resolution Atmospheric Model (ATHAM). We investigate the full diurnal cycle of convection based on the example of the Hector storm over Tiwi Islands, notably the well-characterized event on 30th November 2005. The model performs well in terms of timing and cloud dynamics in comparison to a range of available observations. Also, ATHAM-HYBRID seems to do well in terms of flux partitioning. Whilst awaiting more thorough flux validation, we remain confident that the interactive surface response of both HYBRID and COARE is suited for the purpose of simulating convective-scale processes.

We find the storm system evolution in 3D simulations to be robust with respect to differences in surface configuration and initialization. Within our 3D sensitivity runs, we could not identify a strong dependence on either realistic surface heterogeneity in the island landscape or on the interactive surface response. We conclude that in our case study at least, atmospheric (turbulent) dynamics likely dominate over surface heterogeneity effects, provided that the bulk magnitude of the surface energy fluxes, and their partitioning into sensible and latent heat (Bowen ratio), remain unaltered. This is consistent with 2D sensitivity studies, where we find model grid-spacing and momentum diffusion, governing the dynamics, to have an important influence on the overall evolution of deep convection. Fine grid-spacing is necessary, as the median width of updraught cores mostly does not exceed 1000 m. We associate this influence with the dry air entrainment rate in the wake of rising parcels, and with how resolution and diffusion act on coherent structures in the flow. In 2D sensitivity studies with differences in realistic heterogeneities of surface properties, we find little evidence for a clear deterministic influence of these properties on the transition between shallow and deep convection, in spite of largely different storm evolutions across the various runs. In these runs, we tentatively ascribe triggering to stochastic features in the flow, without discarding the relevance of convergence lines produced by mesoscale density currents, such as the sea breeze and cold pool storm outflows.

Errata

Several figures feature (mass) mixing ratio labels. These should read specific concentrations.

Several figures use q_w to denote cloud droplet liquid water specific concentration. This should read q_l .

Contents

Declaration	5
Summary	7
Errata	9
Contents	10
Acronyms	13
Chapter 1 Preface and motivation	15
1.1 On the relevance of clouds and atmospheric moist convection	15
1.2 A case for high-resolution modelling of convective clouds	17
1.3 Aims and outline of this dissertation	20
Chapter 2 Introduction	24
2.1 Organization, evolution and transition of convection, and the influence of entrainment, dynamics, and surface interactions	24
Triggering and the role of convergence lines, free tropospheric humidity and entrainment	25
Organization of shallow and deep convection and its role in the transition between the two	28
Surface-induced thermal mesoscale circulations, their role in initiating deep convection and considerations about patchiness scale	31
Small-scale circulations and organized turbulence: does surface heterogeneity matter?	35
2.2 Diurnal convection on the Maritime Continent: the example of the Hector storm over Tiwi Islands	37
Chapter 3 The Active Tracers High-resolution Atmospheric Model (ATHAM) and the influence of microphysics, turbulence, radiation and active tracers on a single shallow convective cloud	41
3.1 Model history, formulation, active tracers and radiation scheme	41
3.2 Turbulence scheme and LES capability	43
3.3 Cloud microphysics scheme	46
3.4 Methods	47
Model configuration and initialization	47
Modifications of the equation of state and simulation matrix	50
3.5 Results and discussions	52

Chapter 4	The Hector storm and surface interactions: methods, theory and data	63
4.1	Adopting and interfacing an interactive surface as a model lower boundary	63
	Interface design	66
	Surface wind speed, gustiness and similarity	67
	Radiation and albedo	69
	Surface layer and skin temperatures	69
	Roughness lengths and stability parameterizations	71
	Surface layer flux transfers	77
	Flux enhancement in a preliminary shallow waters parameterization	84
	The mixed blessing of additional complexity	86
4.2	Processing multiple data sources for initializing the surface state	86
4.3	Simulating instrumental data for better model-observations intercomparison	98
4.4	Model atmosphere configuration, setup and initialization	106
Chapter 5	Results and discussions	113
5.1	Comparison of the baseline simulation to cloud-top remote sensing observations	113
5.2	Comparison of the baseline simulation to anvil in situ observations and some insights into convective dynamics, transport and overturning	120
5.3	Comparison of the baseline simulation to radar observations	132
5.4	From shallow boundary layer thermals to deep convective storm cells in 2D: insights and influence of diffusion and grid-spacing	137
	Objectives, setup and simulations performed	137
	Integrated diagnostics	139
	Shallow convection and updraught core statistics	149
	Deep convection and surface interactions	157
	Turbulence and energetics	176
5.5	Deep convection triggering in 2D: influence of surface properties	188
	Objectives, setup and simulations performed	188
	Integrated diagnostics	189
	Surface fluxes, surface layer, atmospheric boundary layer and triggering	192
5.6	The diurnal cycle in 3D: structure in a convective cloud field and the competing roles of surface interactions and self-organizing circulations	203
	Surface fluxes and comparison to measurements and other models	203
	Objectives, setup and simulations performed	208
	Integrated diagnostics and statistics	209
	Structural evolution and storm propagation	212
Chapter 6	Concluding remarks and outlook	219

Acknowledgments	225
References	228
Appendix A: Note on wave parameterizations in COARE	246
Appendix B: New serial/parallel output facilities and model versioning	247

Acronyms

ATHAM	Active Tracer High-resolution Atmospheric Model
CAPE	Convective Available Potential Energy
CIN	Convective Inhibition
COSP	CFMIP Observation Simulator Package
CRM	Cloud-Resolving Model
GCM	Global Circulation Model
GPT	Generalized Plant Type
IWP	Ice Water Path
LAI	Leaf Area Index
LES	Large Eddy Simulation
L(S)T	Local (Solar) Time
LWP	Liquid Water Path
MCS	Mesoscale Convective System
NWP	Numerical Weather Prediction
PBL	Planetary (atmospheric) Boundary Layer
RH	Relative Humidity
SCM	Single Column Model
SGS	Subgrid-scale
SST	Sea Surface Temperature
TKE	Turbulent Kinetic Energy
TTL	Tropical Tropopause Layer
UTLS	Upper Troposphere-Lower Stratosphere

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Chapter 1

Preface and motivation

1.1 On the relevance of clouds and atmospheric moist convection

Clouds, water vapour and aerosols consistently continue to contribute as a major source of uncertainties in future climate predictions (Ramanathan et al. (2001), Stephens (2005), Randall et al. (2007), B. Stevens and Bony (2013)). Current problems include the uncertainty in the global distribution of cloud ensembles that occurs as a response to higher surface temperatures, and non-linear interactions between aerosols and clouds that are difficult to quantify (Andreae and Rosenfeld (2008), Rosenfeld (2006), Rosenfeld et al. (2008), Graf (2004)). Further issues include an incomplete understanding of the interactions of clouds with the Earth energy and moisture budgets and vertical structure, as well as with dynamics and the global circulation patterns, and of the behaviour of convection (e.g. Posselt et al. (2012)). In general, clouds are thought to exert on average a net radiative cooling influence (negative forcing) on our planet, though the vertical (and horizontal) distribution of shortwave scattering (cooling) and longwave absorption (warming) is complicated, given the extreme diversity of clouds and cloud properties in space and in time. Conversely, the net radiative feedback (see e.g. M. J. Webb, Lambert, and Gregory (2013) for climate forcings, feedbacks and sensitivity) due to all clouds in the global climate system has long been uncertain but perceived as possibly (Arking (1991)), and today as likely (Zelinka et al. (2013)) to be neutral or positive. Amongst the more contentious issues remains, for instance, the response of low clouds, in particular of (sub-) tropical oceanic cumulus and stratocumulus, to rising surface temperatures (Xu, Cheng, and Zhang (2010)). Or, a polemical hypothesis that holds that reduced (cirrus) detrainment from tropical cumulonimbus outflows (through arguments about a hypothetical increase of precipitation efficiency) might decrease thermal energy retention in cirrus clouds in a warmer climate. Coined the cloud iris effect, this hypothesis is based on a presumably observed inverse relationship between high-cloud area and mean sea surface temperature (SST) of cloudy regions (Lindzen, Chou, and Hou (2001)). Both examples are related to convective processes. The complete picture of the cloud feedback in a changing climate certainly is complex and remains highly topical (Stephens (2005)).

It is linked at many different time and spatial scales through a wide variety of processes, including different behaviour of high-level, low-level and high-latitude clouds (Zelinka et al. (2013)), and involves potential changes to large-scale circulations and the hydrological cycle. Clouds, therefore, continue to preoccupy scientists as one of the most intricate and intriguing problems in atmospheric and climate research.

On shorter timescales, clouds and cloud systems are of importance to weather forecasting, due to their role in the formation of precipitation, in driving atmospheric motions from the local scale of individual thunderstorms to the global scale of the general circulation via latent heat release, and in producing severe weather events, including local wind gusts, hail, lightning, tornadoes, tropical cyclones, and (flash) floods. Consequently, cloud development and factors driving precipitation, including microphysics, must be understood to properly comprehend atmosphere dynamics. As the most spectacular atmospheric manifestation of the Earth's hydrological cycle, clouds are also important objects from a water resource point-of-view. It is well possible that future shifts in atmospheric hydrological patterns and precipitation intensities, partially linked to aerosol indirect effects, may reveal to be more pertinent of an issue than mere temperature changes, not least because of their role in fresh water supply and food production (Lohmann and Feichter (2005)). In epidemiological investigations, changing rainfall is often associated with the spread of vector-borne diseases (Githeko et al. (2000)), even if the links are complex, often speculative and still poorly understood (Mills, Gage, and Khan (2010)).

Convection, in Earth science, mostly refers to the thermally driven movement of a positively (negatively) buoyant fluid against (in the direction of) gravitational pull, and the associated transport of energy within the fluid's mass. In atmospheric physics, moist convection deals with the vertical ascent of warm and moist air masses, within the planetary boundary layer (shallow convection), and higher up, often reaching the upper troposphere and occasionally penetrating into the tropopause layer (deep convection). Because of the adiabatic cooling of the rising air parcels and the condensation of water vapour contained therein, this phenomenon manifests itself quite dramatically in the form of convective cumulus clouds. Precipitating cumulonimbi prosper in mid-latitude summertime and especially in tropical environments. The speed at which these convective towers may evolve to their fabulous heights leaves an appreciation for the high levels of energy involved. Common vertical velocities of a mere few cm s^{-1} in the surrounding atmosphere may reach several tens of m s^{-1} inside the cloud cells. The most palpable role of convective cumulonimbi in the large-scale circulation may well be that of the gigantic 'hot towers' in the Intertropical Convergence Zone (ITCZ), driving the Hadley cell and teleconnections through enormous amounts of latent heat released in the upper

troposphere, and the associated wave propagation. Tao et al. (2003) claim that the mode in which large-scale disturbances control the evolution of convective cells, cloud ensembles and mesoscale systems, as well as the latter's reciprocal effects on these disturbances, remain indeed amongst the most challenging problems in atmospheric science.

Not unlike giant suction pumps, convective clouds also entrain large air masses from the lower troposphere to upper levels and provide an efficient vertical transport system for momentum, heat, water vapour and atmospheric trace constituents. As such, they contribute to the vertical redistribution (overturning) and long-range advective transport of water vapour and atmospheric tracers, including particles and pollutants (e.g. Andreae et al. (2004)). With their frequently warm cloud bases, or say, lifting condensation levels at temperatures above the freezing point, and cloud tops tens of degrees Celsius below zero, deep cumulonimbus clouds commonly have mixed-phase microphysics; that is, interacting cloud particles of both liquid and frozen thermodynamic phases. When the vertically ascending air masses reach levels of neutral buoyancy or a lid of stably stratified air such as the tropopause, they tend to spread out horizontally, producing large cloud anvils of suspended ice crystals. High altitude cirrus clouds produced from the detrainment from cumulonimbi have important climate implications, since they retain upwelling longwave radiation and contribute with a positive forcing to global warming, as mentioned previously.

1.2 A case for high-resolution modelling of convective clouds

Convective clouds evolve within a turbulent flow, through multiple interactions between dynamic and thermodynamic disturbances, through complex microphysical processes, linked to the absorption, scattering and emission of electromagnetic radiation, and are driven by fluxes from turbulent exchange processes at the surface. Capturing all of these processes from measurements and observations alone, simultaneously in three-dimensional space and over time, is nearly impossible. Experimentation in such a complex and extensive natural system is difficult to implement, and effects are impossible to benchmark, since there is virtually no opportunity for control experiments. Numerical modelling techniques provide a holistic or systems approach to cloud process studies, since these tools offer the much-needed framework for relating fragmentary observations. They make for a closer insight into the intricate physical processes at work in atmospheric convective systems, in a dynamically consistent four-dimensional approach (Tao et al. (2003)). Comprehensive simulations that capture the intricate details of convection and

cirrus formation can illustrate the various interactive processes amongst clouds themselves and their surroundings; between deep tropical convection dynamics, transport and overturning, between cloud microphysics, radiation and the larger-scale circulation (May et al. (2008)). They can be used to investigate tracer transport, and provide a useful support for the design of remote sensing retrieval algorithms. Especially Large Eddy Simulations (LES) and Cloud Resolving Models (CRMs), in their non-hydrostatic formulation and with their explicit treatment of the larger turbulent motions, enable the atmospheric community to determine and quantify relevant physical processes during sensitivity studies, as well as to perform detailed dynamic and thermodynamic budget calculations (Tao et al. (2003)). Already over a decade ago, Moncrieff (1997) emphasized that state-of-the-art CRMs could fairly realistically simulate the various process interactions governing the evolution of cloud systems by explicitly resolving the cloud-scale dynamics, setting them aside from other models used for forecasts and climate studies. Nowadays (and with access to sufficient computing resources), Khairoutdinov et al. (2009) argue that LES results can be used as a benchmark for deep tropical convection dynamics, from the individual large eddy to entire Mesoscale Convective Systems (MCS). According to a review by X. Wu and Li (2008), CRMs to date continue to be extensively implemented for the study of convective processes, in particular in the context of surface precipitation and moisture transport; radiation, microphysics and their interactions; the formation, development and propagation of tropical cloud clusters and the role of gravity waves and cloud mergers; dynamical processes, mostly those associated with vorticity and helicity; the ratio of surface rainfall to vapour convergence and evapotranspiration or vapour condensation and deposition, termed large-scale and cloud microphysics precipitation efficiency, respectively; the diurnal nature of tropical oceanic convection with nocturnal precipitation peaks; the interaction between convective precipitation and ocean stratification; the convective-radiation equilibrium of tropical convection; and many other purposes. Stephens (2005) and B. Stevens (2005) argue that a lot to most progress towards the understanding of clouds has been made through enhanced remote sensing capabilities and CRM/LES, thus clearly emphasizing the utility of very-high-resolution numerical experiments for process studies.

Besides much needed process research, these high-resolution models, based largely on first principles and grounded in theory, but also built upon and validated by observations from field campaigns, will often be used for the development and testing of subgrid-scale (SGS) parameterizations to be included in coarser-resolution models (e.g. Grabowski et al. (2006), Kuang and Bretherton (2006)). In the case of convection, the test-bed for these simplified descriptions, before being implemented in full-blown Numerical Weather Prediction (NWP) and General Circulation Models (GCMs) for climate

simulations, will be typically provided by Single Column Model (SCM) versions. The parameterization of clouds and convection in GCMs remains a challenging matter that is unlikely soon to be tamed in view of current computational limitations; especially since not even the most relevant processes necessary to be captured by such parameterizations have been properly identified (Randall et al. (2003)). Some recently suggested approaches to tackle the topic include, for example, superparameterizations, which explicitly simulate convective processes, feedbacks and mesoscale organization by running 2D CRMs inside each GCM grid-box (Grabowski and Smolarkiewicz (1999)), or parameterizations based on Lotka-Volterra population dynamics, in which individual convective clouds in a grid-column compete for the available instability energy (Wagner and Graf (2010)). CRMs, covering a domain the size of a single GCM grid-box, provide a powerful way of testing single column parameterizations.

High-resolution modelling of localized severe weather events also offers opportunities for studying the sensitivity of deep convection (and its forecasting), to fundamental diabatic processes (and their treatment or subgrid parameterization), such as latent heat release due to cloud microphysics, the turbulent mixing of air masses, the radiative flux divergence, or land and ocean surface processes. High-resolution atmospheric models, coupled to land and ocean models, may be required to investigate the driving forces of the surface boundary, and detailed, realistic interactive feedbacks between the biosphere, the hydrosphere and atmospheric convection. To illustrate the above with an example, heavy rainfall and convective activity near the Mediterranean proved to be quite sensitive to the sea surface flux parameterizations used by Lebeaupin Brossier, Ducrocq, and Giordani (2008), because of the very different air-sea flux values that the parameterizations produced (up to 200 Wm^{-2} differences in latent heat), especially under strong surface wind conditions. Another study found that two-way interactive feedback coupling between the atmosphere and ocean slightly decreased the Sea Surface Temperatures (SST) but produced insignificant differences in accumulated rainfall patterns for the short-term simulations of the same heavy flooding events in southern France (Lebeaupin Brossier, Ducrocq, and Giordani (2009)). This suggests that in the case of water bodies with large thermal inertia, these feedbacks may be irrelevant for NWP. It is well known that the initial state of the system is fundamental for the evolution and forecast of meteorological events. Within the same geographical context as the previous studies, investigations into torrential rain and flash floods revealed that the score of quantitative precipitation simulations could indeed be improved with higher resolutions and more advanced physics, but only with a refined analysis for the initial state of the humidity field and surface data (Ducrocq et al. (2002)).

1.3 Aims and outline of this dissertation

Our set goal is to investigate, and to contribute to a better understanding of the detailed two-way interactions between the most intensive single convective storm systems and the underlying surface and planetary boundary layer (PBL), from the storm systems' emergence out of a shallow convective cloud field and throughout their evolution over the course of a diurnal cycle. Of particular interest, as we shall see hereafter, is the transition between shallow and deep convection. So are possible factors explaining the triggering and organization of deep convection. The structure of the initial shallow cumulus field, besides its obvious relevance to problems related to PBL-scale macro-turbulence and cloud-radiation feedbacks, may also influence emerging deep convection. Recognizing the essential role of the PBL as the link between the surface and the free troposphere, buffering humidity, regulating the hydrological cycle and modulating the transition to deep convection, (as well as affecting chemical trace components, aerosols, the biosphere and human activities), we shall dedicate due attention to the convective PBL of the pre-storm environment and during storm propagation.

To our knowledge, few (if any) studies have so far attempted to simulate both shallow and deep moist convection in a unified high-resolution CRM/LES-framework, fully coupled to sea surface and land surface-vegetation models in a truly interactive way to estimate the turbulent flux exchange between the surface and the atmosphere. Such coupled models have been called for by e.g. Petch (2004) in order to attempt to constrain predictability and location of convection. This dissertation documents the development and testing of such a simulation framework, focused on the technical and physical interface, together with the associated observational data-preprocessing framework necessary to initialize the coupled models. It shall constitute the key reference to the rationale behind the coupled models interface, and as such provide guidelines with respect to future usage, parameter choices, performance, caveats, and a vision for further development. We will also describe several large simulation datasets that are available for further analysis.

This dissertation deals with a project that is by its nature multidisciplinary. It is grounded in computational fluid dynamics, cloud physics, turbulence and atmospheric moist convection, within the overarching discipline of scientific computing, requiring, in a collaborative model development framework, best-practice design, coding, testing and validation efforts. Within the emerging field of Earth systems science, it attempts to disentangle multiple complex feedback mechanisms, and to provide a tool for further investigations into biosphere-hydrosphere-atmosphere interactions. It touches upon soil physics and plant biophysics, cloud microphysics, radiative transfer, but also upon

boundary layer meteorology, mesoscale dynamic meteorology, and radar meteorology. It follows the trace of water, from the ocean or soil, through plant stomata into the interfacial surface layer, and from there through the PBL into the free troposphere to end up in the tropopause layer, in a cirrus cloud, or a precipitation droplet. The vast volumes of model output requires thorough considerations in terms of data handling, analysis, visualization, and excursions into more advanced forms of image processing and (geo)statistics. These new tools were furthermore transposed into the geographic, anthropological and hydrological context of the impact of prehistoric ecosystem change on an island's hydro-meteorological budget, in a separate study performed but not included in this dissertation. Finally, the phenomenon of evolving structure (organization) in convective cloud fields not only triggered scientific curiosity, but also a practical interest for its exploitation in gliding and aviation.

The myriad of areas listed above not only reflects the author's interest in multidisciplinary geophysical systems studies from an inductive, process-based and phenomenological perspective, but also the evolving nature of a research project intimately tied to model development and case studies. The main challenge of the approach is twofold. First, the modelling realm of the problems presented above falls in a category generally recognized as the 'terra incognita' between mesoscale modelling and LES (Wyngaard (2004)), where the length-scale of the energy-producing eddies is of the same order as the affordable grid- (or filter-) spacing, since convection is determined by a highly turbulent regime requiring the resolution of individual eddies over domain scales up to several hundreds of kilometres, defying even today's most advanced parallel computing systems. Second, the turbulent nature of the flow and the amount of interactive processes characterizing the coupled systems, allude to the fact that the system's behaviour is by default complex, and potentially chaotic, such that only conglomerates of extensive sensitivity studies may be providing statistically meaningful results. Since large ensemble runs of computationally extremely expensive single experiments are essentially impossible, we chose to put the focus on capturing details in our few simulations. This makes this more of a process study than a collection of statistics for larger-scale model parameterization development efforts. The investigations presented in this dissertation do not, therefore, follow the typical pathway of robust hypothesis testing based on an initial, unique and limited set of targeted research questions.

The first of the two main foci of this dissertation is on characterizing how our CRM/LES model, ATHAM, deals with spontaneous atmospheric convection, a subtle yet equally ferocious phenomenon for which the model had neither initially been designed, nor previously been tested. The second emphasis is on interactive feedbacks between the atmosphere and the surface boundary, characterized by a complex patchwork of sea

surface, soil and biosphere processes, during periods of convective activity. We have coupled ATHAM to the plant physiology and vegetation dynamics model HYBRID, generally used offline or in coupled climate mode, and to the state-of-the-art sea surface flux algorithm COARE, originally implemented during intensive flux measurements at sea, as well as to a series of new input-output facilities and remote sensing simulators. We have then used this new tool over a broad range of convective regimes, from heavily idealized and highly-resolved warm rising bubbles and interacting convective thermals in 2D, over the organization of shallow convection to an intensive mesoscale tropical island convective storm system in the Tropical Warm Pool, named Hector.

Chapter 2 of this dissertation introduces and summarizes some of the past and present literature dealing with the problems we propose to address, notably the processes and factors that contribute to the organization and evolution of (mostly moist) convection, and to the transition between a shallow regime and deep thunderstorms (section 2.1). The main focus herein is on the role of diabatic processes, in particular that of surface fluxes, and on how these set up boundary layer circulations that may contribute to the triggering of deep convection. Such surface-driven circulations can be contrasted against atmospheric internal circulations. Mostly of turbulent nature, and including cold pool density (gravity) currents, they contribute to the (self-) organization of the flow, independently of the underlying surface. Even within this narrowed scope, the literature covers many decades of research from observational, measurements, theoretical, conceptual, scale-reduced physical and numerical modelling perspectives. It is beyond the scope of this project to provide an exhaustive overview of all research into this field, as many review articles and dedicated textbooks are available. We also present an overview of the Hector storm and our selected case study, used as a test-bed for the coupled models (section 2.2).

In chapter 3, we introduce ATHAM, the model that we will run at grid-spacing between that of an LES and a CRM for our fully-coupled 3D experiments. We introduce some of the more advanced features of ATHAM with respect to other similar models, and how these, as well as the main subgrid-scale physics modules, i.e. microphysics, turbulence and radiation, affect the simulation of a single shallow convective cloud.

Chapter 4 deals with the methods and presents the surface models, HYBRID and COARE, the theory they are based upon, their interface to ATHAM, and shortcomings to be considered in this and future studies (section 4.1). We also introduce the data-preprocessing tool based on the initialization of our case study, along with data sources (section 4.2). Furthermore, we developed an interface to a remote sensing observations simulator package, COSP, which will be used for output data post-processing in a

preliminary effort of model ‘validation’ through the comparison to observed data (section 4.3). In the final part of this chapter, we outline the model setup and configuration used in the baseline simulation (section 4.4).

In chapter 5, merging results, discussions and intermediary conclusions for different problems under investigation, we first proceed with comparing our 3D baseline case study to satellite-based cloud-top remote sensing observations, to gain trust in the model’s performance (section 5.1). Apart from the intercomparison to *in situ* data gathered during a large international field campaign, SCOUT, we will look into storm propagation and evolution, environmental air entrainment and convective overturning, as well as the outflow of air, tracers and humidity within the Upper-Troposphere Lower-Stratosphere (section 5.2). The last step towards model characterization and validation is undertaken by comparing synthesized observations to radar data (section 5.3). The following part of the results chapter investigates the influence of model grid-spacing, in other words the extent to which turbulence is resolved, and of diffusion, on the simulated diurnal cycle of convection in 2D (section 5.4). This investigation serves as a proxy for testing the relevance of internal dynamics, and also provides a much more detailed account of important convective processes, hypotheses regarding convective transition, the interaction with the environment and averaged impacts on the environment. The last part of the results chapter first looks into possible causes for deep convection triggering linked to details in surface properties and its interactive response in 2D (section 5.5). We finally investigate convective statistics, structure and rainfall distributions generated in various 3D sensitivity experiments with different surface configurations (section 5.6), hoping to have contributed to a better understanding of the competing role of internal and boundary processes in the organization of convective cloud fields.

In chapter 6, we converge towards concluding remarks, asking whether interactive surface coupling is really necessary in studies as the present one, and suggesting possible ways forward in terms of further process-integration into the model.

Chapter 2

Introduction

2.1 Organization, evolution and transition of convection, and the influence of entrainment, dynamics, and surface interactions

Atmospheric moist convection is often conceptualized as prevailing in three dominant modes: shallow convection penetrating into the convective boundary layer's capping inversion layer, cumulus congestus, which often extends into the melting layer and preconditions (moistens, Chaboureaud et al. (2004)) the free troposphere for further deep convective events, and deep convection, reaching up to and sometimes above the tropopause inversion layer. Over the course of a diurnal cycle, land-based convection is primarily controlled by changes in vertical stability and atmospheric moisture content that result from solar insolation of the Earth's surface, (unless a large-scale tropospheric forcing dominates over the role of surface fluxes, as documented by G. J. Zhang (2003) for midnight convection). A roughly 3-hourly delay usually exists between the midday peak in surface fluxes and convective precipitation, as shallow clouds and initial congestus towers need to transport moisture from the PBL into the free troposphere, as first updraughts that penetrate through the inversion layers need to grow into precipitation stages and rainfall needs to reach the ground level (Bechtold et al. (2004)). With respect to the Hector thunderstorms over Tiwi Islands that are investigated in this dissertation, J. W. Wilson et al. (2001) note that their detailed evolution depends on the complex and chaotic interplay between sea breezes, cumulus clouds, gust fronts and existing storms. In what follows, we shall present, in a broad overview, several of the key ingredients to moist convection, its structure, organization, and transition from shallow to deep, with a particular focus on dynamic processes (circulations) and the role played by surface (diabatic) processes. As we shall argue from the review of past research, micro- to mesoscale PBL variability is omnipresent and often correlated to deep convection triggering, which is sensitive to even subtle changes (typically 1 K or 1 gkg⁻¹ of specific humidity) in the PBL's thermodynamic state (Crook (1996)). Even in the case of a rather flat and homogeneous island, with seemingly strong and anticipated mesoscale forcings (sea breeze convergence) and a predictable influence of the vertical wind profile and

shear, where some skill in the forecasting of certain storm characteristics exists, this variability still matters. An average description of the state of the atmosphere, as gathered from a radiosounding's thermodynamic profile, may not necessarily strongly correlate with the detailed behaviour, timing and amount of convective activity (J. W. Wilson et al. (2001)).

Triggering and the role of convergence lines, free tropospheric humidity and entrainment

The triggering of deep convection is in dynamic terms often a matter of convergent air masses (e.g. J. W. Wilson and Schreiber (1986), J. W. Wilson et al. (1998)), hence the importance of boundary layer wind and moisture flux convergence lines as preferred areas for convective storm development. If boundary layer air that is conditionally unstable with respect to the free tropospheric profile is forced to ascend to the level of free convection, it can initiate deep convection. Convergent wind fields tend to occur near intersecting boundaries of many different kinds. Orography, soil temperature and moisture contrasts related to heterogeneous surface properties, as well as land-sea boundaries all contribute to local modifications of flow regimes. Apart from topography and mechanical flow interactions with surface roughness elements, mostly diabatic processes are at the origin of these local dynamic perturbations. Differential solar heating of the surface and resulting fluxes of sensible and latent heat, radiative processes in the atmosphere, as well as latent heat release or consumption through condensation, freezing, melting, evaporation and sublimation of water in clouds (modified by aerosol-cloud-precipitation interactions) induce various local circulations that may produce low-level convergence lines. Typically, such circulations include land and sea breezes, urban heat island circulations (related to different surface properties, reduced ventilation and anthropogenic heat production in cities, see e.g. Rozoff, Cotton, and Adegoke (2003)), or gust fronts. The latter often spearhead cold pool density currents spreading radially under a convective storm's evaporatively-cooled precipitation downdraught. They may contribute to the triggering of second-generation convective cells and to their growth into Mesoscale Convective Systems (MCS).

Untangling causality is challenging more often than not. For instance, low-level (moisture) convergence and lifting, though usually tightly coupled to convection, is not necessarily the primary cause of its initiation. In the case of West Pacific Warm Pool oceanic convection, Raymond (1995) favours the hypothesis of a boundary-layer quasi-equilibrium acting on time scales larger than half a day. According to this, convection only occurs as the result of a threshold-exceeding PBL budget of equivalent potential temperature θ_e , a common measure of convective instability. Convection would thus act

as a necessary mechanism to balance the gain of PBL θ_e , due to surface fluxes, by low- θ_e downdraught fluxes from upper layers, with other processes such as turbulent clear and dry air entrainment from the lower-free troposphere only playing a secondary role. In this line of thought, moisture convergence would be the consequence, rather than the cause, of convection. We need to emphasize, though, that in this context, convergence relates more to the synoptic than to the mesoscale sort discussed in the context of individual cloud triggering. Also, the atmosphere in the region under investigation usually remains close to the threshold for convection anyway, such that strong triggering mechanisms may not be all that important.

There is an obvious influence of synoptic-scale forcings on the development of convection, which can result in large regions of continuous triggering (see e.g. Loftus, Weber, and Doswell (2008) for an idealized study and parameterization of such sustained forcing of multicellular convection). Yet, the initiation, evolution and organization of deep convection mainly occur on local to regional scales with processes characteristic of the micro- to mesoscales. Over land and from very high-resolution simulations, C.-M. Wu, Stevens, and Arakawa (2009) synthesized the transition from shallow to deep convection to arise only after clouds in the shallow cumulus layer become, on average, buoyant. Looking into statistics of observational data, Y. Zhang and Klein (2010) found larger relative humidity (RH) in and above the PBL (especially between 2-4 km, from advection) to correlate with earlier and longer precipitation events; RH in the lower-free troposphere bore greatest statistical significance when discriminating fair-weather cumulus from deep convective days by environmental parameters. They also found greater heterogeneity within PBL fields to correlate with larger total amounts and more intensive rainfall. This is consistent with the hypothesized role both of humidity in the lower-free troposphere and of PBL heterogeneity, in accelerating the transition between shallow and deep convection, via a facilitated ascent to the level of free convection. In their analysis, the level of free convection, Convective Inhibition (CIN¹), and the ratio of CIN to Convective Available Potential Energy (CAPE¹) are all considerably lower at 11:30 LT during a deep convection day composite compared to a fair-weather cumulus day, even if CAPE and CIN were not found to be significantly different between the regimes in a statistical sense. Surprisingly, diurnal sensible heat fluxes hardly differ, and the latent heat flux is actually lower on the deep convection composite, even if this may reflect a response to higher PBL RH and lower mean winds. In contrast to the preceding study by Wu et al., they found delayed triggering with higher instability. Even with considerable CAPE and virtually no

¹ In this dissertation, we refer to the definition of CAPE given in Emanuel (1994), chapter 6.3. Where CIN is calculated, it refers to the negative area (NA) on the thermodynamic sounding, between the curves of the density temperature of a parcel lifted pseudo-adiabatically from a given initial level (usually within the PBL) and that of the environment.

CIN, Khairoutdinov and Randall (2006) (hereafter, KR06)'s very-high-resolution simulation of the transition over land occurred gradually, after a considerable period of shallow convection, presumably because initial shallow and congestus clouds are too small to penetrate into the free troposphere and rapidly get diluted through entrainment and mixing. They found that precipitation-driven cold pools generating larger updraughts of a more coherent structure on their gust fronts are needed to trigger deep convection, which is consistent with Grabowski et al. (2006), where transition was associated with larger cloud widths, thus reduced entrainment, and a significant increase of the cloud base and sub-cloud downdraught mass flux. The gradual destabilization of the inversion layer alone, in other words, the build-up of positive buoyancy through a deep layer, may not be sufficient to explain the transition. Rather, cloud growth during the transition may, at least to some extent, be driven through a positive feedback that links updraught widths and precipitation downdraughts through the clustering action of cold pools (KR06). Moreover, KR06 found the effect of tropospheric moistening on subsequent convection to be minor, but only since the affected levels were already quite moist. Tropospheric moistening was in fact identified as the primary reason behind the transition to deep convection over a heated mountain in a region of moderate CAPE and high CIN (Kirshbaum (2011)). This involved the rapid succession of growing clouds through the saturated wake of previous updraughts, and furthermore accelerated seeding of glaciation processes (accretion of supercooled liquid drops by ice particles) in the wake of previous ice clouds. A mountain obviously channels updraughts and provides a triggering mechanism on its own. Yet, the importance of this lower- and mid-tropospheric moistening to convective transition has consistently been confirmed by many other studies at different spatial and temporal scales, the transition simulated for oceanic convection over several days in Kuang and Bretherton (2006) being only one amongst them. From various field experiments and nowcasting experience, the intersection between convergence lines was found to favour storm development, but not to consistently lead to deep convection triggering; conversely, rapid storm intensification was almost always preceded by the geographical presence of clouds (J. W. Wilson et al. (1998)). This potentially points to the presence of local lower-free tropospheric moisture anomalies that would favour cloud growth through reduced dry air entrainment.

Review articles by Bennett et al. (2006) and Weckwerth and Parsons (2006) on atmospheric convection initiation over the UK and the US Southern Great Plains (SGP), respectively, highlighted that limited research had so far been dedicated to the area of convection triggering, that some of the corresponding mechanisms remained poorly understood, in particular with respect to timing and location, and that quantitative (convective) rainfall forecasts continued with low skill scores. The studies underlined the

importance of heterogeneous moisture distributions, boundary layer circulations and convergence lines in the PBL. They highlighted the general difficulty to observe the mesoscale pre-storm environment; hence the need for further high-resolution modelling, varied measurements and complementary datasets to elucidate the processes involved. According to Bennett et al. (2006), three conditions tend to favour the initialization of convective phenomena. First, synoptic and mesoscale forcings or processes in the troposphere should have created an environment sensitive to triggering, involving increasing convective instability maintained in a conditionally stable situation. Next, the instabilities could be released due to localized perturbations in the boundary layer that trigger new convective cells. Last, local modifications to the surrounding environment by parent cells, including gust fronts, tropospheric moisture anomalies and static stability variations due to convectively generated gravity waves, could dominate over other perturbations to generate second-generation cells. Convection initiation due to boundaries, such as drylines, frontal regions, gust fronts, bores, orography, those generated by (organized) turbulent motions and others by surface heterogeneities were the main focus in Weckwerth and Parsons (2006)'s review. In recent times, several extensive field campaigns over increasingly complex terrain, including the International H₂O Project over the SGP (IHOP_2002, Weckwerth et al. (2004)), the Convective Storm Initiation Project in maritime southern England (CSIP, Browning et al. (2007)), and the Convective and Orographically-induced Precipitation Study in mountainous south-western Germany/eastern France (COPS, Wulfmeyer et al. (2011)) bear witness of the large interest in the subject of convection initiation and related processes. Another recent campaign over the SGP in the vicinity of the Gulf of Mexico tackled our understanding about how fair-weather cumulus convection relates to land surface conditions (M. Miller (2010)), with key elements to be investigated including soil-plant-atmosphere exchange processes, land cover small-scale spatial structure, aerosol properties and their interactions with the microphysical and macrophysical properties of convective cloud fields, and the influence of the latter on the depletion of low level water vapour advected from the Gulf of Mexico.

Organization of shallow and deep convection and its role in the transition between the two

Atmospheric moist convection seems to favour a variety of multi-scale organized regimes, with transitions between regimes occurring as wind shear, large-scale forcing and turbulent surface fluxes evolve (Moncrieff (1997)). Mesoscale structures in organized shallow convection are manifold and span many different scales, and can take such forms as e.g. cellular (often hexagonal, distorted by precipitation) and linear patterns (Atkinson

and Zhang (1996), Young et al. (2002)); resulting in heterogeneous advective transport through non-isotropic coherent large eddies (e.g. Lothon et al. (2007)). In their LES grid convergence study, Sullivan and Patton (2011) show a striking visualization of a run at 5 m grid-spacing, revealing how the coherent structure of vigorous thermal updraughts at the top of the convective boundary layer, and at the vertices of a hexagonal open cell, roots in the convergence zones within the surface layer. It also shows the thin downdraught 'sheets' enveloping the updraughts (their Fig 13 and Fig 14). Frequently observed (or simulated) transitions in space and in time (e.g. Atkinson and Zhang (1996), Saito et al. (2001), A. Q. Liu et al. (2004), Peckham et al. (2004), Lothon et al. (2007), Bennett et al. (2010)) happen between the characteristic longitudinal Horizontal Convective Rolls (R. A. Brown (1980), Etling and Brown (1993), Gryschka and Raasch (2005)) and closed or open (Rayleigh-Bénard) cells (Bénard (1900), Pellew and Southwell (1940), see e.g. H. Wang and Feingold (2009), Bennett et al. (2010)). These structures likely depend to some extent on the balance between different forms of PBL instability, which can be of thermodynamic (buoyancy) and dynamic (shear, inflection-point) origins, but also on complex (non-linear) interactions with other processes such as cloud and aerosol microphysics, radiation and surface fluxes (e.g. R. A. Brown (1980), Atkinson and Zhang (1996), B. Stevens et al. (2001)). Such instability is often measured in terms of the z_i/L ratio, with z_i being the inversion layer height and L the Obukhov length (e.g. Weckwerth et al. (1997), Peckham et al. (2004), Gryschka et al. (2008), Ito et al. (2010)). In deep convection, organization often generates the previously mentioned MCS (Houze (2004)), which include the frequently observed linearly propagating squall lines (Houze et al. (1989)). MCS are self-organizing, in as much as they develop mesoscale circulations as they mature, rather than being driven through externally-generated circulations. They are characterized by merged clouds with a very large cirriform structure and a large contiguous rainfall area, involving convective and stratiform precipitation. Organized features may produce upscale and up-gradient transport of momentum and thermodynamic properties of the atmosphere. Efforts to find analytical and conceptual frameworks for their parameterization in coarser-resolution models are on their way (e.g. Moncrieff (1997), Mapes and Neale (2011)). Self-organization on different scales and through multiple feedbacks, involving precipitation (even drizzle, facilitating downdraughts through evaporative cooling), dynamics, gravity waves, radiation, moisture transport and surface interactions, amongst other processes, plays a pivotal role in the evolution of cloud systems. This may result in phenomena such as said cellular convection and associated oscillations (e.g. B. Stevens et al. (2005), H. Wang and Feingold (2009), Feingold et al. (2010)), as well as cell broadening (e.g. Schröter, Raasch, and Jansen (2005), Yamada (2008)). Schröter, Raasch, and Jansen (2005) found the cell diameters

not merely to increase with z_i , but the actual aspect ratio of cells to increase, and associated this change with diabatic processes, condensational latent heat release and cloud top cooling. Strengthening updraughts in growing cells might produce clouds large enough to grow into deep convection (e.g. Yamada (2008)). Self-organization in a deep convective system can eventually result in the clustering (aggregation) of convection in a given area, which might even spawn the genesis of tropical cyclones (Mapes (1993), Bretherton, Blossey, and Khairoutdinov (2005)). Organization and structure in convective cloud fields can favour the transition from shallow to deep convection. For example, horizontal convective rolls are often observed to efficiently moisten and precondition the lower troposphere for deep convection triggering, or to provide the triggering mechanism directly through channelled moist updraughts (e.g. Weckwerth, Wilson, and Wakimoto (1996), Weckwerth (2000), A. Q. Liu et al. (2004)). The dynamic interplay between these features and an additional convergence line from say a density current, may generate the necessary ascent for triggering (e.g. Peckham et al. (2004)). J. W. Wilson and Schreiber (1986) indeed seldom observed horizontal convective rolls to trigger storms in Colorado by themselves. The density current may in turn be the product of a previous or an adjacent organized storm system, generated as a cold pool from evaporating precipitation downdraughts (e.g. Tompkins (2001b), Khairoutdinov et al. (2009)). It often features clear gust fronts on its leading edge, sustained through multiple surges of pulsating storm outflow, shaped by the low-level stratification and flow, the behaviour of the parent storm, surface drag and pressure forces (Goff (1976)). Not only do storm outflows spawn new cells in the vicinity of the gust front convergence line, but new convection may also organize on the density current's upper boundary, prone to (interacting) Kelvin-Helmholtz and inertial gravity waves (Weckwerth and Wakimoto (1992)).

Most of the organization and convective structure discussed above is rooted predominantly in the thermodynamic properties of the atmosphere and in the micro- to mesoscale dynamics of the flow. As processes involved in this organization largely determine the propagation and evolution of storm systems, and since they constitute a crucial link in the transition between shallow and deep convection, capturing them in a simulation of the diurnal cycle is essential. The thermodynamic state of the PBL is forced by some averaged amount of surface fluxes from below. Studies focusing on the structure in convective cloud fields without interactive surface fluxes provide limited insight into the question whether (and to what extent) heterogeneity in these surface fluxes may matter as well.

Surface-induced thermal mesoscale circulations, their role in initiating deep convection and considerations about patchiness scale

Other mesoscale flows regularly associated with the transition to deep convection, clearly result from surface heterogeneities, differential fluxes, and associated baroclinic instabilities. The most notorious of all is the sea breeze (S. T. K. Miller et al. (2003), Crosman and Horel (2010)), judging by the vast literature base. The sea breeze is often linked to deep convection triggering, either by itself (e.g. Baker et al. (2001)), through convergence with other density currents such as cold pools and their gust fronts (e.g. Carbone et al. (2000)), or the interception of organized turbulence in the form of horizontal convective rolls (e.g. Dailey and Fovell (1999), Fovell and Dailey (2001), Fovell (2005)). Surface heterogeneities generating boundary layer circulations do not necessarily originate from such stark contrasts as between land and sea. They may be induced by land cover patchiness or soil moisture gradients set up by previous precipitation, effectively providing a feedback mechanism (see Seneviratne et al. (2010) for soil moisture feedbacks in the climate system). Baker et al. (2001) found soil moisture to focus sea breeze-initiated heavy precipitation over previously wet soil, though this was CAPE-mediated rather than involving a dynamic mechanism. Similarly, even at small spatial scales, deep convection has been found to set up positive hydrologic feedbacks between rainfall and soil moisture (particularly in continental semiarid regions), establishing persistent rainfall patterns at scales of the order of 10 km (C. M. Taylor and Lebel (1998), Clark, Taylor, and Thorpe (2004)). In contrast, a negative dynamic feedback, eliminating soil moisture discontinuities, has been suggested by Avissar and Liu (1996) for shallow convective clouds, wherein a mesoscale circulation is converging over dry areas generating more sensible heat.

The idea of landscape-induced convection initiation and organization is not new. In his review article, Pielke (2001) argues that landscape processes are as much part of the climate system as are atmospheric processes, and that landscape patterning may produce focused regions for deep convection, with the boundary layer acting as the crucial link between landscape and deep convection. Local and mesoscale circulations can set up triggering areas, with reduced CIN. Whilst an increased latent heat flux may boost CAPE and potentially intensify thunderstorms, the correspondingly lesser sensible heat may reduce triggering likelihood. Using a 1D moist PBL model, D. Zhang and Anthes (1982) found that the evolution of the PBL height was most sensitive, in decreasing order, to moisture availability, surface roughness, albedo and surface heat capacity, though vegetation was not included in their analysis. With higher soil moisture availability, the boundary layer tended to be moister, cooler and shallower. Albedo and soil heat capacity had surprisingly small effects on boundary layer development, and hence, potentially, on

mesoscale circulations. Surface evaporation had a dominating influence and moderated sensible heat release even when higher heat energy was available. Convective turbulence would have been favoured by small soil moisture availability, a rough surface in the absence of moisture, a smooth one otherwise, low albedo and a low thermal heat capacity. The effect of soil moisture heterogeneity and sharp discontinuities on thermally induced mesoscale circulations in flat terrain was investigated by Ookouchi et al. (1984), who found that such circulations could reach the strength of the better-known sea breeze, urban heat islands and other terrain features. Such moisture variability could originate from irregular convective precipitation distribution, topography, vegetation cover, but also irrigation. The authors hypothesized that such circulations would play an important role in cumulus convection and air quality. Simulations with regular patches on scales of several tens to hundreds of km by e.g. Chen and Avissar (1994) were in line with other early work supporting the idea that maximum mesoscale heat fluxes are achieved with a forcing heterogeneity of the order of the local Rossby deformation radius (typically about 100 km, e.g. Lynn, Tao, and Wetzel (1998)). Lynn, Tao, and Wetzel (1998) describe simulated deep convection generated over landscape discontinuities. The most-intensive precipitation occurs on sea breeze-like fronts at patch boundaries (inwards of dry patches larger than 10 km) in their 2D CRM, fully-coupled to a land surface model. Geostationary satellite data analysis such as that by M. E. Brown and Arnold (1998) supports the idea that mesoscale baroclinic circulations, forced by gradients in the surface fluxes of sensible and latent heat, might provide the convergence necessary for air masses to penetrate above the level of free convection. The authors noticed a statistically significant spatial clustering of free convective clouds along land cover type and soil moisture boundaries in Illinois, on days with a weak synoptic flow and large PBL humidity.

Weaver and Avissar (2001), using numerical simulations, documented significant and frequent thermally induced mesoscale circulations in the U.S. Great Plains, induced by flux gradients due to characteristic landscape heterogeneity and anthropogenic land use change. From previous theoretical and numerical studies, they argue that such circulations only replace turbulent eddies of the scale of the boundary layer depth when the characteristic scale of patchiness goes largely beyond 5-10 km, as pointed out e.g. by Avissar and Schmidt (1998). At the initial stages of convection, they identified patches of weak updraught on scales of several tens of km, collocated with similar patches of enhanced sensible heat fluxes, and associated convective organization with landscape patterns. Given the relative importance of buoyancy over horizontal pressure gradient forces set up by heterogeneous sensible heat fluxes, Avissar and Schmidt (1998) had previously found that mesoscale circulations predominantly arise when the mean heat flux is small. They concluded that in such cases, the mesoscale organization of individual

eddies removes the randomness of a field of thermal plumes. Based on similar numerical experiments and wavelet analysis, Baidya Roy and Avissar (2000) concluded that a characteristic scale of surface forcing heterogeneity of the order of 5-10 km removes individual buoyant eddies, which coexist with other mesoscale circulations when set up by larger-scale patchiness. Later numerical studies by Baidya Roy et al. (2003) and their analysis in spectral space, suggested that in a natural landscape consisting of a wide variety of patches at different scales, the atmosphere was likely to select a preferential, narrow and intermediate range of scales of mesoscale motion, typically of the order of 10 km. Their simulations did not produce any coherent circulations with spatially homogeneous fluxes. Elongated features, consistently aligned with the background flow, however started to appear over heterogeneous terrain, and intensified into tighter features when the overall sensible heat flux was enhanced. The hypothesis that the authors draw from their study states that convective structure arises from initial pressure gradients set up by differential fluxes, and later is modified by the synoptic-scale mean flow, until the features decouple from their origins, lose their anchor and subsist because of their own inertia. Weaver (2004) found mesoscale circulations associated with heterogeneity in underlying surface fluxes to be occasionally sufficient to trigger shallow or even deep convection, depending on the atmospheric profile, and that, as mentioned before, such heterogeneity could arise solely as a consequence of atmospheric processes (distributed precipitation, for instance). Removing all heterogeneity in both surface characteristics and initial conditions, conversely, resulted in the absence of strong mesoscale circulations.

Concentrating on the convergence zones set up over land cover boundaries, due to mesoscale vegetation breezes set up by Bowen ratio surface flux partitioning, Garcia-Carreras, Parker, and Marsham (2011) endeavoured to identify the mechanism modulating convection initiation using LES. They used a single measured total surface flux diurnal cycle, in other words, a spatially homogeneous equivalent potential temperature (θ_e) flux, partitioned heterogeneously into different sensible and latent heat fluxes. This resulted in enhanced convection (triggering) over the warm crop boundaries and suppression over forests, consistent with the advection, convergence and local concentration of θ_e (or CAPE) in this region and the persistent lifting at the boundary, akin to the mechanisms parameterized by Loftus, Weber, and Doswell (2008) for larger scales. The relative importance of the thermodynamic to the dynamic effect was found to depend on prevailing CIN. Increased turbulent thermals over central areas with higher sensible heat did not trigger convection by themselves. In this study, too, patchiness, although heterogeneous and realistic, was on typical scales of 10 to tens of km.

Model grid-spacing, dictating the smallest eddy a model can actually resolve, may to some extent have influenced previous findings regarding scales of circulation in many of these and older studies. LES studies are now more abundant, but many still rely on idealized flux patchiness. Letzel and Raasch (2003), performing one of the first LES studies with idealized heterogeneity, highlighted damped temporal oscillations in the PBL flow submitted to a sinusoidal surface heat flux forcing; the documented thermally induced mesoscale circulations only produced kinetic energy levels above a homogeneous control when the forcing wavelength was again larger than 5-10 km. Spectrally, the thermally induced mesoscale circulations modified turbulence intensity in a direction- and scale-selective way; in other words, the circulations had different characteristics in a direction parallel and perpendicular to the heterogeneity, and suppressed turbulence at higher wavenumbers (mostly because of induced large-scale subsidence). The vertical velocities were heavily organized into a narrow peak updraught over the peak of the flux wave, and the intensity of all the other usual random convective boundary layer updraughts was strongly reduced. In a sinusoidal setup with phase-shifted surface sensible and latent heat fluxes and a wavelength of 32 km, Kang and Bryan (2011) simulated earlier and stronger convection initiation due to focused mesoscale convergence updraughts over the warm and dry patch with higher heterogeneity amplitudes. From a similarly idealized setup limited to 4 blocks or 3 strips, C. Wang et al. (2011) showed, in line with other but in contrast to the early studies, that even in relatively strong geostrophic winds of 10 ms^{-1} could a mesoscale heterogeneity signal exist, but that the effect is dependent on the direction with respect to patch alignment. Using the common checkerboard idealized flux heterogeneity at scales between 1.2-10 km, G. Liu, Sun, and Yin (2011) investigated the influence of patchiness scale on the dry eddy structure, and the question whether the dominant scale of organized turbulence is set by the surface heterogeneity length scale or z_i . They found limited impact of patchiness on averaged convective PBL characteristics, and an evolution of the structure of organized large eddies, originally espousing the patch pattern through thermal circulations, into typical polygonal cells with a common aspect ratio (around 1.6) as the PBL deepens over several hours.

Landscape patterns have thus long been thought to give rise to focused regions for deep convection triggering, in particular for patch sizes larger than 10 km. Since the convective PBL, through shallow convection, has a moderating function between the surface and deep storm clouds, the connection between surface and upper atmosphere is not straightforward. It is generally believed to involve local erosion of the capping inversion layer, the build-up of a moist energy supply, gradual humidification of the lower-free troposphere that reduces dry air entrainment into burgeoning deeper clouds, and thermally

induced mesoscale circulations that can result in moisture convergence and locally forced ascent. A lot of the cited literature involved idealized non-interacting surfaces, with relatively large patch sizes, or a grid-spacing limiting the explicit resolution of convection. Though recent studies are starting to tackle the problem, the question remains to what extent microscale (<10 km) realistic surface heterogeneity, and an interactive surface response, matter for shallow and deep convection and its organization.

Small-scale circulations and organized turbulence: does surface heterogeneity matter?

At the microscale, the interactions between surface heterogeneity and organized turbulence are therefore also of interest. Indeed, Raasch and Harbusch (2001) had already simulated a high sensitivity of convective PBL secondary circulations (including rolls) to surface heterogeneity at scales as small as z_i (the inversion layer height, see also footnote 28 in section 4.4), even if their patchiness remained regular (checkerboard) as in most of the previous studies, and was characterized by large differences in fluxes, emulating a typical polar marginal ice zone. In some conditions, shoreline geometry (curvature), orography, or surface heterogeneity (producing differential-flux-induced secondary circulations) might even be conducive to roll formation, which can then be perceived as forced rather than purely self-organized turbulent coherence (Tripoli (2005), Kawase, Sato, and Kimura (2005), Gryschka et al. (2008), Ramos da Silva et al. (2011)). From 50 m grid-spacing LES results with forced idealized flux heterogeneities, Inagaki et al. (2006) confirmed results from earlier studies that a minimum heterogeneity-scale equal to z_i was required to induce a mesoscale flux (or circulation). Whilst a strong mesoscale flux component existed for a 2 km length-scale, it completely vanished at 1 km. Also, even a very weak wind of 1 ms^{-1} perpendicular to the boundary in the case of a 2 km patch cut off the circulation. Most recently, Maronga and Raasch (2013) concluded from 100 m LES of dry convection that secondary circulations, partially taking over some of the heat and moisture transfer from the purely turbulent fluxes, do develop over realistic irregular surface heterogeneities (with many superimposed scales), but that sufficient (time and ensemble) averaging is necessary to separate their faint signal from randomly distributed turbulent (primary) convection, the latter being an order of magnitude stronger. Again, increased winds weakened secondary circulations from sensible heat flux heterogeneities, which were in general difficult to relate to the heat flux patterns, and the influence of agricultural land-use heterogeneity on the convective PBL was found to be small. They simulated rolls at higher winds, and emphasize that a heterogeneous heat flux pattern agglomerates into an effective (streamwise-averaged) flux with increasing wind speeds (increased fetch). This correlates well with secondary vertical velocities, the

upstream flux controlling the resulting secondary circulations. They confirmed the dependence of secondary circulations on the ratio of the heterogeneity-scale to z_i (Patton, Sullivan, and Moeng (2005) for example found strongest regular and idealized patch-induced motions for ratios between 4 and 9).

The general theme of the previous review is the relevance of thermodynamic properties and dynamic circulations across a wide range of scales to the transition between shallow and deep convection at the mesoscale, in the absence of synoptic forcing. It is not clear whether triggering happens intrinsically within the atmosphere or is forced by the surface; or, as seen from the last examples, through a combination of both. Contrary to prescribed-surface experiments (such as many of the above), which may lock convection to certain areas (e.g. of high sensible and/or latent heat fluxes), an interactive surface may not behave likewise. Interactive, sophisticated and realistic surface boundaries are now the norm in mesoscale, NWP and climate models, and have been shown to improve the simulation of moist convection (e.g. Lynn et al. (2001)). They are also used to investigate changes in mesoscale atmospheric flow with land-cover change (e.g. C. H. Marshall et al. (2004)). Yet, few have been implemented in CRMs and LES models for studying deep convection (Patton, Sullivan, and Moeng (2005), Courault et al. (2007), H.-Y. Huang and Margulis (2010), van Heerwaarden, Vilà-Guerau de Arellano, and Bou-Zeid (2011), for example, mostly concentrate on PBL processes). Presumably the complexity of the simulated fluid dynamics makes the analysis and interpretation difficult enough, without introducing further feedbacks.

To determine to what extent these feedbacks are relevant for the evolution of convective cloud fields, the generation of structure and the triggering of deep convection shall be the main objective of this dissertation. We ask whether a realistic, interacting (and physiology-based) surface is required to simulate the development, organization, transition and propagation of diurnal convection, using a CRM/LES to explicitly resolve large turbulence and convection.

In other words, are internal or surface-driven circulations the dominant factor? To what extent does land surface variability matter, in the presence of more significant contrasts from land-sea gradients? Do we observe convective storm triggering locked to small-scale heterogeneities, typically found in many landscapes, or is this process rather of stochastic nature? Are persistent convergence lines necessary for the initiation of big storms? Do they remain robust in our simulations and sensitivity studies, or do they depend on a given choice of parameters?

We make no claim on settling these issues, since they depend, as do the results of most of the work cited above, on the context and conditions of the simulations. Our study is set within the particular framework of tropical island convection, where sea breezes and

associated convergence are strong and introduce interesting dynamic interactions, but may overshadow the signal of more subtle land heterogeneity effects, in particular for small-scale patchiness. Island convection is an ideal test-bed for a non-nested limited area model, when not deploying it in homogeneous landscapes. The emphasis on island convection may however limit the generalization of this work into the broader context, where research predominantly focuses on oceanic or continental convection, even if coastal maritime convection has always generated a substantial interest. A further issue is the spatially highly heterogeneous and temporally transient nature of island convection, which limits statistical analysis.

2.2 Diurnal convection on the Maritime Continent: the example of the Hector storm over Tiwi Islands

Globally, extreme convective events are mostly located over land areas, and there is a clear tendency for the most intensive storms over oceans to be adjacent to land masses (Zipser et al. (2006)). A particular case of tropical island deep convection that is often revisited in the literature deals with the diurnally-generated Tropical Warm Pool Hector storm over the Bathurst and Melville (Tiwi) islands, north of Darwin, Australia (e.g. Keenan et al. (1989), Keenan and Carbone (1992)). Hector storms account for the deepest regularly occurring convection identified on the planet, frequently reaching heights well above 15 km. In spite of a complex rugged coastline and the proximity to the Australian continent, Tiwi can in a first approximation be described as an elliptic lowland in a warm sea, with a fairly uniform and homogeneous land cover composed of open eucalyptus forests (open savannah woodlands). Isolated convective complexes can be observed in a clear and undisturbed environment during both the pre-Monsoon transition period from October to December and the Monsoon-break period early in the following year. The pre-Monsoon Hector storm, peaking between 13:00 and 15:00 LST, is thought to be representative of MCSs triggered over the many islands within the Maritime Continent, comprising the Indonesian archipelago (Keenan et al. (2000)), even if the less vigorous Monsoon systems over Darwin are likely more representative of the marine convection dominating the Tropical Warm Pool region. In terms of relevance to the region, Qian (2008) suggests diurnal convective precipitation in the Maritime Continent to concentrate over islands, though the larger islands may play a predominant role here.

Because of these well-documented and impressive storm clouds, the even topography and surface properties, as well as the lack of urbanization, Hectors over the Tiwi Islands provide an ideal and virtually idealized test-bed for modelling studies.

Consequently, a large amount of remote sensing, *in situ* and modelling data are available for comparison. Also, sensitivity studies into the various processes involved in tropical deep convection are much facilitated (e.g. Crook (2001)). Golding (1993) investigated the sensitivity of simulated island thunderstorms to model grid-spacing, island shape and model microphysics; and confirmed convection to be initiated on sea breeze convergence lines and to be intensified around outflow gust fronts, evolving into squall lines. The merger of individual convective elements (see e.g. Tao and Simpson (1984) and D. Fu and Guo (2012) for simulations of lower-level cold pool-induced bridging with new cell activation and upper-level anvil bridging), involving typically less than 10% of their original number, is highly relevant. Cloud merger can produce 90% of the accumulated precipitation, and is multiplicative rather than additive in rainfall production, with strong implications for convection parameterizations in large-scale models (Simpson et al. (1993)). Second-order mergers, defined as the unification of previously merged storm cells, were found to contribute mostly to increased rainfall, through larger precipitating areas and longer lifetimes of the system. The regeneration of new convection and the merger with existing storm cells, due to westward-propagating gust fronts, is deemed to be the primary mechanism increasing the size of Hectors (J. W. Wilson et al. (2001)). The percentage of trailing stratiform rainfall to total rainfall for pre-Monsoon transition Hectors was estimated on average to be of the order of 20%. Due to limited observed vertical shear of horizontal wind, few of the vigorous Hector storms develop into severe local storms. Carbone et al. (2000) explored different types of mesoscale storm organization and evolution, based on data from the Maritime Continent Thunderstorm Experiment (MCTEX), in particular triggering mechanisms and the complex interplay between island-scale sea breeze and cold pool gust fronts which provide a multiple-stage forcing process for deep convection. These mechanisms and interactions were simulated by Saito et al. (2001), whose sensitivity studies further seemed to indicate that even the small orographic undulations, just as the horizontal scale of the island, were relevant for the organization and intensity of convective activity. They also simulated the typical initial shallow convection pattern of Rayleigh-Bénard open cells over the interior of the island, with clouds on the polygonal vertices, and horizontal convective rolls within the sea breezes of the windward coast (a shallow organization that we reproduced with our 3D runs). During MCTEX, the surface energy exchange over the dominant land cover types was measured by Beringer and Tapper (2002). Land surface fluxes of latent heat were deemed insufficient to trigger the observed deep convection, emphasizing the likely relevance of moisture advection from sea surface fluxes. Sensible heat fluxes were confirmed to be critical to the onset of convection, and the surface energy exchange processes generally important for developing the convective PBL that sustains the

Hectors. On the microscopic side of things, Connolly et al. (2006) investigated aerosol-cloud-precipitation interactions and mixed-phase processes, and their implications for the Hector storms' dynamical structure. Sensitivity studies were conducted to shed light onto the aerosols' thermodynamic, glaciation and riming indirect effects, by directly varying cloud droplet numbers (CDN) and ice nuclei (IN). The generally simulated trend for accumulated precipitation was to decrease with increasing CDN, though the relationships between CDN or IN and cumulus development were non-monotonic, suggesting potentially 'optimal' aerosol concentrations for storm enhancement. Interestingly, the simulations revealed that microphysical processes happening over short time-scales during the overall development cycle, such as homogeneous freezing, could dramatically invigorate convection by quickly accelerating updraughts. Although no interactive surface was coupled to the atmospheric model, it was still pointed out that differential land-sea roughness lengths were required to yield the correct timing of convective onset through sea breeze circulations. A more recent mesoscale modelling publication on triggering mechanisms by Ferretti and Gentile (2009), dealing with multiple-cell interactions in Hectors, still supports the role of the sea breeze and of water vapour content for storm initiation. Furthermore, simulated land-use changes, partitioning the surface energy fluxes in favour of an increased latent heat flux or higher soil moisture contents during the Monsoon season, weakened the islands' deep tropical convection.

A typical Hector according to Keenan et al. (2000) and Simpson et al. (1993) starts with widespread shallow convection with a cloud base between 600 and 1000 m, forced by surface fluxes, gradually moistening, mixing and warming the sub-cloud layer, which will support initial convective elements producing warm rain. During the early phase, short-lived shallow organization in the form of random Rayleigh-Bénard cells or weakly-organized rolls have been observed over the centre of the islands. Next, deeper cumulus cells develop along the (lee) sea breeze front and associated convergence lines, with a typical east-west (zonal) and frequently shear-parallel orientation and corresponding showers, intensified by cloud bridging and merging. Finally, explosive growth within the organizing system may generate updraughts with velocities exceeding 40 ms^{-1} (or up to 50 to 60 ms^{-1} , Simpson et al. (1993)), especially within the upper troposphere's freezing region. Convective towers can then be up to 20 km high. Precipitation downdraughts and resulting density currents may redirect the system into a north-south (meridional) and shear-perpendicular orientation, often located over the channel between the islands (Apsley Strait). Perpendicular to the low-level shear, the system will then propagate in a fashion similar to arc-shaped squall lines with trailing stratiform precipitation. Maximum storm intensities are usually reached around this time (May et al. (2009)). The frequently observed initial easterly component in the lower- to middle-tropospheric background flow

is stipulated to play a role in this evolution due to downward transport of easterly momentum in the downdraughts during the mature phase of the storm. With gradually reduced fluxes over the island, the system is often observed to move offshore, where the squall line quickly loses its convective structure. In short, the typical lifecycle of a Hector storm starts with a multicellular field, which then aggregates to form one or more organized MCSs (Keenan et al. (1990)). Statistically, Hector storms tend to produce more rainfall at higher values of CAPE, low CIN and low shear (May et al. (2009)). High shear, associated with high wind speeds, possibly decreases the residence time of PBL air over the island, thus slowing down boundary layer growth, as well as that of individual storm cells. High values of CIN intensified individual updraughts, but only over a reduced convective area.

The Hector storm simulated for this dissertation occurred on 30th November 2005, and has been thoroughly studied as the ‘Golden Day’ during the SCOUT-03/ACTIVE Darwin aircraft campaign. Detailed accounts of the prevailing meteorological conditions can be found in Brunner et al. (2009), Vaughan et al. (2008) and others; the climatological context of the region is outlined by May et al. (2008). Although pre-monsoonal low-level (PBL) winds usually tend to be dominated by easterlies over Darwin and Tiwi Island before shifting to clear westerlies with the passing Monsoon trough, the particular location of the low-pressure system over Western Australia means that the situation towards the end of November was much less clear-cut (see Fig 1(b) in Brunner et al. (2009) and the authors’ reference to the end-of-November ‘mini-Monsoon’ therein).

Observed convection on 30th November 2005 started at the sea breeze front over the east of Melville. It then moved westward with the steering flow at 700 hPa (Brunner et al. (2009)). The outflow was observed with a slight north-eastward drift, producing anvil cirrus generally too thick to probe with the Falcon airborne lidar system, though cirrus above the background deck had been detected up to 18.2 km on the return flight during the decay of the storm. The overflying M55 aircraft observed the mean anvil at 17 km with overshoots reaching up to 18 km and confirming detached cirrus around 18.5 km.

Chapter 3

The Active Tracers High-resolution Atmospheric Model (ATHAM) and the influence of microphysics, turbulence, radiation and active tracers on a single shallow convective cloud

Here, we introduce a first set of important conventional processes in cloud models, governing some of the main interactions within clouds (see e.g. Curry (1986)), i.e. microphysics, turbulence and radiation, as implemented in our CRM/LES, together with the particular treatment of the influence of the condensed phase on the thermodynamics and dynamics of the fluid flow, i.e. the role of the active tracers. Originally implemented with the particular application to dense multi-phase geophysical plumes in mind, we shall test if this particular treatment has any influence on the evolution of a single shallow convective cloud. If so, we'd expect this influence to increase in the case of deep convection with larger cloud condensate and precipitation shafts, which is the main focus of this dissertation.

3.1 Model history, formulation, active tracers and radiation scheme

The non-hydrostatic mesoscale- γ Active Tracer High-resolution Atmospheric Model (ATHAM) had initially been designed for the simulation of explosive volcanic eruption plumes (Oberhuber et al. (1998), hereafter: OH98, Herzog et al. (1998)). It has been used for research into volcanic gas scavenging, particle aggregation and interactions with cloud microphysics (Textor et al. (2006a), Textor et al. (2006b)), and more recently, into the dynamics of large coignimbrite (Herzog and Graf (2010)) and phreatomagmatic (Van Eaton et al. (2012)) eruption clouds. ATHAM has also been successfully applied to case studies of biomass burning plumes (Trentmann et al. (2002)) and related chemical processes leading to the photochemical production of tropospheric ozone (Trentmann, Andreae, and Graf (2003)), the three-dimensional radiative effects in smoke plumes

(Trentmann et al. (2003)), and pyro-convective biomass smoke injection into the lower stratosphere from a large boreal forest fire (Trentmann et al. (2006), Luderer et al. (2006)). It has also been adopted to examine the aerosol indirect effect in contrasting clean and polluted boundary layers during the Second Aerosol Characterization Experiment (ACE-2) and has revealed good agreement between model results and *in situ* observations (Guo et al. (2007)).

ATHAM is based on a modular structure that makes it possible to add specific process modules to the dynamical core. The core solves, in an Eulerian framework, the Navier-Stokes equations of momentum, and the pressure, temperature and tracer transport equations for a gas-particle mixture (OH98). The main special feature of ATHAM is the consideration of active tracers; in other words, of solid, liquid or gaseous components that have their own heat capacities and densities, and influence the mixture's flow by changing its thermodynamic and dynamic properties. Active tracers, such as atmospheric liquid water, ice and aerosol particles, may significantly change the dynamics of the system. Fallout drag for example plays a major part in convective downdraughts. It is thus an important feature of storm clouds, (if to a lesser extent than of volcanic plumes), and relevant to be captured in simulations.

The numeric description of heat and momentum exchange by active tracers in ATHAM sets the model's main assumptions about the existence of thermodynamic and dynamic equilibriums. The former simply means that all constituents have the same temperature. The latter typically requires sedimentation at terminal fall velocities (drag force in balance with gravitational force). Thermodynamic and dynamic quantities are thus exchanged quasi-instantaneously in the mixture, or at least fast enough to reach equilibrium before the time step is incremented. This is evidently only valid for small tracers and if the adjustment times are faster than the model's temporal resolution. Since temporal and spatial resolutions are linked through the Courant-Friederichs-Lewy criterion, these assumptions impose a limit on ATHAM's finest grid-spacing, which is typically on the order of a few tens of metres. Solving prognostic equations only for the volume mean and dealing with the exchange processes diagnostically considerably decreases the computational effort and speeds up simulations. Momentum and tracer equations are described in flux form to guarantee conservation of momentum and mass; the heat transport equation is in advective form. Since ATHAM had to deal with very large density gradients and flow velocities at the volcano vent, approaching or exceeding the speed of sound, supersonic (Mach number) effects had to be considered. ATHAM is therefore formulated as a fully-compressible model capable of resolving sound waves. It uses centred finite differences for the spatial derivatives, and a Cranck-Nicholson implicit time stepping scheme in a 2D or 3D Cartesian grid with possible grid-stretching to refine

the grid-spacing at a focal point of interest. A cylindrical coordinate framework can also be used for axis-symmetric simulations. Initial conditions are specified via a typical sounding profile of temperature, relative humidity and horizontal winds. The no-slip condition is applied at the Earth surface lower boundary. Lateral boundaries can either be cyclic or computed with a no-slip condition, that is, the predicted quantities at the grid-points near the domain boundaries are copied onto the boundary grid-points, such that no pressure gradient exists between these vertical slabs. Vertical velocity at the upper-level boundary is null and a temperature- and pressure-damping sponge layer (increased diffusion) is applied to avoid the artificial reflection of gravity waves. The area-weighted mean temperature, pressure, horizontal and vertical winds at every model level can be nudged towards the initial profile at every time step, applying the respective difference, divided by a nudging time constant, to each grid-point value (White (2008)). This conserves the simulated structures whilst compensating for possible numerical drifts thus improving heat and mass conservation. Large-scale synoptic flow can potentially be applied to the model domain as an average effect, by nudging the domain-averaged wind, pressure and temperature to a time-varying profile.

Interactive radiative forcing is calculated separately for shortwave and longwave radiation. Scattering and absorption (due to H_2O_v , O_3 , CO_2 and O_2) of solar radiation is estimated with a computationally efficient radiative transfer model based on the delta-Eddington approximation (Joseph, Wiscombe, and Weinman (1976)), computed for 18 spectrum intervals between 0.2 and 5.0 μm (Briegleb (1992), Langmann, Herzog, and Graf (1998)). The effects of cloud water droplets have been aligned with Slingo (1989), those of cloud ice crystals with Chou, Lee, and Yang (2002). Longwave radiation has originally been computed with a different algorithm over 50 wavelength intervals (Chou et al. (2001)), though this scheme has for the present simulations been replaced by the frequently referenced RRTM (Mlawer et al. (1997)).

3.2 Turbulence scheme and LES capability

The entrainment of ambient air into a plume or a cloud modifies buoyancy. The generation of surface fluxes and transport through the convective PBL provide the warm and moist air masses that trigger and energize convection. The detrainment from deep convective cloud tops shapes the anvils and largely determines the fate of water vapour and tracers aloft. These processes are governed by mechanic (shear-generated) and convective (buoyancy-generated) turbulence. In models where the numerical grid cannot capture all scales of turbulence, an adequate description of subgrid-scale turbulence is

thus important, especially in the multi-phase multi-component turbulent flow that characterizes any cloud. Of course, turbulence also acts as a kinetic energy sink, which cascades down the scales before it is dissipated into heat at molecular level. Moeng et al. (2009) performed a scale separation (using a Gaussian filter) of an LES-simulated PBL under the influence of deep convection over an ocean, in order to analyse resolved and subfilter-scale fluxes at typical CRM grid-spacing of 1 km. Even with this relatively coarse spacing, they found ‘resolved’ motion (after applying a 1 km-wide filter) to account on average for over half of the moisture transport within the lower PBL (except for the ca. 150 m-thick surface layer). They also compared the calculated subfilter-scale fluxes to those parameterized by a standard simple eddy diffusivity model (see equations (3.3) and (3.4)). They found that the eddy diffusivity model performed better in the lower cloud layer than in the PBL, but largely underestimated the magnitude of the positive subgrid-scale (SGS) fluxes. A possible shortcoming was attributed to the use of a fixed SGS turbulence length scale λ , an issue that ATHAM attempts to address through prognostic prediction (see below).

Subgrid-scale turbulence in ATHAM is parameterized on the basis of a 1.5-order prognostic SGS turbulent kinetic energy (SGS-TKE) closure scheme, which accounts for the local anisotropy between vertical and horizontal motions. TKE anisotropy in the vertical and horizontal directions, related predominantly to buoyancy-production depending on atmospheric stratification, has been shown to produce characteristic ‘pumping’ structures in the ascending region of volcanic plumes (Herzog, Oberhuber, and Graf (2003)).

Starting from a given expression of the classical Navier-Stokes equations, which describe the dynamics of fluids from planetary-scale motions to dissipative eddies on the Kolmogorov microscale η , one can derive, for a model of given grid-spacing, a set of filtered or grid-resolved equations in Einstein summation notation for momentum conservation (Bryan, Wyngaard, and Fritsch (2003)):

$$\frac{\partial u_i^r}{\partial t} + \frac{\partial(u_i^r u_j^r)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p^r}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} \quad (3.1)$$

Here, u_i corresponds to a velocity component, ρ denotes density, p is pressure, and the superscript² r refers to the fact that we describe only the resolved components, available on the grid. Gravity acceleration, including the centrifugal force, and Coriolis terms have been omitted for the sake of simplifying the argument, and the viscous term has been removed since it is acting on spatial scales much smaller than the ones resolved. The stress tensor τ_{ij} accounts for unresolved (residual) subfilter- or subgrid-scale

² We retain the r -s notation to emphasize spatial filtering into resolved and SGS components within LES theory. Spatial filtering differs from Reynolds time-averaging, where we use the notation $\bar{a}$ for the time-averaged value of quantity a and a' for its temporal fluctuation.

(superscript² s) motions and incorporates the Leonard stress, the cross-term stress and a SGS Reynolds-like stress:

$$\tau_{ij} = (u_i u_j)^r - u_i^r u_j^r = \left[(u_i^r u_j^r)^r - u_i^r u_j^r \right] + \left[(u_i^r u_j^s)^r + (u_i^s u_j^r)^r \right] + (u_i^s u_j^s)^r \quad (3.2)$$

This stress tensor must be parameterized along one of many available methods. Often, (explicit³ spectral cut-off) filters are selected such that the Leonard and cross-term stresses are identically zero and an SGS model only needs to account for the Reynolds-like stress (Bou-Zeid, 2013, personal communication). In ATHAM, implicit filtering is done through the finite numerical grid itself⁴. The SGS stress model provides space- and time-dependent forcing to the resolved turbulence that represents the action of the unresolved motions on the resolved ones, as opposed to the mean effects of the entire turbulent spectrum onto a mean flow, as implemented in large-scale Reynolds-Averaged Navier-Stokes (RANS) models. Traditional LES models, meant to partially resolve fully turbulent flow, should be configured with filter- or grid-spacing Δ_{fg} set well in between the large energy containing and producing scale l and the Kolmogorov microscale η , ideally within the inertial subrange. Practically, for geophysical flow, this may not always be feasible.

The original Smagorinsky-Lilly model (Smagorinsky (1963)) aims to relate the deviatoric part of the Reynolds-like stress to the resolved strain-rate tensor S_{ij}^r and a SGS eddy viscosity (or turbulent transfer coefficient K). The eddy viscosity can also be based on additionally-computed local values of SGS-TKE, as in Deardorff (1980). The anisotropic SGS-TKE scheme in ATHAM uses in effect 2 different scalar turbulent transfer coefficients K_j for horizontal and vertical fluxes⁵. The SGS turbulent correlations of the Reynolds-like stress are then parameterized through a gradient approach, under the assumption of incompressibility, and assuming that turbulence acts like a strong diffusion on momentum and scalars:

$$\tau_{ij} \cong (u_i^s u_j^s)^r = -K_j \frac{\partial}{\partial x_j} u_i^r \quad (3.3)$$

Note that no summation over index j is implied above in equation (3.3). Given the SGS TKE and its horizontal and vertical components expressed as $TKE = (u_i^s u_i^s)^r$,

³ Explicit low-pass spatial filters have a characteristic width $\Delta_f > \Delta_g$, and help the solution to converge to the true solution of the filtered equations at the expense of computational cost compared to implicit filtering, which could be spent on further increasing the model resolution.

⁴ Although implicit grid filtering is technically not equivalent to a spectral cut-off filter (Bou-Zeid, 2013, personal communication), we assume for practical purposes that it is, such that only the Reynolds-like term needs to be accounted for in equation (3.2).

⁵ K_j is actually a 2D matrix assumed diagonal, with one principal axis aligned vertically and another one with the mean wind; $K_j = K_{ij} \delta_{ij}$ (Herzog, Oberhuber, and Graf (2003))

$TKE_{hor} = (u_1^s u_1^s)^r + (u_2^s u_2^s)^r$ and $TKE_{ver} = (u_3^s u_3^s)^r$, respectively, the turbulent transfer coefficients are set proportional to a turbulent length scale λ and the square root of TKE:

$$\begin{aligned} K_1 = K_2 = k_{hor} &= c_0 \lambda \sqrt{3/2 TKE_{hor}} \\ K_3 = k_{ver} &= c_0 \lambda \sqrt{3 TKE_{ver}} \end{aligned} \quad (3.4)$$

where c_0 is an empirical constant. The eddy diffusivities for the various scalar tracers in the model are obtained from K_j via the inverse turbulent Prandtl number.

A prognostic set of three coupled equations for horizontal and vertical SGS TKE and for the characteristic turbulence length scale λ of eddies is solved separately from the resolved flow, treating the main history-dependent non-local effects of turbulence, as outlined in Herzog, Oberhuber, and Graf (2003). For SGS TKE, these equations include advection, turbulent diffusion, wind shear production, buoyancy production, redistribution and dissipation. For λ , they include advection, turbulent diffusion and ‘nudging’ towards an equilibrium term. The equilibrium length scale λ_0 is the smallest value amongst the mean grid-spacing Δ_g , $2/3$ of the distance of the grid-box centre to the ground and an equilibrium length determined by stability (see Deardorff (1980)). Higher-order terms are parameterized, making for a 1.5 order scheme; turbulence decays along a timescale $\tau_0 = \lambda / \sqrt{TKE}$ and active tracers intervene in the buoyancy production of TKE.

3.3 Cloud microphysics scheme

Current mixed-phase cloud microphysics are based on a simple prognostic bulk Kessler-type approach, predicting cloud droplets, rain, ice crystals and graupel as mass per unit volume only (Herzog et al. (1998)). Cloud droplets and ice crystals are assumed monodisperse, with a prescribed radius (10 μm). Rain drops and graupel follow a Marshall-Palmer distribution, and their respective fall velocities are derived diagnostically from their mean radii. Since the width of the droplet spectrum is prescribed, broadening due to autoconversion processes cannot be captured, which might give false precipitation estimates. No aerosol microphysics or activation/nucleation mechanisms are presently implemented. Supersaturation does not exist beyond one time step and the parameterization does not resolve initially small droplets or capture solution and curvature effects. Ice sublimation/deposition is temperature-dependent and only occurs well below freezing level, though ice nuclei (IN) are implicitly supposed to be present at sufficient quantities for heterogeneous deposition and formation of new crystals to occur. Cloud ice melts instantaneously below the freezing isotherm; graupel melts through heat transfer. Supercooled cloud and rainwater are parameterized through a statistical

freezing relationship. A warm-rain two-moment scheme (predicting mass specific concentrations and number densities) is also available, but not used in this study, and current development focuses on a new two-moment mixed-phase cloud microphysics scheme. Additional ATHAM modules include gas scavenging and ash aggregation, emissions, and chemistry.

3.4 Methods

Model configuration and initialization

In order to investigate the influence of the aforementioned physics parameterizations and of the active tracers on moist convection in a controlled environment and with little computational effort, we implemented a new 2D ATHAM configuration. This incorporates the warm, cold, double and Gaussian dry ‘bubble’ test configurations (see Robert (1993)) into a more generic framework in terms of model initialization and the possibility to use any of the available physics modules. It facilitates the setup both of an idealized atmospheric state and of an idealized anomaly initialization.

The idealized state initialization can replace a homogeneously-replicated measured profile (such as from a radiosounding) by an idealized convective PBL capped by an interfacial inversion layer. Rather than using a piecewise-linear potential temperature θ and water vapour specific humidity q_v profile with discontinuous breaks at the bottom and top of the inversion layer, we modelled the inversion that caps a perfectly mixed PBL with a sigmoid (logistics) function f , to emulate the ‘realistic’ capping inversion presented in Deardorff (1979). The advantage over the simpler piecewise-linear treatment resides in removing the necessity of a convective spin-up to remove the discontinuities. Consequently, if θ_{ref} denotes the user-specified mixed reference θ throughout the convective PBL, if $\Delta\theta$ is the user-specified θ jump across the inversion layer, $k-k_i$ is the grid-point distance from the interface midpoint or the sigmoid ‘s inflection point at index k_i (where the latter has a value of $\frac{1}{2}$), h_{zi} is the thickness of the inversion layer (specified as a percentage of vertical grid-points, giving the vertical grid-point index k_{zi}), and where h_{free} is the thickness of the free troposphere above the inversion (specified as a percentage of vertical grid-points, giving k_{free}), the θ profile (Fig 1(a)) in the interface evolves as

$$\begin{aligned} \theta(k) &= \theta_{ref} - f_{tol} \cdot \Delta\theta + f(k - k_i) \cdot \Delta\theta, \text{ for } k_{zi} < k \leq k_{free} \\ f(k - k_i) &= \left(1 + e^{-\alpha(k - k_i)}\right)^{-1}, \text{ with } 0 \leq f \leq 1 \end{aligned} \quad (3.5)$$

The logistics function only tends towards 1 for large values of $k - k_i$, which is why we introduce a further user-specified tolerance parameter f_{tol} that effectively determines the

width of the central part of the sigmoid used, i.e. $f_{tol} \leq f \leq 1 - f_{tol}$, and hence the shape of the inversion profile and the lapse rate of the free atmosphere above. The α parameter then follows as:

$$\alpha = \frac{-\ln\left(\frac{f_{tol}}{1-f_{tol}}\right)}{\left(k_{free} - k_{z_i}\right)/2} \quad (3.6)$$

A large value of f_{tol} effectively yields an almost piecewise-linear profile and a small value a fully sigmoidal interface. The free tropospheric lapse rate follows by assuring a continuous function at the upper end of the interface through differentiation of the logistics function, for $k > k_{free}$:

$$\theta(k) = \theta(k-1) + \Delta\theta \cdot \alpha \cdot f\left(\left(k_{free} - k_{z_i}\right)/2\right) \cdot \left(1 - f\left(\left(k_{free} - k_{z_i}\right)/2\right)\right) \quad (3.7)$$

For the sake of simplicity, we make the q_v profile follow the inverse evolution of the θ profile. Since our idealized initial profiles with capping inversions were not in hydrostatic equilibrium and produced domain-mean vertical oscillations, we updated the original algorithm to compute the hydrostatic pressure profile. This improved the results considerably (by a factor of roughly 10), but an initial damped oscillation remains over roughly the first 10 simulated minutes (see also Bryan and Fritsch (2002) on the topic and difficulties of a moist hydrostatic initialization).

Convective bubbles with different properties can be released into this idealized (or alternatively a realistic) environment, with the possibility to selectively include cloud microphysics, turbulence, radiation and surface fluxes. To emulate a single thermal that may be released from a hypothetical warm patch on the ground, we superimpose a further thermal anomaly onto the θ -field within the surface layer, confined to a Gaussian envelope. To this purpose, we compute a Gaussian distribution envelope of user-specified standard deviation σ_G and amplitude A_G , and create a temperature anomaly that decreases exponentially with height from a user-specified ΔT near the ground towards and across the local height of the envelope. In this preliminary study, we used $h_{z_i} = 20\%$, $h_{free} = 40\%$, $\theta_{ref} = 303.15$ K, $q_{ref} = 19$ gkg⁻¹, $\Delta\theta = 4$ K, $\Delta q = 9$ gkg⁻¹ and $f_{tol} = 0.05$ for the profile, and $\sigma_G = 100$ m, $A_G = 50$ m and $\Delta T = 1$ K for the anomaly. These parameters yield a convective PBL that is in essence similar in depth, heat and moisture content to the initial PBL over the Tiwi Islands studied later, use the same reference potential temperature as in the standard bubble test case, albeit with a strong inversion (Sullivan et al. (1998)), and have been optimized to produce a convective cloud from the surface-forced rising thermal. The resulting initial thermodynamic profiles, as well as the superimposed thermal anomaly, are given in Fig 1(a) and (b), respectively.

In order to simulate the boundary layer with an eddy cut-off within the inertial subrange, D. E. Stevens, Ackerman, and Bretherton (2002) warrant a grid-spacing on the order of 10 m to model eddies responsible for lateral and penetrative entrainment and corresponding mixing processes in individual small cumulus clouds. We did not add any damping layer at the model top boundary, and used a 2D Cartesian grid with open lateral boundaries, 3km large and 2 km high, with homogeneous grid-spacing of 10 m in each direction. Typical simulation time was 60 minutes with full model data-field dumps to file every minute. No mean wind was imposed.

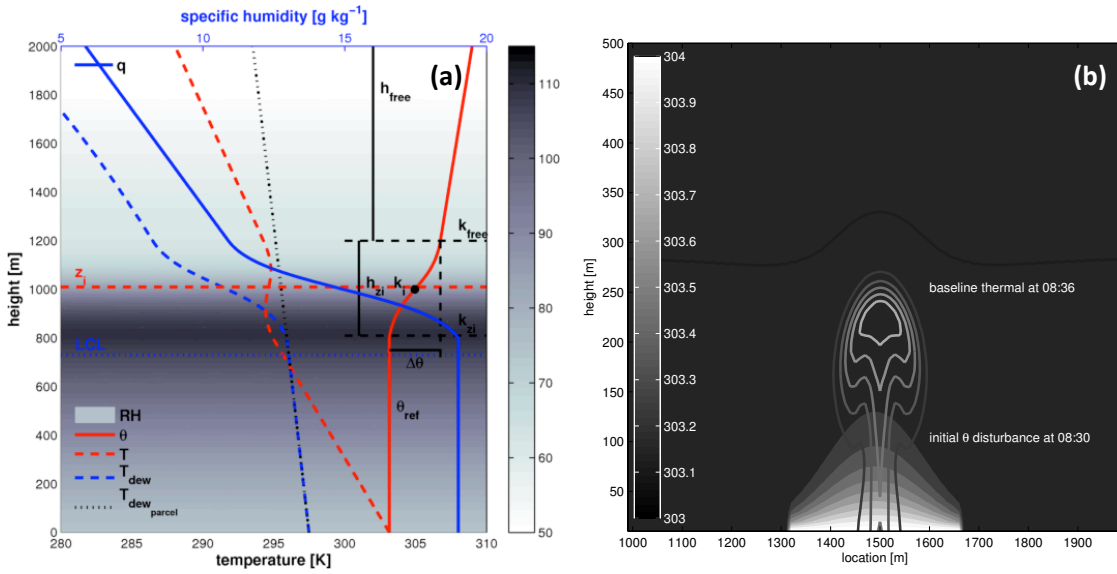


Fig 1 (a) thermodynamic initialization of the model domain. The solid red and blue lines correspond to the idealized θ and q_v profiles, respectively, the associated temperature and dew point temperatures are dashed. Relative humidity is shaded and illustrates the stratified cloud layer around 800 m. Since the convective PBL is well-mixed and given the heat and moisture levels, condensation occurs below the start of the inversion, and the Lifting Condensation Level (LCL), computed for a parcel lifted from the surface layer, cooling dry adiabatically, thus coincides with the cloud base of the predefined cloud deck. PBL height (z_i) is estimated here through the gradient method, taking the level of the maximum value of the virtual potential temperature (θ_v) gradient. Here, this obviously coincides with the sigmoid midpoint and not the lower level of the inversion layer (see Sullivan et al. (1998) for various z_i selection methods); (b) Gaussian thermal anomaly (as θ shading) used to initialize the convective updraught (thermal). The rising thermal is also shown through θ contours after 6 minutes of simulation

Note that our particular model initialization results in a thin supersaturated layer and therefore represents in effect a ‘stratocumulus’ cloud under a strong inversion perturbed by a single convective updraught originating above a warm land surface. A conceptually similar cloud deck, together with the relevant physical processes that will be investigated here, is sketched out in Fig 2(a), albeit for different values of heat and moisture (taken from B. Stevens (2005)). Closed shallow convection cells are sometimes thought to result from the breakup of a stratified cloud deck. Since the stepwise inclusion of the aforementioned processes in this preliminary study leads essentially to a similar

cascade of events and the eventual breakup of the deck as reviewed by Atkinson and Zhang (1996), we take the freedom to use their reproduced Fig 10(a) for reference (Fig 2(b)).

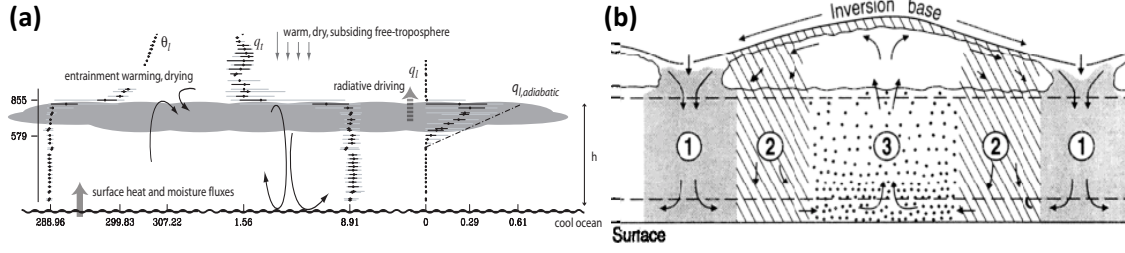


Fig 2 (a) depiction of a well-mixed non-precipitating stratocumulus layer, with airborne measurement statistics of total and liquid water specific humidity (q_t and q_l), and liquid water potential temperature (θ_l), (taken from B. Stevens (2005), their Fig 4); (b) reproduction of a vertical cross-section through a closed cell with a region of warm dry inversion layer air entrainment into the PBL and adiabatic warming (1), of cloud top radiative cooling, convective turbulence generation, sinking, mixing and further evaporative cooling (2), and of longest exposure to surface heat fluxes (3), (taken from Atkinson and Zhang (1996), their Fig 10(a))

Modifications of the equation of state and simulation matrix

Density perturbations, governing the fluid's buoyancy, are intrinsically linked to compositional changes, and compositional effects on the gas constant cannot easily be neglected (B. Stevens (2005)). In particular, the gas constant for a moist fluid (gas) $R_g = c_{p,g} - c_{v,g}$, where $c_{p,g}$ and $c_{v,g}$ denote specific heat at constant pressure and volume, respectively, is often expressed in terms of the parcel's specific humidity in vapour form q_v , the residual dry specific concentration q_d , and the corresponding dry air and water vapour gas constants (R_d and R_v) as:

$$R_g = R_d q_d + R_v q_v = R_d \left(1 + \frac{R_v}{R_d} q_v - q_t \right) \quad (3.8)$$

Herein, q_t denotes the total water specific concentration, which includes the condensates and vapour. The specific heat of water vapour and liquid, however, have traditionally been ignored in most numeric models (Bryan and Fritsch (2002)). Their study demonstrates that neglecting moisture-related terms in thermodynamic and pressure equations can have dramatic impacts on idealized rising thermals, although the authors found a much lesser (albeit potentially relevant) impact in realistic deep convection simulations. With the aim to express relationships in terms of dry gas properties, a virtual temperature is then often defined as $T_v = T(1 + (R_v/R_d)q_v - q_t)$. It represents the temperature of dry air having the same density as moist air at temperature T , which is less dense due to the smaller molecular weight of water in comparison to dry air. Following this, the virtual potential temperature θ_v , obtained when bringing an air

parcel at initial virtual temperature T_v and pressure p adiabatically to a reference pressure p_0 (typically 1013hPa), can then conveniently be defined as:

$$\theta_v \equiv T_v \left(\frac{p_0}{p} \right)^{R_d/c_{p,d}} \quad (3.9)$$

where $c_{p,d}$ represents the specific heat of dry air at constant temperature. If the concept of virtual (potential) temperature is useful for analysis, ATHAM rather relies directly on the mean properties of the mixture.

R_g is used in the ideal gas law $p_g = \rho_g R_g T_g$, which couples the thermodynamics to the dynamics (momentum and pressure equations, see Herzog (1998) for a detailed discussion). In ATHAM, under the assumptions of dynamic and thermodynamic equilibrium, the pressure and *in situ* temperature of the gas (and all other) components p_g and T_g are assumed equal to their volume mean values p and T (OH98, Herzog (1998)). The gas density ρ_g differs from the volume mean density ρ used for the dynamics; the latter is derived diagnostically from the tracers' specific concentrations and respective densities.

Passive tracers constitute components of the fluid that are assumed not to modify the dynamics of the flow via changes of the thermodynamic state. Active tracers, on the contrary, may occur at sufficiently large concentrations that their influence on the thermodynamic state and directly on density can no longer be neglected, resulting in associated impacts on the dynamics (OH98). In ATHAM, designed for the study of dense multi-phase/multi-component plumes, the thermodynamic state is computed via an iterated solver of the equation of state, which incorporates the effects of the active tracers. In our case of convective clouds, these reduce to water in its various phases (vapour, liquid, ice).

In order to estimate the sensitivity of our cloud simulations on one of these compositional effects, not necessarily included in other similar atmospheric models, we have selectively removed the influence of the condensed-phase active tracers on the mass of the volume mean. The required source code modification ("no A.T. in density") consists in the removal of the incompressible active tracers' contribution to the volume mean density ρ . We effectively expected this change to result in a reduction of 'precipitation drag' and therefore in weaker cold pool density currents, through a reduction in vertical momentum, not rain drop frictional drag (which is not parameterized in ATHAM). Simply, ρ in equation (17) in OH98 was reduced to the local density of the gas (i.e. moist air) only, the gas to total volume ratio was set to 1, and the gas specific concentration used for model dynamics was also set to 1.

Further alterations to investigate the thermodynamic influence of the condensed-phase active tracers, not implemented here, would consist of their removal from the

volume mean heat capacity c_p , used throughout the model wherever diabatic heating processes occur, and which would therefore reduce to that of moist air, i.e. to $c_{p,g}$ in equation (15) in OH98. Note that the density perturbation due to vapour, i.e. the effect often captured by the virtual temperature concept, still remains under such an alteration. Simultaneously, the conversion from the conservative volume mean potential temperature θ (defined in equation (10), OH98, as a total heat content) into the *in situ* temperature T , as spelled out in equation (16), OH98, would reduce to its common form (equation (14), OH98) in the absence of condensed-phase active tracers. An additional simplification, not related to the latter, would consist in replacing the moist $R_g/c_{p,g}$ exponent in equation (16), OH98, by a dry air version $R_d/c_{p,d}$, a simplification adopted for convenience by Bryan and Fritsch (2002) for their moist benchmark simulation without noticeable degradations of accuracy. Our own tests with this simplification also produced hardly perceptible differences, which is why they will not be further discussed below.

We have performed several sets of simulations, sequentially switching on the (diabatic) physics modules of Kessler microphysics (“**K**”), turbulent diffusion (“**T**”), and short- and long-wave radiative transfer (“**R**”). In each case, we run a baseline simulation, followed by the aforementioned source code modification affecting the active tracer compositional effect on density (“**no A.T. in density**”) and by a further test with no latent heat exchange during phase changes (“**no LHR**”). The experiments with source code modifications are only shown for simulations with all physics modules active (“**KTR**”), as the effects are similar throughout the various sets. In terms of solar shortwave radiation, the experiments were started at 08:30 LT on 30th November, at a latitude -11.55°S. The experiments have been produced using an ATHAM branch⁶. Model configuration and setup have been specified in the previous section.

3.5 Results and discussions

For brevity, we only show a few characteristic snapshots (Fig 3 to Fig 5) to highlight the diabatic, turbulent mixing and compositional effects, at the times of precipitation downdraught onset and the initial development and spreading of a small density current. The focus is on gaining a qualitative and process-based understanding of the interplay between model physics, thermodynamics and dynamics, which will be relevant to the complex realistic simulations following hereafter. As stated above, results are only shown for the 5 out of 9 simulations that differ most. In terms of bulk diagnostics,

⁶ Branch named ah519_moistbubble at revision 683; see Appendix B

the differences are astounding. Integrated over the entire 3 km domain, the total ground-level deposited rain (per unit-m in domain depth) at the end of the runs is by far largest with 38.6 kg when latent heat release is switched off (KTR-no LHR). This is largely due to the drainage of the existing stratified cloud layer, and does in essence not represent a physically possible scenario. Using cloud microphysics only, but retaining latent heat release (K), this amount decreases by not quite an order of magnitude to 6.9 kg. Adding SGS turbulence (KT) decreases that by half to 3.5 kg; further including radiative processes (KTR) reduces it by another order of magnitude to 0.3 kg. More startling still, removing the active tracer compositional effect on density (KTR-no A.T. in density), presumably a small change, dramatically increases the accumulated rainfall over 70-fold to 21.2 kg; whilst in return, the influence of adding turbulence and radiation is now reversed, i.e. the amount increases from K (9.1 kg) through KT (13.8 kg) to KTR! This dramatic difference is to some extent incidental, in as much as a substantial amount of precipitation in the baseline KTR evaporates before reaching the ground. Bulk quantities do not reveal the full story here, and may not be the best approach to evaluating runs with different processes included. Indeed, as will emerge from the following discussion and figures, this dramatic increase with no A.T. in density is partially the result of a successful break of the cloud through the inversion layer, thus, in essence, of the transition from shallow to deeper convection. A measure of maximum cloud top height increased from 1180 m to above the domain limit at 2 km between the 2 KTR runs with and without the active tracer compositional effect on density.

Several interesting features, some more, others less expected, are worth pointing out. Under the sole action of microphysics (K, Fig 3), condensational latent heat release, particularly strong within the rising thermal's topmost outer spherical shell, conveys an additional boost to the thermal, which penetrates into the stable inversion layer, before effectively collapsing in its centre. Since it is hard to imagine how resolved eddies should mix dry and warm air into the rising bubble's top (unless through bubble deformation or induced secondary vortices) and produce evaporational cooling, we speculate that this collapse is the result of excessive liquid water mass loading, captured by the density of the active tracers. Indeed, whilst cloud droplets concentrate around the outer edges, rain drop specific concentrations are highest in the centre of the cloud (not shown), and an identical simulation with the active tracers' density effect removed (hereafter: no A.T.(ρ)) does not produce the same central collapse (not shown). Note that this concentration of condensate is consistent with large gradients of other tracers (e.g. θ) simulated in the "arch connecting the two rotors" of dry thermals (Bryan and Fritsch (2002)). SGS turbulence (T in KT) acts by design as diffusion and produces mixing within the cloud and to some extent with outside environmental air. Cloud condensate is now much better

distributed throughout the cloud, resulting in a vertically layered droplet distribution (not shown). This distribution, presumably with dilution through environmental air entrainment and consequential partial re-evaporation and positive buoyancy loss, results in a delayed onset and less intensive precipitation rate (Fig 6(c)), as well as less intensive vertical velocities (Fig 6(a) and (b)). If we were to calculate the resolved TKE, we'd expect the KT simulation to have weaker small-scale resolved TKE than the K counterpart, due to turbulent diffusion of momentum, which produces a cascade down the eddy energy scale and ultimately leads to dissipation of momentum. Indeed, spectral analysis of the horizontal velocity deviations $u' = u - \langle u \rangle_{hor}$ and of w' within the inversion layer⁷, (where cumulus cloud mixing occurs), shows a strong drop of spectral energy density in KT with respect to K towards the larger wavenumbers (not shown). In both K and KT, the main entrainment mechanism is strikingly evident in terms of a Hill's vortex capping the rising thermal and vortically entraining air from levels just below the location of the main updraught core. The effect of radiation (R in KTR) is particularly striking. Cloud top longwave radiative cooling strongly destabilizes the bottom of the inversion layer interface (darkest shade of blue in Fig 3). This results in a thin layer of negatively buoyant air which engulfs in a rapidly collapsing and sinking motion, (with again the characteristic vortices), towards the edges of the cumulus cloud. This particular location is possibly the result of initial downward forcing due to the cloud's Hill's vortex. It induces a complex dynamical pattern with 3 vertically stacked centres of rotation. Upon approaching the ground, the lowermost vortex effectively cuts off lateral surface layer air supply to the rising thermal whilst feeding it with top-of-the-convective-PBL air. The question how this would act upon stationary versus pulsating thermal updraughts in wind-still conditions with a presumed 'continuous' energy supply in terms of sensible heat fluxes over a significantly warmer surface patch would require further investigation. Note that reality is more complex still, given the heterogeneity of the wind speed that ultimately drives the fluxes. Below the thermal core, convergence reduces wind, and surface energy to feed the updraught would need to originate laterally. As we shall mention later, another question is if the drag law parameterizations used to parameterize surface fluxes are valid for individual thermals at all. In essence, in all 3 simulations (K, KT, KTR), the forming cumulus breaks up the original stratified cloud deck, which starts to decay at the edges of the new cloud, somewhat alike the sketch in Fig 2(b). However, we simulate very little warm inversion layer air entrainment into the convective PBL (as in region 1) besides that forced by negatively buoyant downward branches, and a much more complex dynamics field with potential impacts on energy supply and surface fluxes. Our results agree with

⁷ We use the notation $\langle a \rangle$ for spatial averaging

those discussed by D. E. Stevens, Ackerman, and Bretherton (2002), who suggest that cloud top cooling provided much of the turbulence necessary for the rise of the inversion layer by entrainment. Indeed, for stratus clouds, large values of the liquid water path near cloud top, and small droplet sizes, have long been shown to produce large radiative cooling rates, the latter in turn favourable to enhanced entrainment processes (Curry (1986)). Previous studies established that cloud-top radiative cooling might result in mixed-layer convection if balanced by a sensible heat flux from below, compensated by local latent heat release due to the condensation associated with the radiative cooling, and also compensated by turbulent entrainment of sensible heat from above the cloud layer.

Without latent heat release (KTR-no LHR), the thermal cannot penetrate into the inversion and spreads out laterally below the capping layer. Simultaneously, intense cloud top radiative cooling, not offset by compensating condensational latent heat release, destabilizes the deck. This quickly produces a distributed set of negatively buoyant ‘fingers’, reinforced by liquid water mass loading, that sink into the PBL, producing strong turbulent mixing.

The balance between radiative and evaporative cooling, both potentially contributing to the destruction of the cloud deck through turbulence enhancement (the first if latent heat effects are excluded, both if they are included), are interlinked through non-trivial feedbacks (see e.g. Yamaguchi and Randall (2008)), and cannot be gauged from these simulations. Many of our simulations exhibit a pronounced roughly 2-min high-frequency periodic oscillation in the domain-mean w field, embedded in a lower-frequency (8-min) damped oscillation (not shown). Based on an in-depth analysis, we tentatively attribute some of this behaviour to the iterative solver of the equation of state implemented in the model. Suffice to say in this context that the absence of latent heat release dramatically amplifies (and phase-shifts by a factor of π) this signal (not shown). Presumably, this may be linked to our initialization design, in which the high RH below the inversion results in immediate condensation and drop formation, followed by strong mass loading sinking motion and precipitation downdraughts, since the compensating effect of condensational warming is missing. The strong initial rainfall can be seen in Fig 6(c).

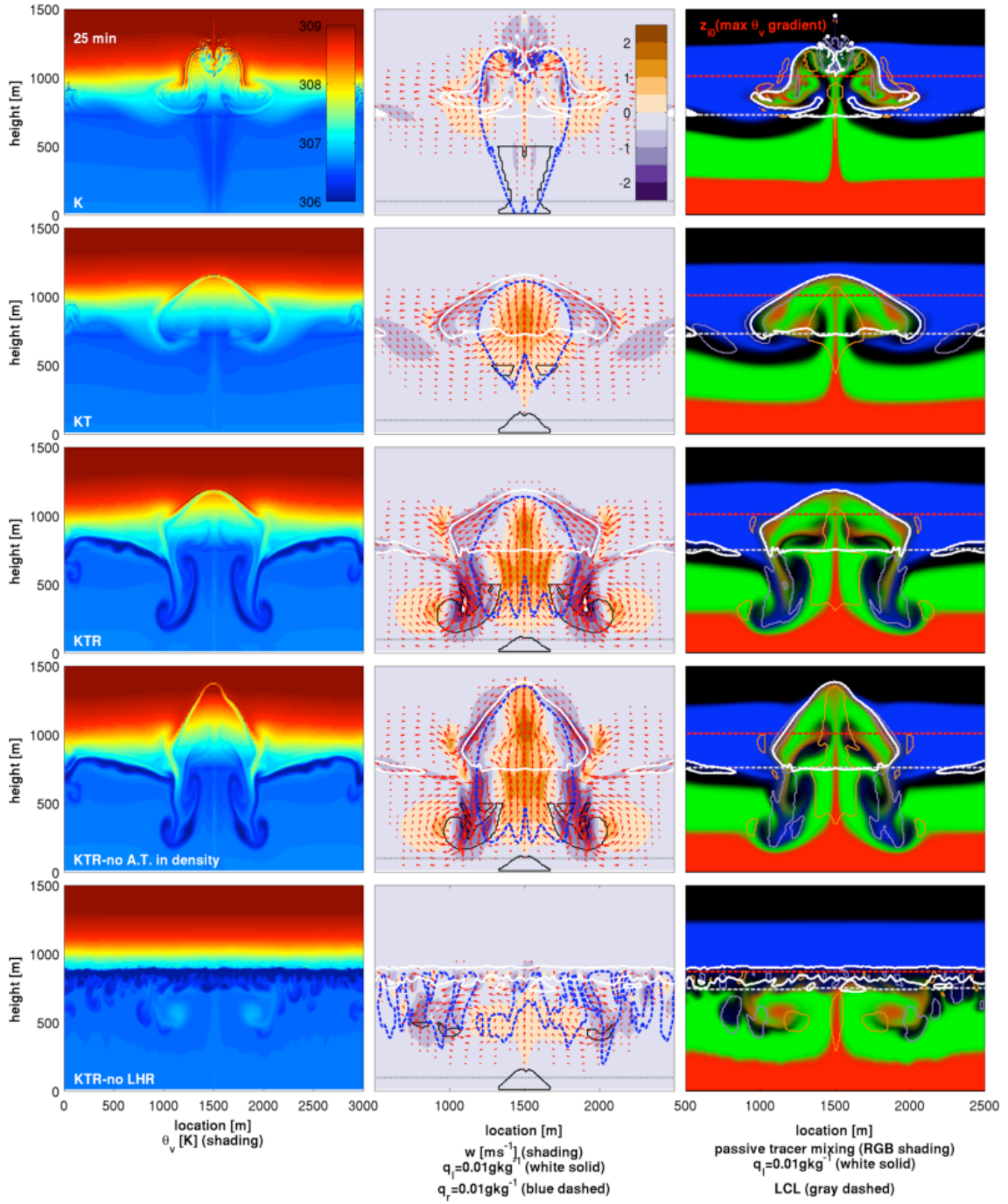


Fig 3 Thermodynamics (θ_v , first column), dynamics (w and wind field, second column) and mixing (passive tracers, third column) of a simulated convective thermal penetrating into a stratified cloud layer at $t=25$ min. Experiments (rows) are identified as follows: K, Kessler microphysics, T, turbulence, R, radiation; KTR is the baseline. “No A.T. in density” and “no LHR” (latent heat release) correspond to corresponding source code modifications. The wind field arrows in the second column are plotted where flow speed exceeds 0.2 ms^{-1} . Cloud droplet and rain drop outlines are overlaid as white solid and blue dashed lines, respectively. The black contour outlines the density anomaly mask used for estimating the density current. If $\Delta\rho = \rho - \rho_0$ is the anomaly of the density field with respect to its initial state, the mask is defined where $\Delta\rho > \langle \Delta\rho \rangle + 0.5\sigma_{\Delta\rho}$, where $\langle \rangle$ and σ denote spatial mean and standard deviation, respectively, and applying an upper cut-off height set to 500 m. The density current mean velocity plotted in Fig 6(d) corresponds to the surface layer (defined up to a maximum height of 100 m, black dotted line) horizontal winds averaged over the mask. The mixing plots in the third column are composite RGB images where the colour is computed from the specific concentrations of surface layer (red), mid-PBL (green) and inversion layer (blue) air masses within each grid-box. The initial z_i (red dashed) and

instantaneous lifting condensation level (grey dashed) are computed as in Fig 1. Also shown are the mask outlines of convective core updraughts (gold) and downdraughts (purple) used to calculate their conditional mean w in Fig 6(a) and (b). Core masking will be described later in this dissertation.

Unexpectedly but not surprisingly, the KTR baseline with no A.T.(ρ) produces a deeper cloud driven by a more vigorous updraught thermal (Fig 6(a)), as the condensate mass loading remains unaccounted for. The updraught succeeds in piercing through the idealized inversion layer and penetrates into the free troposphere (Fig 4). A bubble of condensate, generating rainfall, is injected above the inversion layer. It eventually disconnects from the lower-level moisture supply through rotating dynamics and precipitation downdraughts. It does thus not evolve into a deep convective plume but may contribute to the moistening of the lower free troposphere. As the bubble rises higher and faster, adiabatic cooling intensifies, resulting in the production of more intense rainfall reaching the surface (Fig 6(c)) and prolonged downdraughts (Fig 6(b)). This in turn invigorates the spreading density current (Fig 6(d)), which is contrary to our initial expectations to find a reduced density current. It also strengthens the forced ascent on the gust front convergence lines, which is reflected in slightly larger updraughts-averaged w in Fig 6(a) after 28 min. Note here that the density currents in KTR simulations predominantly incorporate radiatively-cooled negatively buoyant air, whilst evidently rainfall-induced outflow currents are best seen in the K and KT simulations (Fig 5). The density current strengths evolve identically with and with no A.T.(ρ) in KTR as the radiative effects are similar, but the additional increase in the latter is due to rainfall.

All the precipitation shafts are submitted to various extents of splitting due to the upward motion of the thermal below and secondary circulations induced by the negatively buoyant sink on radiatively-cooled cloud edges (Fig 4). Ultimately, most rainfall cores (not shown) regain the centre, except in simulation K. Here, after the central collapse of the cumulus, rainfall is produced in both remaining lateral clouds, giving rise to 2 streaks initially merging slantwise towards the centre as they approach the ground. Presumably because of strong convergence in the very centre, these streaks then quickly separate again after they reach the ground and move laterally, into the system shown in Fig 5. In the baseline (KTR), hardly any precipitation actually reaches the ground (Fig 6(c)).

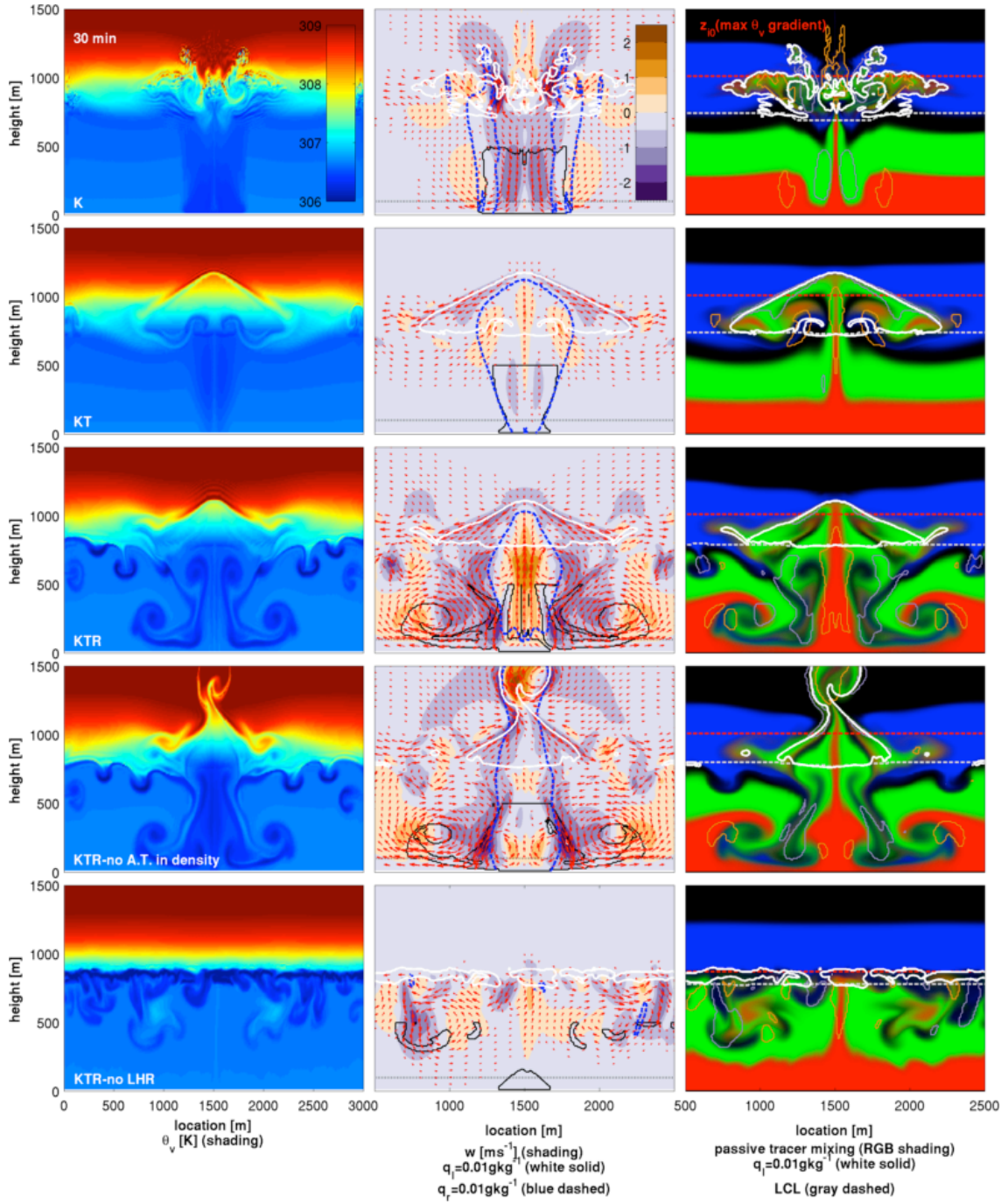


Fig 4 Same as Fig 3, but for $t=30$ min

Entrainment⁸, followed by mixing, matters for several reasons, as discussed above. Tracing the origins of air masses with different properties helps to investigate their fate and potential effects. For instance, if aerosols, acting as cloud condensation nuclei, are concentrated in a thin horizontal layer, cloud evolution may critically depend on whether this layer is ingested into the cloud or not.

⁸ Entrainment is here loosely defined as air transiting through an interface into an air mass with different characteristics, such as a thermal, a cloud, or through the interface between the PBL, the inversion layer and the free troposphere

An interesting way to visualize the mixing of several (max 3-4) horizontal layers, defined by relative specific concentrations of passive tracers, originally confined to predefined pressure levels, consists in using these to produce composite RGB images (Fig 3 to Fig 5). In theory, strong mixing and diffusion should result in a large and varied colour palette. The fact that this is not the case suggests that even with parameterized SGS turbulent diffusion, small-scale mixing (that changes the properties of a given grid-box) on time scales of an hour might not be intense, and that the entrainment of warm and dry inversion layer air (blue) is limited and restricted to cases with radiatively produced negative buoyancy. More generally, the whole convective overturning of the PBL in our simulations is heavily dependent on radiation. If streamers with different air mass origins are possibly least blurred in simulation K because of the absence of SGS-induced diffusion, after cloud break-up, resolved TKE ultimately leads to the best-mixed inversion in this case. Surface layer air (potentially with highest moisture content in the presence of surface latent heat fluxes) originally concentrates around the outer shell of the convective Hill's vortex. Only little inversion-layer air gets engulfed into the cloud, and mostly from below, such that cloud condensation nuclei concentrated herein may have limited influence on cloud evolution. The core of the convective cloud seems to consist mostly of mid- an upper-level PBL air, although we need to point out that in these simulations, supply from the surface layer is limited to an initial pulse.

In the 2 KTR simulations (KTR, KTR-no A.T.(ρ)), cloud-top radiative cooling and the associated enhanced mixing and high- θ air entrainment have led to an almost complete dissipation of the clouds (Fig 5). Surprisingly, the cumulus in KT submitted to SGS parameterized turbulence remains whilst the cloud in K has almost completely vanished. At first sight, this seems counterintuitive, as we would have expected enhanced turbulent diffusive mixing of environmental thermodynamic properties to contribute to faster cloud dissipation. In line with what we argued above, we tentatively attribute this finding to 2 interlinked factors. First, SGS-induced mixing has worked against the concentration of condensate and the associated collapse. Second, without this collapse, less resolved turbulence (vortex motions) has been induced and enhanced dissipation of resolved turbulent momentum under the very action of the SGS parameterization have both effectively reduced environmental air entrainment, mixing and cloud break-up.

The surface layer immediately above the ground (taken as the lowermost grid-point level, not shown), is finally about 1 gkg^{-1} drier in KTR simulations than it is in simulations without radiation, due to enhanced mixing, with obvious impacts on potential surface fluxes and thus on future convective clouds. θ -depressions, characteristic of cold pool downdraughts, exist in all experiments, except in that without latent heat release; this depression is weakest in the KTR baseline. The interesting feature is that the surface layer

in the cold pool is slightly moister in K and KT than outside, whilst this is less pronounced or even reversed in KTR. This is because all the cold pool air in simulations K and KT comes directly from within the cloud, where concentrated moisture is released during sub-cloud re-evaporation. In KTR, a large quantity of cold pool air comes from the dry inversion. This lateral intake will be much more dramatic in big storm systems, as we shall see later in this dissertation.

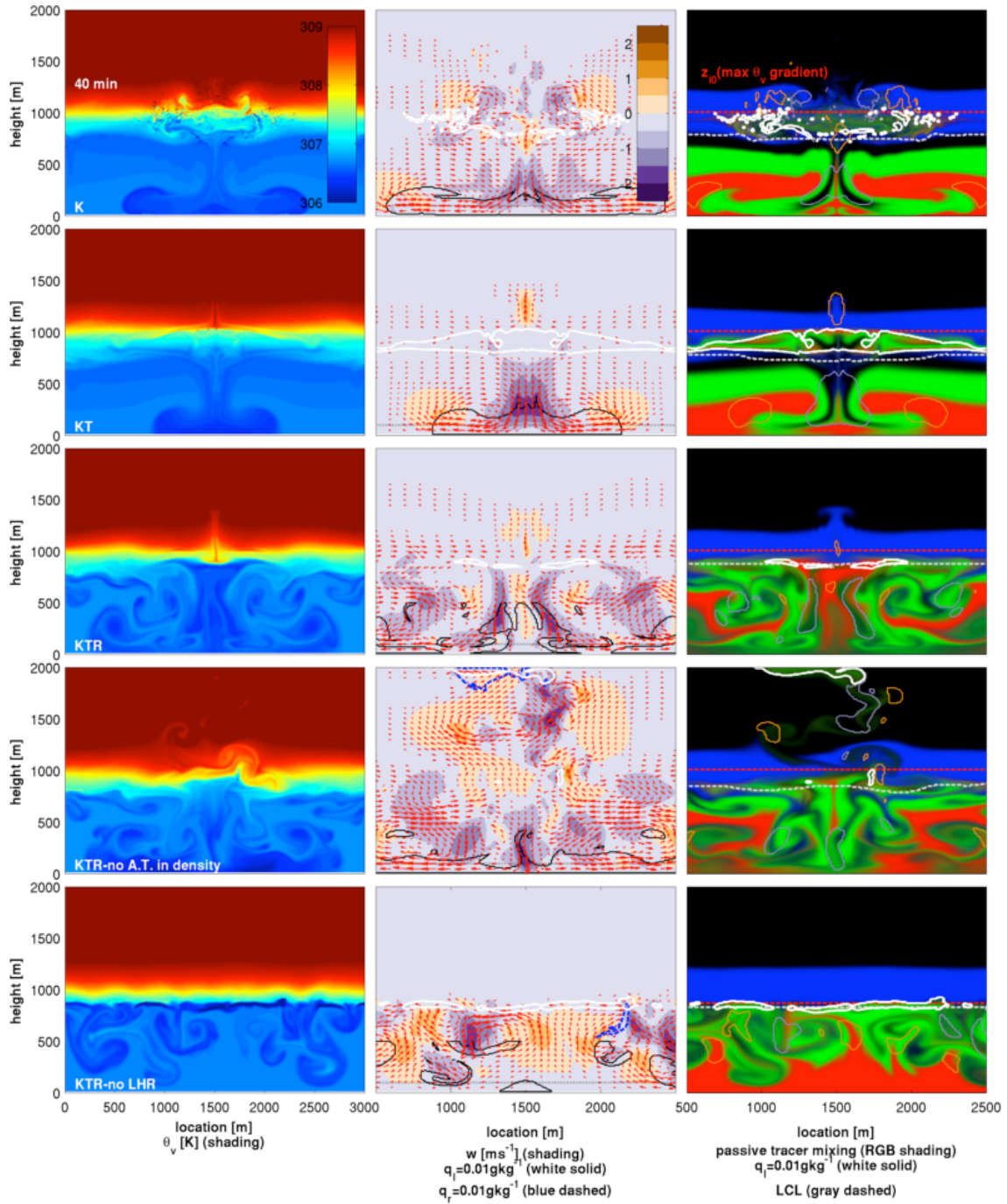


Fig 5 Same as Fig 3, but for $t=40$ min

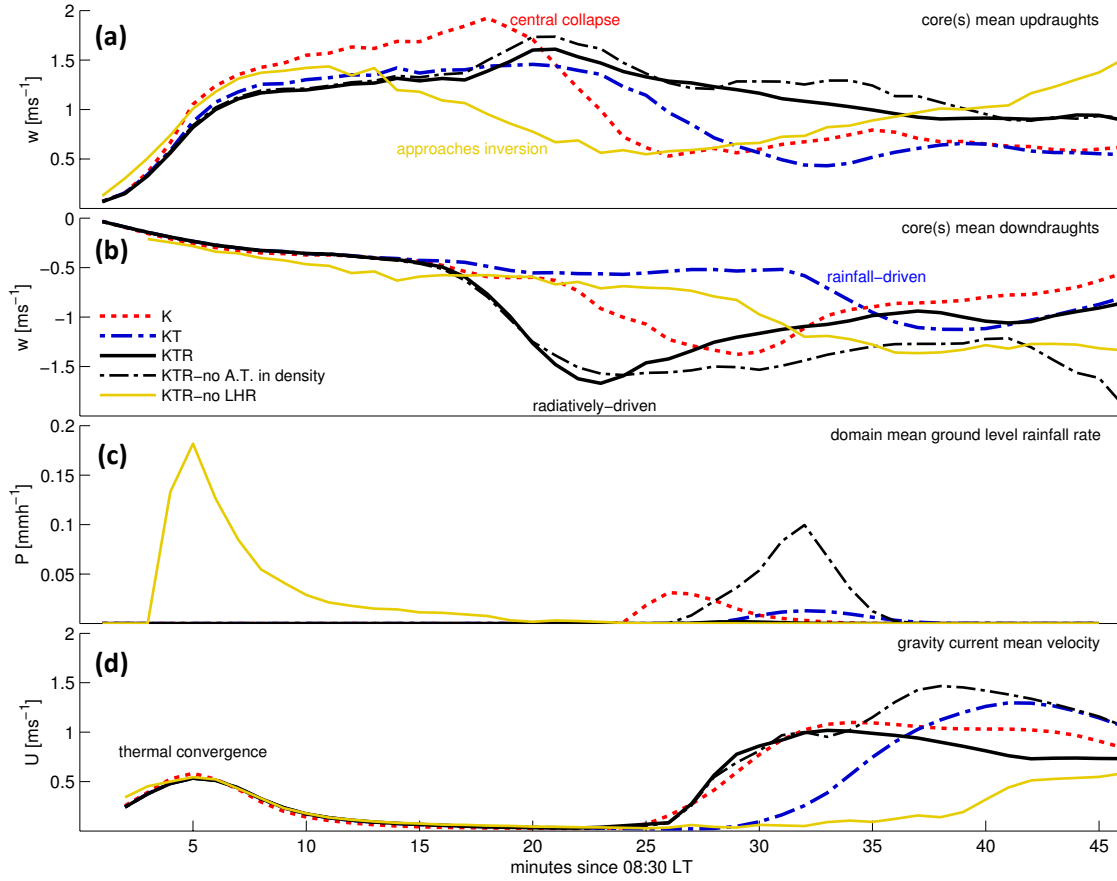


Fig 6 Time evolution of spatially averaged convective ‘core’ (a) updraught and (b) downdraught velocities, (c) ground-level rainfall rate and (d) density current (as defined in Fig 3) horizontal mean velocity. Note that the initial peak is not a diverging outflow but a converging air mass drawn into the thermal updraught.

Within a 2D Cartesian idealized framework of a convective PBL capped by a stratified cloud layer below a strong inversion layer, disturbed by a single finite thermal updraught rising from the surface, we have investigated the interactions between cloud microphysics, turbulence, radiation and dynamics, as captured by the ATHAM model. A particular emphasis has been put on the active tracer (i.e. here the cloud condensate) formulation of ATHAM, although we have only looked into their effect on density, and not on heat exchange.

In our simulation, shallow convection detrains lower PBL air into the inversion layer, potentially leading to moistening and erosion, but the produced rainfall is not responsible for mixing inversion layer air downwards. Downward entrainment is primarily the consequence of negative buoyancy from cloud-top radiative cooling, a process already identified in many previous studies. Although the SGS parameterization of turbulence leads to diffusive tracer mixing, we find that at the very high grid-spacing adopted for this study, the SGS turbulent diffusion of momentum also leads to the dissipation of resolved eddies (i.e. resolved-scale TKE), which effectively reduces the entrainment of environmental air into the cloud and significantly changes its lifetime and dynamics. In other words, without parameterized SGS-

TKE, there is more structure, more shear, more TKE and more entrainment on the resolved scale.

Neglecting condensate mass loading significantly increases buoyancy and does not seem to have the initially expected consequence of attenuating precipitation downdraughts and density current formation. Of course, the influence of active tracers on the dynamics will be just as important or even stronger for cloud systems with larger condensate contents. A further simulation of a prescribed-surface Hector storm produced total rainfall roughly 2.4 times higher when run without considering tracers in density, compared to the baseline. It also resulted in earlier storm onset, stronger updraughts, and a significantly larger and higher anvil (not shown), whilst the initial dry shallow convection phase remained identical.

Our analysis may be limited by our choice of a 2D Cartesian, as opposed to a 3D (or even 2D cylindric, i.e. pseudo-3D) domain. In particular, for an axis-symmetric convective cloud as simulated herein, core updraughts are necessarily stronger than the ‘cylindrical’ sink surrounding the core, unless concentrated in a thin shell. Extending this work to 3D would therefore be useful, as would be a sensitivity study into how the inversion layer properties relate to the triggering of deeper convection, or a coupling of the surface model documented hereafter.

Chapter 4

The Hector storm and surface interactions: methods, theory and data

4.1 Adopting and interfacing an interactive surface as a model lower boundary

Since ATHAM did not include an interactive surface boundary to simulate the turbulent energy, momentum and matter exchange between the atmosphere and land and ocean surfaces, we have developed an interface layer designed for coupling it to various sophisticated hydro- and biosphere models. Our rationale behind the interface design was to avoid substantial changes to the adopted surface code structures, in order to facilitate subsequent updates. Also, without the capability to independently and thoroughly test the surface models' sub-components against field and published data, we refrained from substantial modifications to the physics that would deviate from a published reference, in spite of relevant issues that will be briefly discussed hereafter and may need to be addressed in future work. Nevertheless, some significant modifications in terms of structure had to be carried out to improve code integrity and consistency with ATHAM's computing arithmetic and numerical precision, to isolate core modules, to adapt them from single-column formulations to ATHAM's grid structure, and to clearly separate model initialization, integration and termination. The surface models currently implemented in ATHAM, and on which this dissertation is based, include the vegetation dynamics and terrestrial primary production model HYBRID, version 6.5 (Friend and Kiang (2005), Friend (2010)), which provides the link between soil-plant-hydrodynamics and the atmosphere, as well as the state-of-the-art bulk air-sea flux algorithm COARE, version 3.0 (Fairall, Bradley, Rogers, et al. (1996), Fairall et al. (2003)). COARE ranked first in an intercomparison of ocean surface turbulent flux algorithms according to Brunke et al. (2003)'s assessment, and has been successfully introduced in e.g. the Goddard Cumulus Ensemble (GCE) model (Tao et al. (2003)). HYBRID's main strength is its new realistic physiology-based leaf-level photosynthesis and stomatal conductance scaled to the canopy, which is expected to perform well in simulating the latent heat flux due to

evapotranspiration. Friend and Kiang (2005) suggested that the specification of canopy stomatal conductance over rain forests was critical for a valid simulation of surface energy budgets and regional hydrology. The vegetation submodel's conductance responds to atmospheric moisture, where an increased gradient between internal leaf air spaces and atmospheric specific humidity reduces stomatal conductance, and to carbon dioxide concentrations, which will be kept constant in this study. It also varies with the soil water potential, and the CO₂-saturated potential rate of canopy photosynthesis, which accounts for light, temperature, and photosynthetic capacity. Soil physics in HYBRID are represented within a simple two-layer model (Friend (2010)), which acts as a water and energy reservoir. It is based on the Goddard Institute for Space Studies (GISS) GCM II (Hansen et al. (1983)). Interception of rainfall by vegetation cover is not captured. A schematic overview of some of the parameterized processes discussed hereafter is given in Fig 7.

Before addressing some of the detailed theoretical considerations in the preceding models that are of direct relevance to the flux transfer into ATHAM, we note that the flux parameterizations are based on 3 bulk transfer equations for momentum (τ [Nsm⁻²s⁻¹]), sensible heat and humidity. These rely on mean profile (stability correction) functions (Ψ in integral form, see footnote 13 on page 72), to incorporate the influence of atmospheric stability on turbulent transport in a similarity theory framework. The bulk transfer relationships rely on mean gradients of velocity (U [ms⁻¹]), (potential) temperature (T or θ [K]) and specific humidity (q_v [kg_v · kg_a⁻¹]), which in a modelling framework are usually taken between the lowermost model level and the surface. If we consider that the horizontal flow is null at the lower boundary (no slip condition), only surface temperature (T_s) and humidity (q_s) are unknown. As we will see, the estimation of stability generally implicitly requires the knowledge of the fluxes themselves, usually in terms of the friction velocity (u^* [ms⁻¹]) and the sensible (f_h [Wm⁻²]) and latent (f_e [Wm⁻²]) heat flux, which adds a further 3 unknowns. Also, for the nowadays well-established logarithmic profiles within the dynamic sublayer, (the lowermost part of the atmospheric surface layer), the roughness lengths for momentum (z_0 [m]), heat (z_{0h} [m]) and water vapour (z_{0v} [m]) will need specification. These are the heights at which the atmospheric value for the given quantity is equal to the surface value. Roughness parameters are critical for flux estimations and are best determined experimentally. For modelling purposes, we will try to parameterize z_0 as a function of surface characteristics; the scalar z_{0h} and z_{0v} are in similarity theory often assumed the same and expressed as a function of z_0 . Fluxes and roughness parameters are often incorporated into transfer coefficients ($C_{d,h,e}$) that quantify the flux for a given gradient.

We thus have 3 equations with 5 unknowns and further parameters. Surface humidity is usually assumed saturated at surface temperature ($q_s = q_s^*(T_s)$), or parameterized as a function of temperature and further variables. Surface temperature can be modelled by considering one further equation, the surface energy budget constraint, given in Brutsaert (2005) as:

$$(R_s(1 - \alpha_s) + \varepsilon_s R_{ld} - R_{lu}) - f_e - f_h + L_p F_p - G + A_h = \frac{\partial Q}{\partial t} \quad (4.1)$$

T_s intervenes in most of the terms in the energy budget, not least in the rate of change of the heat content Q of the upper surface layer if it is of finite thickness. R_s is the shortwave incoming solar radiation, R_l denotes the downward and upward longwave radiation, α_s is the surface albedo, ε_s the emissivity. L_p is the thermal conversion factor for fixation of CO_2 at the specific flux F_p (neglected here), G is the ground specific energy flux (leaving the layer) and A_h are advected heat fluxes. The latter include precipitation and run-off heat fluxes, and are taken into account in our budget equations.

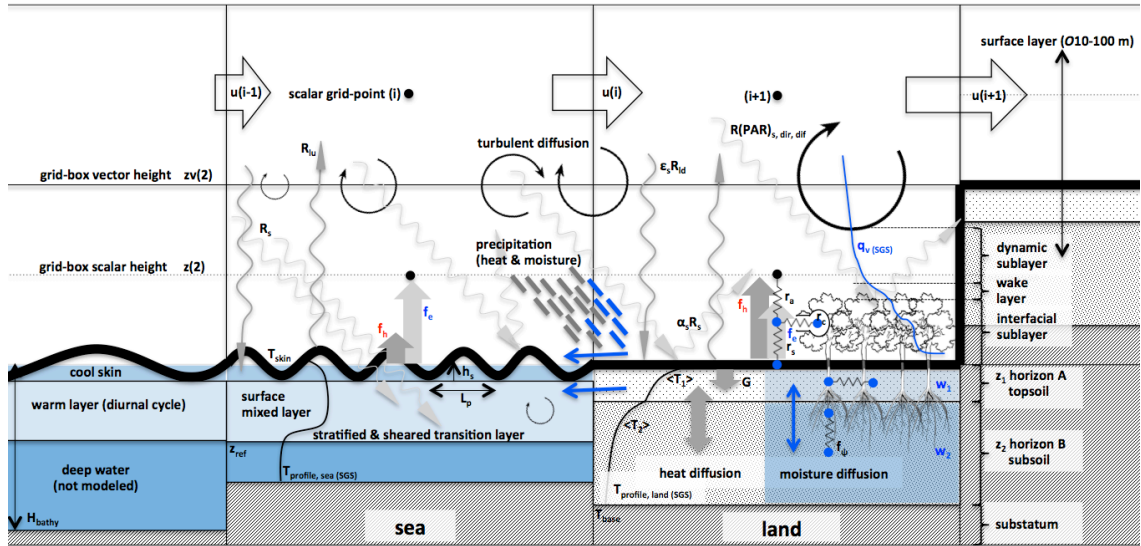


Fig 7 Schematic representation of the atmosphere-biosphere-hydrosphere coupling and of the most important parameterized processes. Variable names follow those in the text.

The flux transfer parameterizations adopted in the surface models coupled to ATHAM are appropriate for coarse grid-spacing and are built on a theoretical framework rooted in the assumption that turbulent fluctuations are sufficiently averaged to represent a turbulent spectrum in equilibrium. In other words, such parameterizations are built for models that solve the Reynolds Averaged Navier-Stokes (RANS) equations. It is obvious that this assumption is not met at the very-high spatial and temporal resolutions of CRM/LES models, which resolve part of the turbulence spectrum (section 3.2). We will come back to this issue several times. Below the blending height, i.e. the height at which the influence of surface heterogeneity of a particular quantity on the vertical profile of that

quantity becomes small, turbulence is not horizontally homogeneous, and the application of similarity theory may not be justified (H. -Y. Huang and Margulis (2009)). However, van Heerwaarden, Vilà-Guerau de Arellano, and Bou-Zeid (2011) found, (in the context of a smooth, even and homogeneous grassland under a convective PBL), that the surface energy balance and turbulent statistics were surprisingly insensitive to the numerical formulation of a land surface model coupled to an LES. Even in the limit of free convection, in which the large-scale-averaged velocity vanishes, they found limited sensitivity of PBL statistics to the land surface model formulations. The heat capacity of the canopy layer, model grid-spacing and subgrid-scale treatment near the surface were also found to have minimal influence, and van Heerwaarden concluded that the formulations currently implemented in NWP models could readily be transposed into LES models, at least for a convective PBL over grassland. It is possible that these conclusions are not valid for heterogeneous surfaces. Here, we simply assume that the formulations should be appropriate both over land and over sea and in heterogeneous situations, but testing of this assumption and validation against measured data (as in H.-Y. Huang and Margulis (2010) for a simpler land surface scheme) will eventually be required.

Interface design

In terms of implementation, the top-level interface provides a generic framework to couple any given surface model to ATHAM. It provides function calls for the models' initialization, preset and allocation, including new input file reading facilities; integration during each ATHAM time step; and termination and deallocation at the end of a run, as well as function calls for dynamic ocean albedo estimation (see below). An urban model and hydrology network model could also be coupled here. We have currently implemented urban areas as special bare soil grid-boxes with corresponding parameters within HYBRID. Date, time and geographical location synchronization are now handled through a new centralized UTC time manager in ATHAM. During model integration, this top-level interface loops over each grid-point of the domain (or subdomain on a parallel architecture) and executes the single-column surface models iteratively. We have performed performance assessments to ascertain that this does not constitute a performance bottleneck. This procedure was necessary since the adopted surface models were not coded as spatial array structures. In order to keep the required data in memory, we have implemented model-specific multidimensional data array modules and associated pointer functions, which are called during each grid-point iteration to point towards the required set of variables in memory. These data array modules are also used by the new surface model restart-file read-write facilities that are called during initialization and termination.

For each grid-point and during each time-step, we start by preparing ATHAM atmospheric variables required by the surface models as input. These include lowest-level air temperature, pressure, density, specific heat capacity, specific humidity, precipitation and horizontal wind speed. We have assigned rainfall to liquid precipitation and, in the absence of a snow microphysics category, graupel as the only frozen species to solid precipitation, expressed as equivalent liquid precipitation in ms^{-1} units. If the air temperature is below freezing, we also treat ATHAM's rain as solid precipitation. Inconsistently, solid precipitation falling into water bodies is treated as rainfall assumed at wet-bulb temperature, in order to estimate the sensible heat transferred to the ocean surface by precipitation (see Fairall, Bradley, Rogers, et al. (1996)). Heat loss due to melting is not included.

Surface wind speed, gustiness and similarity

HYBRID's resistance-based flux parameterizations (documented below) depend critically on horizontal surface wind speeds. They break down under weak wind conditions and in stable atmospheres, which arise particularly after sunset or rapid ground-surface skin cooling. Weak winds frequently occur in local convergence zones, where non-stationarity invalidates similarity theory on which flux parameterizations are based. At the risk of further deviating from similarity theory, we have therefore added a user-defined (untested) dimensionless parameter $\beta_{TKE} \geq 0$ (typically order of or less than 1) to include SGS TKE in the horizontal wind speed U passed to HYBRID, in terms of an additional gustiness or turbulent velocity scale. This is loosely based on Mahrt (2008)'s proposition of a meso-velocity scale, meant to account for unresolved mesoscale circulations and to enforce non-vanishing fluxes. Similarly, we imply to introduce unresolved turbulent circulations through:

$$U = \sqrt{U^2 + w_{TKE}^2} = \sqrt{U^2 + \beta_{TKE}(TKE_h + TKE_v)} \quad (4.2)$$

where we deliberately chose to include vertical TKE to account for free convection buoyancy-generated turbulence, and more importantly, shear turbulence generated by forced ascent in local convergence zones and orographic areas.

This modification of grid-box wind is not applied for COARE, since the air-sea flux algorithm applies in an analogous fashion a gustiness velocity $w_g = \beta W_*$ in unstable atmospheres. It is proportional to the Deardorff (1970) convective scaling velocity W_* , following e.g. Godfrey and Beljaars (1991) and Beljaars (1995). In our implementation, the required inversion layer height z_i is hardwired to 600 m, the default COARE value, as no suitable diagnostic is available directly within ATHAM. W_* is given in Fairall, Bradley, Rogers, et al. (1996) as:

$$W_* = \left(\frac{g}{T} \left[\frac{f_h}{\rho_a c_{pa}} + 0.61T \frac{f_e}{\rho_a L_e} \right] z_i \right)^{1/3} \quad (4.3)$$

Sensible and latent heat fluxes are denoted here by $f_{h,e}$, g is gravity, T is air temperature, ρ_a and c_{pa} are air density and specific heat at constant pressure, and L_e is the latent heat of vaporization. A minimum w_g of 0.2 ms^{-1} is imposed in stable conditions, when a convective velocity is not defined; the proportionality factor β is set to 1.25.

It may be argued that scaling velocities as outlined above should not be required in an LES model, and that more importantly, Monin-Obukhov similarity theory may not be applicable in the highly transient flow simulated within an LES or a CRM. Similarity theory may be violated by double-counting turbulence when including it as a gustiness term in the mean wind. Indeed, van Heerwaarden, Vilà-Guerau de Arellano, and Bou-Zeid (2011) state that the use of a gustiness velocity is undesirable in LES, since part of the horizontal motion induced by convective turbulence is actually resolved. However, as long as a more appropriate framework for surface-atmosphere transfer is not available and bulk flux parameterizations rely on horizontal winds, they may break down under weak wind conditions, leading to numerical instabilities and necessary remedies.

Since Monin-Obukhov similarity theory is based on the concept of a fully-developed turbulence spectrum in equilibrium over a homogeneous surface with a sufficiently large fetch, it is not guaranteed to hold for increasing spatial (and temporal) resolutions. Based on referenced experimental studies in shoreline transition regions, suggesting relatively small turbulent adjustment time scales, (after which an internal equilibrium between surface fluxes and local vertical gradients is established and similarity theory becomes applicable), Mahrt (1987) gives an example of a typical length scale for turbulence equilibrium, $L = V l_{eddy} / w_{TKE}$. Here, V is a scale value for the speed of the mean flow, w_{TKE} represents the turbulence velocity scale and l_{eddy} a length scale of the main eddies. Considering the height of an internal boundary layer ($O100 \text{ m}$) as an appropriate value for l_{eddy} , Mahrt estimates an adjustment scale of the order of 500 m . It is obvious that with similar or even smaller CRM/LES grid-spacing, we need to be aware of potential theoretical shortcomings when applying similarity theory to convection-resolving models. We argue that at least as long as we do spatially average over many dynamic sublayer⁹ and surface layer¹⁰ eddies, for which the characteristic length scales are small, in other words, as long as we set the first model level within the surface layer¹¹ but do not actually resolve it, the similarity framework may remain appropriate.

⁹ Where profiles are logarithmic, see Brutsaert (2005)

¹⁰ Where profiles deviate according to stability

¹¹ This will not be possible in highly stable situations (Kondo, Kanechika, and Yasuda (1978))

Radiation and albedo

From the radiative transfer models, we also pass the sun's zenith angle, the surface-level total, direct and diffuse solar radiation fluxes, as well as the downwelling longwave radiation flux through the interface. In HYBRID, solar radiation is converted into direct and diffuse photosynthetically active radiation (PAR), which governs photosynthesis, and therefore, stomata fluxes. The shortwave broadband albedo is required both in ATHAM's radiation and in the surface models. The ocean's albedo, and hence its energy balance, is highly variable, and depends critically on the solar zenith angle, the slope of surface wave facets, direct versus diffuse radiation, and ocean colour given by the chlorophyll concentration. We implemented these dependencies using the look-up tables (LUT) described by Jin et al. (2004), with the surface wind speed from ATHAM, and the cloud broadband optical depths as estimated in ATHAM's shortwave radiation code. The aerosol optical depth, in the absence of aerosol active tracers, as well as the chlorophyll content, are both given as user-defined input variables. In this study, they were set to their default values of 0 (no aerosol optical depth offset, i.e. a clean atmosphere) and 0.2 mgm^{-3} (global ocean average), respectively. For land surfaces, a solar factor (sf) is used to modify the surface albedo as a function of the cosine of the zenith angle μ , using $sf = 1.4 / (1 + 0.4\mu)$, as simplified from Briegleb (1992). This factor is currently applied indiscriminately of surface type, even if certain surfaces, in particular densely vegetated ones, exhibit a weak albedo-dependency on the sun's zenith angle. HYBRID can now be initialized with a measured visible broadband albedo field or a homogeneous estimate. Alternatively, the model's original implementation included a composite value estimated from the subgrid-scale fractional areas of various Generalized Plant Types (GPTs, see below). In vegetation dynamics mode, (which is neither fully functional nor required in the current version), this value is changing over time, and can be passed to ATHAM.

Surface layer and skin temperatures

After each time step, the surface model returns its skin temperature and sensible and latent heat fluxes, the latter as an evapotranspiration rate in $\text{kgm}^{-2}\text{s}^{-1}$ or mms^{-1} . Skin temperature is used for estimating outgoing longwave radiation in ATHAM and for calculating the fluxes in the surface models.

COARE's ocean skin temperature either remains invariant and identical to the initialized Sea Surface Temperature (SST), or it is modified on a diurnal cycle basis through warm layer and/or cool skin physics. A diurnal cycle may result from upper-ocean warming and stabilization through the absorption of solar radiation. This limits the

destabilizing downward penetration of turbulent wind mixing, and locks air-sea fluxes of heat and momentum to a surface-mixed warm layer of a given depth, particularly around noon (Price, Weller, and Pinkel (1986)). Warm layers are most pronounced under very low winds, when the trapping depth may be as thin as 1 m. They may incubate surface layer temperature amplitudes up to 2-3 K, a value that decreases to a few tenths of a degree with the more typical trapping depths of the order of 10 m. The heat budget of the layer also includes precipitation fluxes, which may be significant in case of intensive convective rainfall.

Conversely, the uppermost mm of the ocean are generally cooler than the subsurface, which is directly relevant for longwave emission and air-sea exchange (P. M. Saunders (1967)). This fact is related to arguments about the energy balance at the interface, and typical observed temperature differences for tropical areas are of the order of 0.3 K (less during daytime). Warm layer and cool skin corrections are available in the COARE algorithm to remove measurement biases (Fairall, Bradley, Godfrey, et al. (1996)). They may be used as a first-order approximation of the diurnal response of the sea surface layer and skin to diurnal heating and cooling, if the initial sea temperature corresponds to a bulk measurement. The warm layer is then superimposed as a diurnal cycle upon a sea temperature at depth presumed constant and invariant. Consequently, sea temperatures within ATHAM-COARE are not allowed to drift over several days. The available solar radiation absorption parameters correspond to the turbidity values measured during the TOGA-COARE campaign, and have not been linked to the user-defined chlorophyll content for estimating the ocean albedo.

In ATHAM-COARE, warm layer and cool skin physics have to be compiled explicitly, by including the WARM_OCEAN_LAYER precompiler flag in the model's Makefile.COMPILE. The warm layer is built up incrementally through a heat energy integration starting at sunrise, and is functional only if the model is started before 06:00 LST of a given cycle. Therefore, although the model used in this study has been compiled with the corresponding algorithms, **warm layer effects are not included in the simulations presented here.**

HYBRID's original skin temperature was identical to the 10 cm upper-layer bulk soil temperature. The 2 nominal soil layer thicknesses and thermal properties are such that when implemented in a GCM, the soil physics allow to simulate the diurnal surface temperature change with sufficiently large time steps, whilst retaining seasonal heat storage to emulate a valid intra-annual cycle (Hansen et al. (1983)). Even if such a simple 2-layer scheme makes causal relationships in heat variations easier to identify and attribute, our diurnal experiments with fast-varying surface-atmosphere interactions make it hard justify the lack of a proper high-amplitude and fast-response skin

temperature. To remediate this issue, a simple parameterization based on a subgrid-scale quadratic temperature profile extrapolation has been added to HYBRID. This gives a diagnosed skin temperature, at the expense of needing to provide a deep-soil initial bottom temperature (Gerken et al. (2012)). This modification has been shown to greatly improve modelled surface temperatures and fluxes on the Tibetan plateau, and was switched on in this study, along with the new diffusion length scale for heat transport described therein.

Roughness lengths and stability parameterizations

COARE returns the dynamic roughness length z_0 , which is a crucial parameter for boundary layer momentum transfer by surface drag in ATHAM. B. Stevens et al. (2001) reported for the simulation of trade wind cumuli, that a more realistic implementation of surface similarity theory, using a Charnock-like model for surface roughness, changed surface winds, and therefore fluxes and buoyancy. This presumably also changed the balance between thermodynamic and dynamic generation of turbulence, changing turbulence structure from a more streak-like to a more plume-like regime. The wind-induced z_0 is valid within an extended wind range up to $U = 20 \text{ ms}^{-1}$ (Fairall et al. (2003)). At its lower limit of aerodynamically smooth flow ($U_{10m} \leq 2 \text{ ms}^{-1}$), it is made dependent on a constant roughness Reynolds number of $R_r = 0.11$, when surface stress is supported through viscous shear, characterized by the kinematic viscosity of air ν . For higher wind speeds and rough flow ($U_{10m} \geq 8 \text{ ms}^{-1}$), ocean surface roughness, due to wind-generated waves, is given as a function of stress through the Charnock (1955) relationship, with a Charnock constant α . Correspondingly, roughness in COARE is given in Fairall, Bradley, Rogers, et al. (1996) following Smith (1988) as:

$$z_0 = 0.11 \frac{\nu}{u_*} + \alpha \frac{u_*^2}{g} \quad (4.4)$$

where u_* denotes the friction velocity, linked to the surface shear stress τ through $\tau = \rho u_*^2$. The base value of α is set to 0.011 for wind speeds below 10 ms^{-1} ; this is increased to 0.018 for winds over 18 ms^{-1} , and linearly interpolated in between, although revised analyses have shown this increase with wind speed to be controversial (Fairall et al. (2003))¹².

The relationship between z_0 and u_* (interlinked furthermore with the scalar, i.e. heat and water vapour, transfer scaling parameters T^* and q^*) is solved iteratively for

¹² For further possible roughness parameterizations, see Appendix A for available wave parameterizations in COARE, which have not been used in this study.

stability. This involves the gustiness velocity in equation (4.3) and the actual flux calculations (equations (4.9) below), and relies on Monin-Obukhov similarity theory. An iteration starts with a first guess using a bulk Richardson number (Ri_b) approach (Grachev and Fairall (1997)), which reduces the loop to 3 iterations only. Ri_b is defined as the finite difference form of the gradient Richardson number ($Ri_g = \left(\frac{g}{\theta_v} \frac{\partial \theta_v}{\partial z} \right) / \left(\left(\frac{\partial U}{\partial z} \right)^2 \right)$), i.e.:

$$Ri_b = -\frac{gz_r}{T} \frac{[\Delta\theta + 0.61T\Delta q_v]}{U^2} \quad (4.5)$$

for surface-atmosphere differences in temperature (adjusted to surface values from potential temperature θ) and in specific humidity q_v . θ_v is the virtual potential temperature. Without going into all the details, this approach is further based on the dimensionless stability parameter $\zeta = z_r/L$, where z_r is the measurement or reference height, here equal to half the grid-box height. L is the Obukhov length, characterizing atmospheric stability through the ratio of shear- to buoyancy-generated turbulence and incorporating the sensible and latent heat fluxes, i.e.:

$$L = \frac{-u_*^3}{\kappa \frac{g}{T} \left[\frac{f_h}{\rho_a c_{pa}} + 0.61T \frac{f_e}{\rho_a L_e} \right]} \quad (4.6)$$

where κ is von Karman's constant (0.4 in COARE, 0.35 in HYBRID, in line with the profile functions used for stability). In a neutral atmosphere, most turbulence is generated mechanically, and L tends to be large. Unstable atmospheres have a negative L tending towards 0, stable atmospheres are characterized by the opposite; small values may also arise in the limit of low wind speeds. ζ is introduced into Monin-Obukhov similarity theory profile functions $\Psi_{m,h,e}$ ¹³. These in turn are used to adjust turbulent transfer coefficients from their values calculated for neutral conditions. For more information on the form of the profile functions used, (a blended form of the Kansas-type (Businger et al. (1971)) and of convective limit functions in unstable conditions; Beljaars and Holtslag (1991) in stable conditions), and on the exact iterative procedure implemented, we refer to Fairall, Bradley, Rogers, et al. (1996) and Fairall et al. (2003).

Over terrestrial areas, and particularly over highly heterogeneous landscapes, most of the boundary layer turbulence is generated over the roughest patches. High variability of small-scale patchiness has been simulated to correlate with a higher equivalent surface

¹³ Given here in integral form, integrated from the “universal” $\phi_{m,h,e}$ functions for momentum, heat and humidity: $\Psi(\zeta) = \int_0^\zeta [1 - \phi(x)] dx/x$, for a dummy integration variable x . The universal functions define the respective dimensionless gradients of momentum, heat and humidity, e.g. $(k(z - d_0)/u_*) \cdot d\bar{u}/dz = \phi_m(\zeta)$.

roughness (Bou-Zeid, Parlange, and Meneveau (2007)). As above, an accurate estimation of z_0 is directly relevant for the turbulent transport of scalars and momentum in the lowermost atmospheric layers, and for the potential generation of internal boundary layers, although these may not be resolved with realistic model grid-spacing.

In HYBRID version 6.5, discussed in Friend (2010), vegetation dynamics has been switched off (static version) and single fixed-size individuals are simulated on each vegetated surface, with a uniform canopy height of 1 m. The original implementation in vegetation dynamics-mode foresees for each GPT a z_0 that is a linear function of simulated (or fixed) canopy height between a minimum desert value of 0.005 m and a maximum tropical rainforest value of 2 m (when trees are 30 m high). We have introduced optional GPT-specific average roughness lengths. These are ingested along with the other plant physiology parameters during model initialization, and we use them in this study. Subgrid-scale heterogeneity in terms of vegetation cover for each HYBRID grid-box is dealt with using a mosaic approach as laid out in Avissar and Pielke (1989). Herein, individual subgrid-scale patches or tiles, sized by their fractional area coverage, are supposedly homogeneous and vegetated by a single GPT. They get treated individually, independently and sequentially, as much for the associated surface energy and water balance and prevailing micrometeorological fluxes, as for the vegetation's physiological processes. If this can certainly be justified in large-scale models, where individual tiles have significant spatial extents and may be thought of as representing a similarly patchy coverage in the physical world, it is not obvious if individual micrometeorological treatment is still appropriate at the much higher spatial resolution of a CRM. In particular, fractional GPT covers may be used to define new types of composite ecosystem surfaces, spread homogeneously over the entire grid-box (as opposed to covering several subgrid homogeneous tiles), such as savannahs composed of grass, trees and bushes. In such instances, the stability and turbulence of the atmosphere above, governing the net ecosystem exchange, should be evaluated for the mean composite surface as a whole, rather than separately for the individual subgrid tiles.

In the case of small-scale yet isolated homogeneous surface patches in a flat heterogeneous landscape, a possible extension for a more robust estimation of surface roughness could be implemented to model an effective surface roughness z_{0e} (and a boundary layer blending height) as a function of individual patch fractional areas, roughness lengths and a characteristic variability length scale, as documented by Bou-Zeid, Parlange, and Meneveau (2007). In a CRM, such an approach could be implemented on the subgrid-scale of each individual grid-box, or alternatively applied as an average over several grid-boxes, though it requires additional spatial information regarding the variability length scale. In the absence of validation data, we retain the original

implementation within HYBRID for the purpose of scalar flux calculations. We apply individual roughness lengths for each subgrid-scale GPT-tile, before calculating a weighted average of the scalar fluxes in terms of fractional areas. Optionally, and in this study, we first calculate a simple area-weighted grid-box mean z_0 over the GPT-generic z_0 values, and use this indiscriminately for the flux calculations over each subgrid-scale tile, an approach which seems more appropriate for composite surfaces. We also transfer this single grid-box z_0 value to ATHAM for TKE estimation and the calculation of momentum loss due to surface drag. We only transfer z_0 once during the initialization, as fractional areas remain invariant in the static version of HYBRID. The treatment is identical for the zero-plane displacement height d_0 , which for each vegetated GPT-tile is set to 70% of a corresponding generic plant height, before performing an area-weighting.

In HYBRID, the influence of atmospheric bulk stability on transfer coefficients follows the implementation in Hansen et al. (1983). Here, deviations from neutral stability, (giving $C_{dn} = \kappa^2 / \ln^2(z_r - d_0/z_0)$ for neutral momentum transfer), are estimated through non-iterative approximations to analytic integrations of the Monin-Obukhov similarity relations. Such approximations are a function of a surface layer bulk Richardson number, as described in Deardorff (1968) for the air-sea interface. The approximated empirical profile functions for unstable conditions (Dyer and Hicks (1970)) are the same as the Businger et al. (1971) formulation used for COARE, albeit with a modified γ -value of 16 instead of 15 in $\phi_m = (1 - \gamma\zeta)^{-1/4}$ (for momentum), and without the modification for free convection in very unstable situations. For stable conditions, an early form from series expansion (Brutsaert (2005)), the log-linear profile, $\phi_m = (1 + \beta_u \zeta)$ (for momentum), has been used by Deardorff (1968) in the analytic integrations, with a suggested $\beta_u = 7$ based on McVehil (1964). Note that this form, with $\beta_u = 5$ in a more common version, has been found to describe experimental data only for low values of stability, typically $\zeta \leq 0.5$ (Dyer (1974)), $\zeta \leq 1.0$ (E. K. Webb (1970)), $\zeta < 5/7$ or $Ri_g < 0.243$ (Kondo, Kanechika, and Yasuda (1978)) for $\beta_u = 7$. The last study also found turbulence to virtually cease beyond $Ri_g = 2$. This is relevant since a parameterization based on a bulk Richardson number is prone to produce extreme values of stability for a finite temperature inversion when the wind vanishes. An iterative solution using the Obukhov length (equation (4.6)) is less susceptible to this problem as simultaneously smaller fluxes essentially keep L at bay. Beljaars and Holtslag (1991) recommended dropping bulk transfer coefficients as a function of Ri_b in favour of profiles expressed in terms of z/L .

The surface layer bulk Richardson number in HYBRID deviates from equation (4.5) in as much as it subtracts the zero-plane displacement height d_0 from z_r , uses a surface-air temperature difference rather than a virtual potential temperature difference, and surface (skin) rather than air temperature on the denominator for the basic state temperature scale T . A new configuration flag however can be set to force a conversion from T to an approximated value of θ , which makes a difference for a large vertical grid-spacing in the boundary layer (a 50 m grid-box height produces a difference of about 0.25 K). Crucially, the surface temperature is taken as estimated from the heat budget for bare soil physics, with the optional skin temperature extrapolation, and not as the canopy interfacial sublayer temperature. For heavily vegetated surface areas, in particular forests, which should benefit most from the detailed physiology of HYBRID, this presents an obvious problem, since the thermal ‘inertia’ and properties of vegetation cover are not captured. Consequently, we can expect the estimated atmospheric stability, expressed through Ri_b , to fluctuate strongly with a highly variable surface skin temperature.

The momentum, heat and moisture transfer coefficients for a non-neutral stratification are given in unstable conditions ($Ri_b < 0$) as:

$$C_d = C_{dn} \cdot \sqrt{\frac{(1 - a \cdot Ri_b)(1 - b \cdot Ri_b)}{(1 - c \cdot Ri_b)}} \quad (4.7)$$

$$C_h = C_e = C_d \cdot 1.35 \cdot \sqrt{\frac{(1 - d \cdot Ri_b)}{(1 - f \cdot Ri_b)}}$$

and in stable conditions ($Ri_b > 0$) as:

$$C_d = \frac{C_{dn}}{1 + (11.2 + 90 \cdot Ri_b) Ri_b} \quad (4.8)$$

$$C_h = C_e = \frac{C_d \cdot 1.35}{1 + 1.93 \cdot Ri_b}$$

The parameters a , b , c , d and f are listed in Hansen et al. (1983)’s Table 7 as a function of $\log((z_r - d_0)/z_0)$. Heat and moisture transfer coefficients are assumed equal. These functions are drawn in Fig 8(b) and (c), for typical values used in this study. Deardorff emphasized that only a narrow range of Ri_b -dependent transfer coefficients was actually supported by data at the time of publication, with observed stratified-to-neutral drag coefficient ratios of roughly 1.3 in unstable conditions ($Ri_b = -0.1$) and of 0.5 in stable conditions ($Ri_b = 0.05$), see Fig 8(b) for lowest z_0 (thin dash-dotted line). Anything beyond should be considered as extrapolated estimations. He suggested a critical Ri_b of 11/49 at which turbulent transfer vanishes, and the validity of the log-linear stable profile to probably cease much before this. Louis (1979) found that for Ri_b beyond the critical value, a modelled surface energetically disconnected from the stable atmosphere, leading to

unrealistically low night-time ground temperatures and possibly to insufficient atmospheric cooling from the downward heat flux. Mahrt (1987) notes that turbulence-suppression for Richardson numbers greater than 0.25 (i.e. the numbers above) usually refers to the usage of local gradient Richardson numbers. Using layer Richardson numbers from aircraft measurements at flight levels between 20 and 100 m (more akin to our model setup), ranging typically between 0 and 10, very stable stratifications with weak turbulence were actually associated with $Ri > 3$. We therefore cannot exclude a considerable discrepancy between the early experiment-based relationships and their implementation in our coupled models.

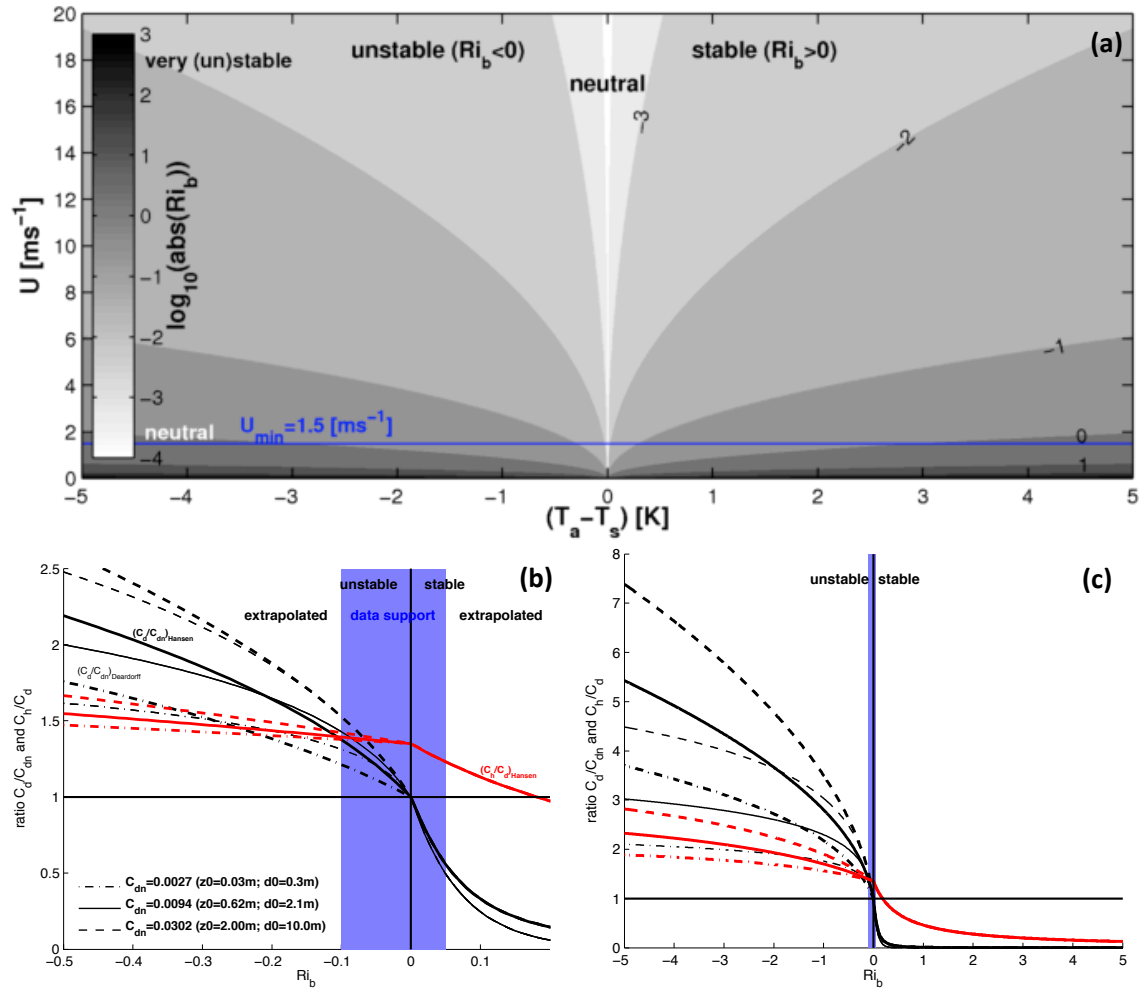


Fig 8 (a) estimated Ri_b (depicted in log-colour scale) as a function of ΔT (between surface and overlying air) and the lowest-level wind speed, as implemented in HYBRID. The reference height z_r has been set to 25 m (half the grid-box height), from which a d_0 of 2.1 m (average over Tiwi Islands) has been subtracted; air temperature T set to 300 K, κ to 0.35; (b) and (c) ratios of momentum transfer (drag) coefficient C_d to its neutral value C_{dn} (black) and of heat transfer coefficient C_h to C_d (red) as a function of Ri_b , (c) is an expanded version of (b). The set of 3 curves corresponds to typical z_0 and d_0 values found in our study, for grassland (dash-dotted), Tiwi open forest composite (solid) and tropical rainforest (dashed). The thick lines correspond to equations (4.7) and (4.8) from Hansen et al. (1983) used in HYBRID, the thin lines follow equations (25) and (26) in Deardorff (1968). The blue shaded area delimits the Ri_b -range supported by data in Deardorff (1968).

It is clear from Fig 8(a) that an estimation of stability around Ri_b , based on model-simulated differences between surface skin and first model-layer temperatures, divided by the surface layer wind velocity squared, readily produces large to extreme values ($Ri_b \gg 1$), especially for vanishing wind speeds. This is likely to produce significant flux uncertainty in the extrapolated regions of the relationships without much data support (Fig 8(b) and (c)). To constrain the surface fluxes and to maintain numerical stability, we set a user-defined minimum wind speed in equation (4.5). By default, this is set to $U_{min}=1.5 \text{ ms}^{-1}$, a ‘weak’ wind according to Mahrt (2008) if taken at 10 m. From Fig 8(a), this avoids Ri_b larger than 01-10, even for a large ΔT . We have also added a configuration flag to use a grid-box mean Ri_b to estimate stability, rather than separate values for each GPT tile, simply by applying the area-weighted T_s for each tile. This should be more appropriate for homogeneous composite land covers. Note that the practice of area-averaging the variables needed to estimate mean grid-box stability and exchange coefficients will yield different results to area-averaging said coefficients, because of the non-linear relationships (Mahrt (1987)). In this study, we retain the original tile-specific Ri_b implementation in HYBRID, mostly to keep our model results consistent with the original design.

Surface layer flux transfers

Turbulent surface fluxes of sensible and latent heat in COARE are computed under simple turbulence similarity assumptions from bulk variables and transfer coefficients, as outlined above, iteratively solving the classical bulk parameterizations applied to mean vertical gradients:

$$\begin{aligned} f_h &= -\rho_a c_{pa} u_* T_* = \rho_a c_{pa} C_h U (T_s - \theta) \\ f_e &= -\rho_a L_e u_* q_* = \rho_a L_e C_e U (q_s - q_a) \\ \tau &= -\rho_a u_*^2 = \rho_a C_d U (u_s - u) \end{aligned} \quad (4.9)$$

The transfer coefficients for drag, heat and water vapour $C_{d,h,e}$ are estimated for a given atmospheric stability from their respective roughness heights $z_{0,0T,0e}$ by using the Monin-Obukhov similarity theory profile functions mentioned before. Gradients in temperature and moisture are calculated between the surface state and the lowermost model scalar level, the free water surface layer being saturated ($q_s = q_s^*(T_s)$). For obvious reasons, there is no surface current u_s in a single-column model, which is therefore set to 0, although it could be made a function of u (here the same as U).

The sensible heat flux (f_h) in HYBRID follows the same drag law parameterization as given in equation (4.9). As already mentioned in the context of stability, the surface temperature in the drag law parameterization for f_h is set to either the upper soil-layer

mean temperature, which for the purpose of the energy balance is supposed to contain the complete vegetation structure (Friend (2010)), or to a parameterized soil skin temperature, but not to a canopy or interfacial sublayer temperature. It is legitimate to ask if the first option is not to be favoured over heavily vegetated, and in particular over forested areas. It provides damped temperature fluctuations, albeit for the wrong physical reasons, since the heat capacity corresponds to that of a moist soil with a certain simulated water content. The complex dependency of fluxes (here, of f_h) on atmospheric stability, included in C_h , is illustrated in Fig 9. Interestingly, the parameterization allows for a sort of ‘free convection’ regime in which f_h increases for a given positive finite ΔT when U tends towards zero. This very unstable situation corresponds to a large negative Ri_b where only buoyancy generates turbulence and the mechanical generation term is removed. It will not occur with U_{min} set to 1.5 ms^{-1} . Very large wind speeds always create a regime akin to neutral stratification, in which f_h varies as a linear function of both U and ΔT . Fig 9 also highlights the strong dependency of fluxes on roughness and displacement height parameters, chosen here to represent typical values within our simulations. Essentially, areas with large z_0 will generate a very elevated f_h that will quickly reduce the ΔT at its origin in a negative feedback mechanism.

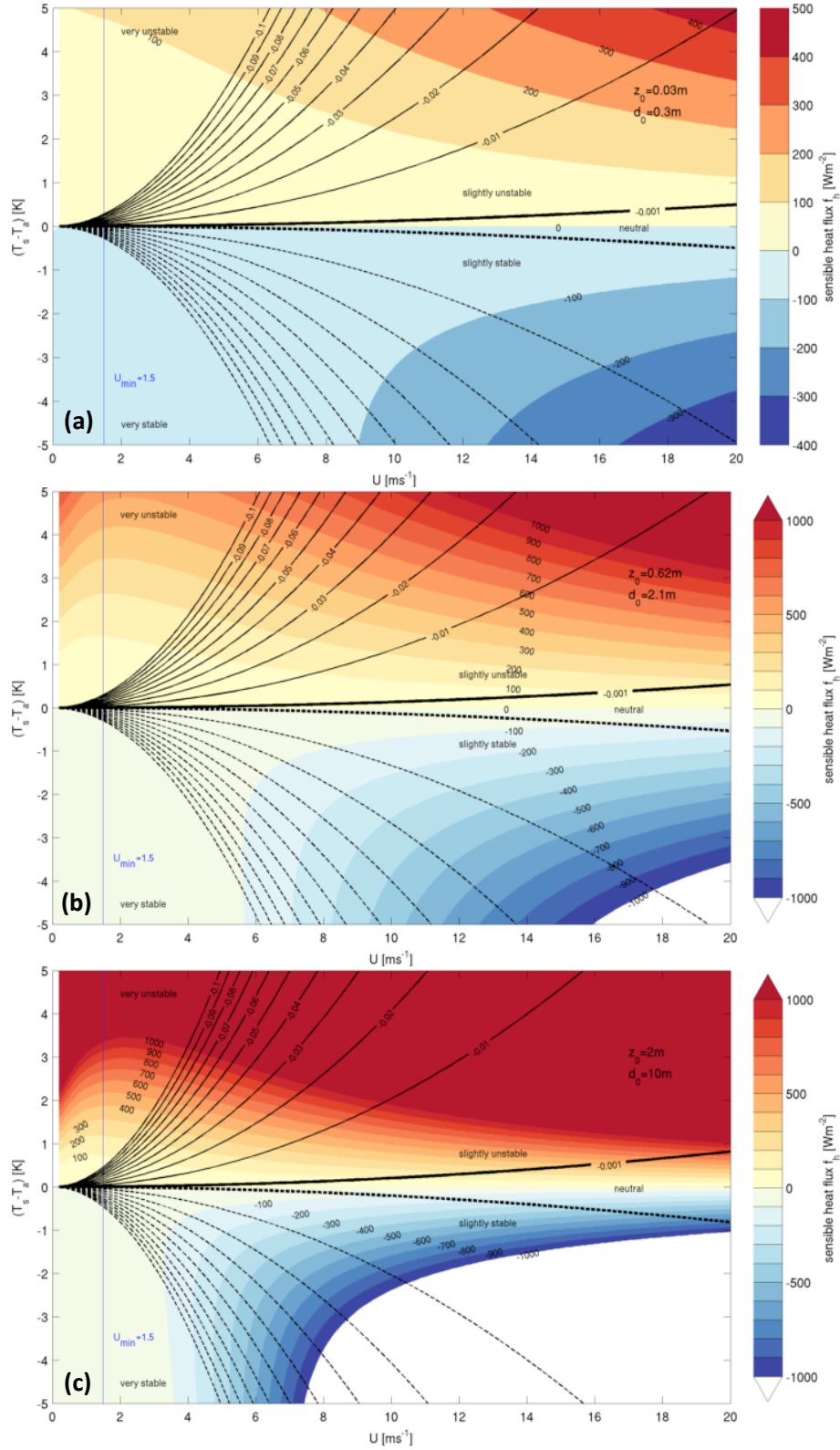


Fig 9 Theoretical land surface fluxes following eq. (4.9) for the same parameters used in Fig 8 and with $\rho_a = 1.2 \text{ kgm}^{-3}$ and $c_{pa} = 1004.64 \text{ Jkg}^{-1}\text{K}^{-1}$ (dry air), as a function of wind speed and surface-air temperature difference. The black contours indicate modelled surface layer stability in terms of the surface bulk Ri_b ; solid lines are negative (unstable), dashed lines are positive (stable). The thick contours delimit an arbitrary region of near-neutrality. The 3 plots differ only in roughness (z_0) and displacement height (d_0).

The latent heat flux (f_e) in HYBRID needs to consider both evaporation (in $[\text{kg m}^{-2}\text{s}^{-1}]$ or $[\text{mm s}^{-1}]$) from the bare soil (E_{ground} , upper soil layer (1) only) and plant transpiration (E_{canopy} , all soil layers (i) penetrated by roots, here $i=2$):

$$f_e = L_e \cdot \left(E_{ground,1} + \sum_i E_{canopy,i} \right) \quad (4.10)$$

It is based around a serial resistance concept for soil evaporation and the canopy conductance approach described in Friend and Kiang (2005) for transpiration. Evapotranspiration is parameterized to occur in unfrozen soils only. The simulated potential bare soil evaporation follows the formulation in the Simplified Simple Biosphere Model SSiB (Xue, Zeng, and Adam Schlosser (1996)), before being further reduced through foliage retention as a function of the Leaf Area Index (LAI):

$$E_{ground} = \rho_a \cdot \frac{1}{r_s + r_a} \cdot \left(RH_s q_s^*(T_s) - q_a \right) \cdot \exp^{-0.7 LAI} \quad (4.11)$$

Here, the surface-level specific humidity at saturation q_s^* , given at either soil skin or first model-layer temperature T_s , is adjusted to the soil's actual mean specific humidity through the relative humidity of the air at the soil surface (Camillo and Gurney (1986)):

$$RH_s = e^{\frac{100\psi_g}{T_s R_v}} \quad (4.12)$$

when $q_s^*(T_s) > q_a$; else, RH_s is set to 1. $R_v = 465.1 \text{ m}^2\text{s}^{-2}\text{K}^{-1}$ is the water vapour gas constant. This relationship considers soil capillary forces or soil water retention by relying on the soil water potential (suction) ψ [MPa] (multiplied by a factor of 100 to convert to pressure head in [m]). The latter is expressed in terms of HYBRID's prognostic upper-layer ratio of water content to field capacity $w_1 = \theta_1 / \theta_{fc}$ following the empirical power curve in Clapp and Hornberger (1978):

$$\psi = \psi_s \left(\frac{\theta}{\theta_s} \right)^{-B} \approx \psi_{fc} \left(\frac{\theta}{\theta_{fc}} \right)^{-B} \quad (4.13)$$

with the parameters ψ_{fc} (at field capacity) = -0.01 MPa and $B = 5$ (representing a sandy to silty loam), and the validity of the relationship for water content to fc being an assumption. Note that within the context of soil physics, θ exceptionally denotes the unitless volumetric soil moisture content (see Seneviratne et al. (2010)), and that the parameters depend strongly on soil characteristics, notably texture. They have not been changed from HYBRID's default values in this study.

The surface resistance r_s accounts for obstructions to the flow from the source within the soil layer to the surface. In SSiB, it is parameterized as a curve-fit to upper-layer soil moisture based on the results of Camillo and Gurney (1986):

$$r_s = 101840 \cdot \left(1 - \left(\frac{\theta_l}{\theta_s} \right)^{0.0027} \right) \approx 101840 \cdot (1 - w_l^{0.0027}) \quad (4.14)$$

Besides this empirical fit being obviously specific to a particular soil, the direct implementation in terms of w_l is conceptually flawed in as much as when the water content is at fc, i.e. still below saturation, r_s cancels. In general, $\theta/\theta_s < \theta/\theta_{fc}$, therefore r_s will be too low, and we can expect this to produce an overestimated E_{ground} .

The aerodynamic resistance r_a parameterizes the stability-dependent atmospheric surface layer turbulent transfer and reduces to the usual form in the drag law parameterization:

$$r_a = 1/(C_e \cdot U) \quad (4.15)$$

Bare soil evaporation in equation (4.11) is limited to upward-positive values. Dew formation is currently not included in the model. Dew constitutes an important reservoir for early morning latent heat transfer to the atmosphere, but in order to be captured by the model, requires this reservoir to be carefully coupled to the water and energy budgets. A dew and interception reservoir would probably be made a function of LAI.

Assuming that the leaves' internal air space is saturated in moisture at the prevailing canopy temperature¹⁴, plant transpiration from each soil layer i can be parameterized in terms of a mean canopy stomatal conductance to moisture (or the inverse resistance $r_{c,i}$), $g_{can,i} = 1/r_{c,i}$, which accounts for the cross-stomata transfer (Friend and Kiang (2005)):

$$E_{canopy,i} = \rho_a \cdot \frac{1}{r_{c,i} + r_a} \cdot (q_s^*(T_s) - q_a) \quad (4.16)$$

In HYBRID, $g_{can,i}$ [ms^{-1}] for each GPT-tile is taken as the sum over each plant individual (in vegetation dynamics mode only, else over the unique individual) for the wetter one of the 2 soil layers only. For a given individual, the total canopy conductance to moisture g_{can} is a decreasing function of the gradient of specific humidity between internal air spaces and the air on the outer leaf surface ($f_{\Delta q,leaf}$), a decreasing function of leaf internal CO_2 (f_{CO_2}), a decreasing function of canopy height ($f_{hcanopy}$), an increasing function of the soil water potential or water availability (f_ψ), is scaled with the net photosynthetic capacity ($A_{cap}[\mu\text{mol}_{\text{CO}_2} \text{m}^2_{\text{ground}} \text{s}^{-1}]$), i.e. the gross capacity (based on Kull and Kruijt (1998)) with unlimited CO_2 supply minus mitochondrial respiration, and multiplied by a constant of proportionality $\alpha [\text{m}^3_{\text{H}_2\text{O}} \text{mol}^{-1}_{\text{CO}_2}]$:

¹⁴ Set here to the upper-soil level or surface skin temperature ($T_{can} = T_s$), such that the leaf internal specific humidity reduces to $q_{can} = q_s^*(T_s)$

$$g_{can} = \alpha \cdot f_{\Delta_q \text{ leaf}} \cdot f_{CO_2} \cdot f_{h_{canopy}} \cdot f_{\psi} \cdot A_{cap} \quad (4.17)$$

A_{cap} varies with light, temperature and photosynthetic N. Canopy stomatal conductance is limited to a GPT-specific range, typically $0.06 - 6 \cdot LAI \text{ mm}_{H_2O} s^{-1}$. Friend and Kiang (2005) note that they assume a minimum of 30 min for stomata apertures to switch between these 2 extremes. Since we could not identify a corresponding limit to the rate of change within the model, we assume that this might have been implicit with the typical large time steps in a GCM. The very high temporal resolution of ATHAM and rapidly varying atmospheric processes might violate this response time.

The leaf internal CO_2 concentration (C_i) is finally calculated through an iterative procedure (over sub-time steps t) such that CO_2 supply at a given stomata aperture (canopy conductance) balances net fixation by photosynthesis (A_{can}), computed across several canopy layers with gradual light extinction by the foliage. Then, if C_a is the atmospheric CO_2 , we have:

$$A_{can}(t-1) = \frac{C_a(t-1) - C_i(t)}{r_{tot}(t-1)} \quad (4.18)$$

with $r_{tot} = 1.6(1/g_{can} + r_a)$ being the combined resistance to CO_2 flux from surface level atmospheric air into leaf internal air spaces. From this last equation, considering equation (4.8) for atmospheric stability and the particular implementation of the iterative solver in HYBRID, we found C_i to tend towards very large values after sunset in stable atmospheres, so as to balance a finite negative net photosynthesis (i.e. respiration) A_{can} , when r_{tot} became increasingly large due to aerodynamic resistance. This could possibly be resolved by including a missing inhibition process on respiration in A_{can} for large C_i concentrations, since respiration is currently unaffected by internal CO_2 -forced displacement of available O_2 (Friend 2009, personal communication). It is not clear to us to what extent abnormally high C_i further affects the simulation, in particular the turbulent fluxes, if at all. At night-time, the modelled A_{cap} becomes negative, and stomata close to avoid water loss (equation (4.17)), respectively get set to a default minimum conductance value; therefore C_i does not modify transpiration through g_{can} . Conversely, high atmospheric stability during daylight hours produces realistic convergence, since essentially, decaying turbulent flux transfer cuts off CO_2 supply to the plant, leading to a quick depletion of C_i . The solution then converges to an equilibrium of very low C_i , no cross-stomata exchange and shut-down photosynthesis.

In our view, however, this behaviour illustrates a broader issue, which may well affect a number of models, namely that boundary layer similarity theory is used outside the remit for which it has been developed. Although turbulent fluxes might decrease dramatically in very stable atmospheres within the surface layer, it seems less obvious

that transpiration within a plant canopy in the interfacial sublayer should be heavily limited by decreasing turbulent fluxes aloft. Molecular diffusion, by contrast, might play an increasingly relevant role for large gradients of gases within a forest canopy microclimate. We could imagine using a modified r_a based around diffusion, or parallel resistance coupling between turbulence and diffusion, within a currently missing interfacial sublayer. This issue with transpiration was the main reason behind our choice to add TKE to the mean wind in equation (4.2) and to impose a minimum wind speed during the estimation of Ri_b . Arguments about the interfacial microclimate set aside, note also that transpiration will be heavily influenced by soil water stress, requiring soil physics, hydrology, properties and initialization to be captured in a much more realistic way than they currently are.

Lastly, and most importantly, the sensible and latent heat fluxes are incorporated as potential temperature, specific humidity and pressure perturbations into ATHAM's lowermost grid-boxes, for any finite ATHAM time-step dt . The potential temperature perturbation $\delta\theta_1$ [K] is computed from the sensible heat flux as:

$$\delta\theta_1 = \frac{f_h \cdot dt}{\rho_a c_{pa} \cdot \Delta_{zv}} \cdot \left(\frac{p_{s0}}{p} \right)^{R/c_{pg}} \quad (4.19)$$

where $\Delta_{zv} = 2z_r$ is the grid-box height of the staggered vector grid, p is the pressure in the grid-box, p_{s0} is the reference surface pressure in the domain, R [$\text{J} \cdot \text{kg}^{-1} \text{K}^{-1}$] is the gas constant for the total mixture and c_{pg} the specific heat capacity at constant pressure for the gas mixture. The specific humidity perturbation δq_{v1} [$\text{kg}_v \cdot \text{kg}_a^{-1}$] is calculated from the latent heat flux, or rather directly from the surface evaporation or evapotranspiration E [$\text{kg}_v \cdot \text{m}^{-2} \text{s}^{-1} = \text{mm} \cdot \text{s}^{-1}$] as:

$$\delta q_{v1} = \frac{E \cdot dt}{\rho_a \cdot \Delta_{zv}} \quad (4.20)$$

By differentiating the equation of state for an ideal gas, $p\alpha = RT$, where α [$\text{m}^3 \cdot \text{kg}^{-1}$] is the specific volume, we get:

$$pd\alpha + \alpha dp = RdT \quad (4.21)$$

According to the first law of thermodynamics, the general expression for the conservation of energy is written as:

$$dq = c_v dT + pd\alpha \quad (4.22)$$

where the specific heat at constant volume c_v is related to c_p and R by $c_v = c_p - R$, and where dq exceptionally denotes a change of heat per unit-mass of gas. For adiabatic processes, no energy is exchanged between the system described by equation (4.22) and

the exterior, such that $dq = 0$. Combining (4.21) and (4.22), taking $\gamma = c_p/c_v$, and since $d\alpha/\alpha = -d\rho/\rho$, we obtain:

$$dp = \gamma p \frac{d\rho}{\rho} \quad (4.23)$$

The pressure perturbation δp_1 [Pa] induced by increasing the atmospheric density through the addition of water vapour mass (specific humidity) is then simply:

$$\delta p_1 = \gamma_a \cdot p \cdot \delta q_{v1} \quad (4.24)$$

Note that an additional pressure change will arise through the temperature perturbation $\delta\theta_1$ from the sensible heat flux. This perturbation is directly accounted for in ATHAM's dynamical core and added to the other pressure perturbations, including (4.24), when solving for pressure waves. Naturally, temperature perturbations and changes in molecular composition, (water vapour having a lower molecular weight than dry air), will influence a parcel's buoyancy, which is accounted for during a following update to the equation of state during an integration step.

Within the realm of a computationally achievable model grid-spacing required to simulate both shallow and deep convection, it is not possible to resolve near-wall turbulent stresses, and any adopted vertical grid-spacing is certainly outside the inertial subrange (Bou-Zeid et al. (2008)). Consequently, besides the actual sensible and latent heat transfer from the surface to the atmosphere, handled by the surface parameterizations, the vertical flux through the few grid-boxes in the surface layer and through the lower boundary layer will critically depend on the subgrid-scale turbulence model.

In terms of future improvements, a consistent treatment of atmospheric stability to be used in the surface layer by all coupled models for heat, tracer and momentum flux parameterizations would be advantageous.

Flux enhancement in a preliminary shallow waters parameterization

COARE is an algorithm designed for deep seas with a wind speed-dependent aerodynamic roughness in equilibrium. In uniformly shallow water bodies, such as shallow lakes, the mean-square wave heights are empirically proportional to water depth (Davidan et al. (1985), cited in Panin et al. (2006)). We have adopted the parameterizations proposed by Panin et al. (2006) to adjust COARE's estimated sensible and latent heat fluxes to shallow bathymetries through:

$$f_{h,e}^{sw} \approx f_{h,e} \cdot \left(1 + k_{h,e}^{sw} \cdot \frac{h_{rms}}{H_{bathy}} \right) \quad (4.25)$$

Here, $f_{h,e}^{sw}$ denote the shallow waters-adjusted sensible and latent heat fluxes, $k_{h,e}^{sw}$ are empirical coefficients, set both to 2, H_{bathy} is the depth of the water body, and h_{rms} is the mean-square wave height, given in a depth-dependent form as $h_{rms} \approx \frac{0.07 \cdot U^2 \cdot (gH_{bathy}/U^2)^{3/5}}{g}$, where g stands for gravity¹⁵.

Wind speed U should be provided at the standard 10 m, but for consistency with the rest of the code, is taken at the model's lowest atmospheric scalar grid-point. Very crudely, this formulation may also reproduce a behaviour similar to shoaling in coastal waters, increasing fluxes as depths decrease. Like the warm layer physics, these shallow water corrections have to be compiled explicitly, by including the SHALLOW_WATER precompiler flag in the model's Makefile.COMPILE, and require an additional bathymetry input data set. Their inclusion in the algorithm has not been tested and might be inconsistent with the original formulations in Fairall et al. (2003). Furthermore, in our implementation, when the warm layer is wiped out and where the maximum trapping depth (currently 19 m) exceeds the local water depth, we equate the average fraction of absorbed solar radiation for the calculation of a new warm mixing layer to unity, rather than the original fixed fraction of $\frac{3}{4}$ in COARE. The shallow water adaptation of warm layer physics thus assumes that all solar radiation is absorbed if a wiped-out mixing layer reaches the seabed, and that no radiation is reflected off the seabed to leave the water body.

COARE's wave parameters¹⁵ were not used above since depth-independent. Note that an alternative (and physically more consistent) way forward would be to adapt the wave parameters therein to shallow waters, applying, for example, standard equations for the dispersion relationship for a more elaborate treatment of coastal waters (P. K. Taylor and Yelland (2001)). This can be easily implemented in the model, and the Panin et al. (2006) parameterization then exclusively used for shallow lakes, after thorough testing.

By way of a summary of surface and interface features additionally implemented in the coupled models and actually used within this study, we refer to Table 1.

¹⁵ See also Appendix A

Table 1 Summary of currently available surface interface features; value refers to this study

Model	Feature	Parameter	Eq.	Reference	Value
HYBRID	<i>gustiness/turbulent velocity scale</i>	β_{TKE}	4.2		1 [-]
HYBRID	<i>skin temperature from quadratic SGS profile</i>	-		Gerken et al. 2012	included
HYBRID	<i>modified diffusion time scale for heat transport</i>	-		Gerken et al. 2012	included
HYBRID	<i>area-weighted mean z_0 for composite vegetation</i>	-			included
HYBRID	<i>minimum wind for stability estimation</i>	U_{min}	4.5		1.5 [m s ⁻¹]
HYBRID	<i>grid-box mean Ri_b for stability estimation</i>	-	4.5		not used
ATHAM-COARE	<i>dynamic ocean albedo</i>	τ_{aeros} / chlorophyll		Jin et al. 2004	0.0 [-] / 0.2 [mg m ⁻³]
COARE	<i>cool skin (use precompiler flag)</i>	-		Saunders 1967	included
COARE	<i>warm layer (use precompiler flag)</i>	-		Price, Weller, and Pinkel 1986	not used
COARE	<i>wave parameterization for surface roughness</i>	-	7.1-2	Taylor and Yelland 2001, Oost et al. 2002	not used
COARE	<i>shallow waters flux enhancement (use precompiler flag)</i>	-	4.25	Panin 2006	included

The mixed blessing of additional complexity

A large amount of detailed additional processes have been added within the newly coupled modelling system, which increase the range and complexity of potential feedbacks. To our knowledge, this might be one of the first integrated ‘Earth systems’ models running at the scale of a CRM/LES, permitting simulations in the realm of dry PBL convection as of deep moist convection. However, many further parameters need specification, and they might not be trivial to determine. Beljaars and Holtslag (1991) write in the context of land surface parameterizations that in spite of more accurate physics, they find simpler schemes often to be preferable. More complicated and physically realistic parameterizations hence provide a substantial scope for further sensitivity studies, and an even greater need for individual component validation, preferably in idealized model setups. Houze (1994) writes that insights into the dynamics of thunderstorms have been largely gained from the analysis of 3D fully-compressible numeric simulations, based on models undergoing gradually-increasing sophistication. The coupling described in this dissertation aims at contributing to this effort, by introducing a physiologically-driven interactive biosphere response to both subtle and intensive convective processes in the atmosphere. In this study, and within the context of the Hector storm simulation, we maintain the maximum level of complexity to produce a realistic simulation with a carefully chosen initialization, but with no ‘tuning’ to optimize the results.

4.2 Processing multiple data sources for initializing the surface state

If ATHAM is run in interactive mode with HYBRID and COARE, the coupled models will require a larger set of initial conditions and specification files that describe the characteristics and set the state of the lower boundary. Most community or operational modelling suites include data assimilation procedures, standard datasets and/or preprocessors to initialize a run from observed or re-analysis data sources. We have

produced such a preprocessing package specifically for ATHAM-HYBRID-COARE, called *buildsurface*¹⁶.

Buildsurface reads in gridded observational surface data (file paths set in INPUT_surface_preprocess) and user-defined surface model parameters (defined in INPUT_surface_preprocess), and exports the single column initialization variables required by HYBRID and COARE as arrays matched to the ATHAM stretched grid. Amongst the exported ATHAM-HYBRID-COARE initialization files, the land-sea mask and topography files can also be used for uncoupled, (including prescribed-surface), ATHAM runs in various configurations. It is possible to initialize the entire domain with homogeneous (averaged or idealized) conditions to simplify the setup. The corresponding variables are called single value defaults (SVDs, if substituting spatial data) and single value parameters (SVPs, if no spatial data can be used), and are all defined in *buildsurface*'s INPUT_surface_preprocess namelist file. Single value defaults are also used to fill in data gaps. Input observations need to be provided in a format specified in *buildsurface*'s documentation, output files are formatted such that the coupled models can read them; both are in netCDF format¹⁷.

Several idealized simulation scenarios can be created by the preprocessor. Currently, these include circular or elliptic islands or lakes in an otherwise flat environment, or volcanic cones. In all other situations, the fundamental file to set up a scenario, (provided it includes both land and water areas), is the land cover dataset, since it defines the land-sea mask. All other observational datasets will be referenced to this land-sea mask. Data gaps, or otherwise inconsistent data-points identified with respect to this mask, are replaced by default values. An associated quality control file (QC_surf_gapmap.nc) will be output by the preprocessor. The land cover dataset will be used to define fractional GPTs for each grid-box, over areas identified as containing natural landscape. The four nearest neighbours will make up the fractional land cover classes in a model grid-box, with weighting according to distance. Since various land cover datasets can be used according to the modelling purpose, the corresponding classes

¹⁶ *Buildsurface* is now delivered with every standard ATHAM release, and is compiled using a standard *make* in ATHAM's top-level directory. See Appendix B for the new model versioning system. Since *buildsurface* needs to recreate the grid that will be used for a specific experiment within any given ATHAM configuration, *make buildsurface* will compile the full coupled models, and incorporate parts of the ATHAM code in the preprocessor. For the same reasons, running *buildsurface* will also require access to the same INPUT_atham_setup namelist file that will be used for the experiment and that defines the grid. Because of a specific issue in the code, the flag *config_surf_from_file* in INPUT_atham_setup needs to be set to *false* when running the preprocessor only. The total number of grid-points therein, $(nt_{x,y})$, should be defined such that no further adjustment is necessary in a parallel configuration, that is, given a required number of processors in each direction $(np_{x,y})$, the number of grid-points per processor, $n_{x,y} = \left((nt_{x,y} - 2) / np_{x,y} \right) + 2$, should be an even integer.

¹⁷ See Appendix B

need to be remapped into HYBRID's GPTs, usually resulting in a composition of several different plant types. The table providing the remapping key needs to be provided in the required format with the MAPPING_surf_landcover namelist file (see below and Table 2). The yearly maximum of the monthly mean 24h maximum temperature from climate data is used to assign herbaceous species to either C_3 or C_4 photosynthetic pathways. As in Friend (2010), a threshold of 31°C is used, above which all herbaceous plants are associated with the C_4 pathway. Special categories can also be defined. We currently include high- and low-density urban areas, water bodies, snow- and ice-covered regions as well as wetlands in special categories. If the fractional area of any such category exceeds a user-specified threshold (the default is 0.5), the entire grid-box is assigned to this class. All water bodies are simulated using COARE. Urban areas currently get treated as barren grid-boxes using HYBRID's soil physics, after applying special parameter sets. A snow-ice mask is defined to be used within HYBRID. Wetlands are given increased soil moisture field capacity values (see below) and are water-saturated.

Within *buildsurface*, all water bodies are necessarily flat and set at a unique user-defined altitude, independently of the topography observations. In case different water bodies at different altitudes are present, this will need to be adjusted through post-processing of the topography initialization file. Topography is readjusted to relative heights with respect to the lowest model grid-point, then translated into grid-box units. Single grid-box depressions in any horizontal direction are removed since they create singularities in ATHAM; this results in some smoothing.

Because of the very short simulations ATHAM has been designed for, the photosynthetic biomass of vegetated grid-boxes, estimated through the Leaf Area Index (LAI), is currently ingested as an 'instantaneous' (typically 16 days) operational LAI product. This is assigned onto HYBRID's monthly mean climatological LAI structure for all the months. Obviously, a true average can be used, or alternatively *buildsurface* adapted to read arrays with a further monthly time dimension.

Surface albedo is generally different for direct and diffuse sun light. The zenith angle-dependent direct insolation albedo is termed black-sky albedo, diffuse insolation albedo is known as white-sky albedo. In the absence of a consistent 'blue-sky' treatment of these separate values for direct and diffuse sun light across ATHAM and HYBRID, we are currently reading in either a black- or a white-sky observational grid, and use this as a total solar broadband albedo surrogate. As mentioned previously, this can be used to replace the composite albedo computed internally as a function of vegetation cover, and might be more representative of the real surface. It then implies a homogeneous solar energy partitioning across a grid-box. This can be either more or less realistic than GPT-dependent albedos, depending on whether subgrid-scale vegetation patchiness is well-

distributed, such as in a savannah or sparse forest, or confined to separate tiles, as is more typical for anthropogenic landscapes. Surface and bare soil albedo values for grid-boxes masked by snow or ice are readjusted to a value of 0.8.

In terms of the soil's capacity for retaining moisture and actual water content, HYBRID is implemented with a volume fraction of condensed soil water at field capacity (θ_{fc}). Field capacity (fc) is the maximum amount of water the soil can naturally retain against gravity. It is a useful property for defining a well-drained soil, but much less useful if the water table reaches the upper-soil horizons. We have therefore introduced a special user-defined default soil porosity that replaces θ_{fc} in areas of perennially saturated soils, such as marshlands or rice fields. In these areas, soil physics within HYBRID will continue to be modelled in terms of a maximum water retention defined by fc, but the choice of a larger value for porosity, independently of the true nature of the soil, will make the available water amount proportionally larger. In our study, this resulted in increased evapotranspiration fluxes over coastal mangrove areas. A soil moisture field from a previous HYBRID spin-up run, i.e. using the same 2 soil-layers configuration, can be ingested if available.

Without dedicated field measurements, soil properties are hard to come by. The FAO Harmonized World Soil Database (Nachtergaele, van Velthuisen, and Verelst (2009)) provides a globally consistent dataset, including gridded data of observed available water storage capacity (AWC), the water that can be held in the rooting zone between the plant wilting point and fc. We have implemented this as the default parameter expected by *buildsurface*. Conversion into θ_{fc} has been aligned with Friend (2010) using a multiplier of 1.75, and defining a default value for undefined grid-boxes of 100 mm m⁻¹.

In terms of skin temperatures, SST is now routinely available at very high temporal resolution from satellite observations. Land surface temperatures are more difficult to estimate because of uncertain emissivities; furthermore, HYBRID requires an estimated temperature profile. A user-defined single value default land surface 'skin' (i.e. upper-layer) temperature can be distributed across the grid, with an optional random component, provided the original 2-layer parameterization is used. If the new skin-extrapolation described by Gerken et al. (2012) is selected, initializing with an identical soil temperature profile for every land surface grid-point is currently mandatory.

Bilinear interpolation of nearest neighbours is used to populate the initialization files from the observational datasets. This produces most representative results if the original dataset resolution roughly matches ATHAM's grid-spacing. Particularly, the original resolution should not be much finer than ATHAM's grid-spacing. If it is, averaging should be performed prior to running *buildsurface*. ATHAM uses a 3D Cartesian reference framework, and observations are to be provided in a geographical coordinates system

(GCS). A latitude-longitude map will be built from the Cartesian grid using simple spherical geometry, assuming that the x-direction is west-east aligned and the y-direction south-north. The geographical position of the grid-centre is specified by the user, and for each grid-point, the distance to the centre of the Earth is derived from a World Geodetic System (WGS) 1984 ellipsoid. Geographical coordinates are then computed for each ATHAM grid-point in the new projected framework. Note that this is only used for the interpolation of observations; ATHAM's native output remains in a Cartesian reference system. Here, single-valued offsets (latitude and longitude of grid origin) and scale-factors ($180/\pi r_E$ for latitude, $180/(\pi r_E \cdot \cos \phi_{c,rad})$ for longitude, where r_E is the Earth ellipsoid radius at the grid centre and $\phi_{c,rad}$ is the grid-centre latitude in radians) are generated and added as attributes to the output file dimension vectors. They can then be used to rapidly convert Cartesian coordinate vectors into geographical ones. This works fine as long as ATHAM's domain remains small relative to the Earth radius ($O100$ km), especially in the north-south direction, and is significantly away from the poles.

Ideally, for efficient surface setups, the preprocessor should be linked to a database (DB) of preformatted geospatial data required as input, or provide access to corresponding operational data servers. We have started to populate a corresponding Geographical Information System (GIS) DB with large data files representing static conditions, typically topography, bathymetry, soil properties, climate data, land cover, and so on. In practice, users will want to use their own data sources and need to use timely information that characterizes the observed state in specific case studies, e.g. LAI, surface albedo, soil temperature and moisture profiles, SST. We also found processing observational data to the required format so that it can be used by *buildsurface* to be rather tedious in a GIS framework¹⁸. We have therefore also developed a suite of tools in scripting language to import observational data from a variety of sources and to export it within the specifications required by *buildsurface*.

For convection-resolving simulations, the land cover datasets usually used for HYBRID simulations have too coarse a resolution. The highest-resolution globally-classified and independently validated land cover dataset currently available is derived from ENVISAT-MERIS full-resolution imagery. The GlobCover initiative (Arino et al. (2007)) provides a global map for the year 2005-2006 at 300 m resolution, with a 22 class thematic legend compatible with the UN/FAO Land Cover Classification Scheme (LCCS). Even if other products are available, a definite advantage of using a globally-homogeneous

¹⁸ Such processing may include format conversions, geo-referencing and dataset projection (into a WGS 1984 GCS), information extraction, smoothing, interpolation, dataset size reduction or raster merging, joining attribute tables, creating rasters from vector features, averaging time records, and so on.

(and regularly updated) dataset is the possibility to easily transfer the model to other locations, or to perform land-use change sensitivity analyses without having to resort to major GPT-re-mapping updates. We have used a GlobCover version 2.2 regional map over Australia with over 50 regionally-tuned sub-classes for this study, with the re-mapping key given in Table 2. This also includes case study-specific values for roughness lengths z_0 and displacement heights d_0 , attributed to each GPT. These values fall into a similar range as the 10% of canopy/crop height used by Prabha, Karipot, and Binford (2007) and Maronga and Raasch (2013) for similar LES studies focused on the PBL. As discussed previously, these will be used together with fractional GPT-coverage to estimate rough ‘effective’ averages for each grid-box. The average fractional GPT-coverage over Tiwi Islands is composed of 14.70% NLEVs, 25.51% BREVs, 23.57% BREVt, 0.03% BRDDt, 34.25% C4, 0.85% BRCDt, 0.01% moss and 0.13% NLCDt (see Table 2 for abbreviations). This results in an average z_0 of 0.62 m and d_0 of $0.7 \cdot 3$ m. Sensitivity simulations with a homogeneous land cover are initialized with this composition.

Table 2 Re-mapping table between GlobCover regional classes and HYBRID Generalized Plant Types (GPTs), as used within this study (MAPPING_surf_landcover namelist file)

		NLEVs	NLEVt	BREVs	BREVt	BRDDt	C3/C4	BRCDt	moss	NLCDt
roughness length	z_0 [m]	0.30	1.00	0.30	2.00	1.00	0.03	1.50	0.01	1.50
displacement height	d_0 [m]	1.0	10.0	1.0	10.0	10.0	0.3	10.0	0.1	10.0
LCCS level 1 category	(sub-) class									
		cultivated terrestrial areas and managed lands (A11)								
<i>post-flooding or irrigated croplands</i>		11	-	-	15	-	15	50	-	-
	shrub or tree crops	12	-	-	30	-	30	-	-	-
<i>rainfed croplands</i>	herbaceous crops	13	-	-	-	-	100	-	-	-
		14	-	-	15	-	15	50	-	-
	herbaceous crops	15	-	-	-	-	100	-	-	-
	shrub or tree crops (vinyards, olive, archards,...)	16	-	-	30	-	30	-	-	-
<i>mosaic cropland (50-70%) / vegetation (20-50%)</i>		20	-	-	20	-	60	10	-	10
	grassland or shrubland	21	-	-	40	-	60	-	-	-
<i>mosaic vegetation (50-70%) / cropland (20-50%)</i>	forest	22	-	-	-	-	60	20	-	20
		30	-	-	15	-	55	15	-	15
	grassland or shrubland	31	-	-	30	-	70	-	-	-
	forest	32	-	-	-	-	40	30	-	30
		natural and semi-natural terrestrial vegetation - woody/trees (A12)								
<i>closed to open broadleaved evergreen or semi-deciduous forest</i>		40	-	-	-	65	-	35	-	-
	closed broadleaved evergreen and/or semi-deciduous	41	-	-	-	100	-	-	-	-
	open broadleaved semi-deciduous and/or evergreen forest with emergents	42	-	-	10	20	-	70	-	-
<i>closed broadleaved deciduous forest</i>		50	-	-	-	-	-	100	-	-
<i>open broadleaved deciduous forest</i>		60	-	-	-	-	-	70	30	-
<i>closed needleleaved evergreen forest</i>		70	-	100	-	-	-	-	-	-
<i>open needleleaved deciduous or evergreen forest</i>		90	-	15	-	-	-	70	-	15
	deciduous	91	-	-	-	-	-	70	-	30
	evergreen	92	-	30	-	-	-	70	-	-
<i>closed to open mixed broadleaved and needleleaved forest</i>		100	-	-	-	-	-	35	35	30
	closed	101	-	-	-	-	-	50	-	50
	open	102	-	-	-	-	-	70	15	15
<i>mosaic forest or shrubland (50-70%) / grassland (20-50%)</i>		110	-	-	30	-	-	40	15	15
<i>mosaic grassland (50-70%) / forest or shrubland (20-50%)</i>		120	-	-	20	-	-	60	10	10
		natural and semi-natural terrestrial vegetation - shrubs (A12)								
<i>closed to open shrubland</i>		130	30	-	35	-	-	35	-	-
	broadleaved or needleleaved evergreen	131	30	-	35	-	-	35	-	-
	broadleaved evergreen	132	-	-	65	-	-	35	-	-
	needleleaved evergreen	133	65	-	-	-	-	35	-	-
	broadleaved deciduous	134	-	-	65	-	-	35	-	-
	closed broadleaved deciduous	135	-	-	100	-	-	-	-	-
	open broadleaved deciduous	136	-	-	30	-	-	70	-	-
		natural and semi-natural terrestrial vegetation - herbaceous (A12)								
<i>closed to open herbaceous vegetation (grassland, savannas or lichens/mosses)</i>		140	-	-	-	-	10	65	-	10
	closed grassland	141	-	-	-	-	-	100	-	-
	closed grassland with sparse trees or shrubs	142	-	-	4	-	4	92	-	-
	open grassland	143	-	-	-	-	-	30	-	-
	open grassland with sparse trees or shrubs	144	-	-	4	-	4	30	-	-
	lichens or mosses	145	-	-	-	-	-	-	100	-
		natural and semi-natural terrestrial vegetation (A12)								
<i>sparse vegetation</i>		150	-	-	4	-	-	4	-	-
	grassland	151	-	-	-	-	-	8	-	-
	shrubland	152	-	-	8	-	-	-	-	-
	trees	153	-	-	-	-	8	-	-	-
		natural and semi-natural aquatic vegetation (A24)								
<i>wetland: closed to open broadleaved forest, fresh or brackish water</i>		160	-	-	-	65	-	-	35	-
	(semi-)permanently flooded land	161	-	-	-	65	-	-	35	-
	temporarily flooded land	162	-	-	-	65	-	-	35	-
<i>wetland: closed broadleaved forest or shrubland permanently flooded, saline or brackish</i>		170	-	-	-	100	-	-	-	-
<i>wetland: closed to open grassland or woody vegetation</i>		180	-	-	-	30	-	35	-	35
	woody vegetation, fresh or brackish water	181	-	-	-	65	-	-	35	-
	woody vegetation, temporarily flooded	182	-	-	-	65	-	-	35	-
	woody vegetation, permanently flooded	183	-	-	-	65	-	-	35	-
	woody vegetation, waterlogged	184	-	-	-	65	-	-	35	-
	grassland, regularly flooded or waterlogged	185	-	-	-	-	-	65	-	35
	grassland, temporarily flooded	186	-	-	-	-	-	65	-	35
	grassland, permanently flooded	187	-	-	-	-	-	65	-	35
	grassland, waterlogged	188	-	-	-	-	-	65	-	35
		artificial surfaces (B15)								
<i>artificial surfaces and associated areas (urban>50%)</i>		190	-	-	-	-	-	-	-	-
		bare areas (B16)								
<i>bare areas</i>		200	-	-	-	-	-	-	-	-
	consolidated bare areas	201	-	-	-	-	-	-	-	-
	non-consolidated bare areas (sandy desert)	202	-	-	-	-	-	-	-	-
	salt hardpans	203	-	-	-	-	-	-	-	-
		inland water bodies, snow and ice (B28)								
<i>water bodies</i>		210	-	-	-	-	-	-	-	-
<i>permanent snow and ice</i>		220	-	-	-	-	-	-	-	-
		perennial snow or ice								

The mnemonics used for GPTs are: NLEVs – needleleaved evergreen shrub, NLEVt – needleleaved evergreen tree, BREVs – broadleaved evergreen shrub, BREVt – broadleaved evergreen tree, BRDD – broadleaved dry deciduous tree, C3 – C₃ pathway herbaceous, including crop, C4 – C₄ pathways herbaceous, including crop, BRCDt – broadleaved cold deciduous tree, moss – bryophytes, NLCDt – needleleaved cold deciduous tree. Values are in %, bare soil adjusts the total to 100%. Class and level 1 legend as in Appendix II and III of Bicheron et al. (2008), level 2 legend given therein. Closed means >40%, open 15-40%, closed to open >15%, sparse <15%. Trees are typically >5 m, shrubs <5 m. See text for

climate-dependent re-assignments between C_3 and C_4 . Special categories are in bold. Roughness lengths z_0 and displacement heights d_0 , have been specifically assigned to the vegetation for this case study (adapted from Brutsaert (2005)). All physiological parameters remain the same as specified in Friend (2010) and associated references. This table has been compared qualitatively against main vegetation types it derives for Tiwi Islands; it shall by no means be applied to other regions without further validation, especially if a robust vegetation physiology is required.

Topography has been derived from the SRTM 90m dataset, processed from the original data to a seamless continuous digital elevation model (Jarvis et al. (2006)). The coarse-resolution bathymetry dataset we accessed from a global database provided unreliable depths in coastal areas. We derived a mean depth of 47 m and favoured a homogeneous ocean around the islands to avoid inconsistent treatment at the model's lateral periodic boundaries.

Soil properties have been derived from the online digital Atlas of Australian Soils (McKenzie et al. (2000)), accessed and downloaded through the Australian Soil Resource Information System, an open soil GIS DB. This includes a soil profiles DB, containing descriptions of soil type, morphology, chemistry, and some physical properties. Because of the crude parameterization of soil thermal and water diffusion processes in HYBRID, *buildsurface* currently only reads single default values for soil properties. We therefore used the geospatial data for computing area-weighted averages of the latter. Since only one value can be assigned to each of the two layers for bare soil characterization, we used averages computed for the non-saturated areas only. Values given correspond to area-weighted medians of the principle/dominant soil profile form, with the 5th to 95th percentile confidence interval in between parentheses. Overall, Tiwi Islands soils have been classified as of lateritic tropical rainforest type (Keenan et al. (1989)), overgrown with Eucalyptus sub-tropical savannah-grassy open forests. Laterite soils, typical for hot and wet tropical areas, develop by intensive weathering of the underlying parent rock, and are therefore often porous and slightly permeable. The littoral wetlands, mainly in mangrove regions, are saturated hydrosols. A full characterization of the soil's A- and B-horizons for average Tiwi 'drylands' and 'wetlands' (Fig 10(d)) is given in Table 3.

Table 3 Average Tiwi Islands soil properties computed for unsaturated soils and wetlands as area-weighted averages, using data from the Atlas of Australian Soils

	Drylands horizon A	Drylands horizon B	Wetlands horizon A	Wetlands horizon B
<i>Horizon thickness [m]</i>	0.3 [0.1-0.5]	1.2 [0.3-2.5]	0.15 [0.1-0.3]	1.5 [0.8-2.0]
<i>Soil classification</i>	Kandosol [Vertosol]	Kandosol [Vertosol]	Hydrosol	Hydrosol
<i>Texture group</i>	Sandy loams	Clay loams	Light clays	Light clays
<i>Clay content [%]</i>	15 [5-30]	40 [15-50]	50 [40-70]	50 [40-70]
<i>Silt content [%]</i>	[0-20]	[20-40]		
<i>Sand content [%]</i>	[60-80]	[20-40]		
<i>Organic carbon content [%]</i>	[2-3]	[0-1]	[3-4]	[>5]
<i>Grade of pedality</i>	Massive	Massive	Massive	Strong
<i>Bulk density [Mg/m³]</i>	1.29 [0.7-1.5]	1.39 [1.1-1.59]	1.29 [1.1-1.6]	1.39 [1.2-1.7]
<i>Saturated hydr. cond. [mm/h]</i>	300 [100-1000]	100 [10-1000]	0.3	0.3
<i>Vol. water content at 0.1 bar</i>	0.25	0.29	0.33	0.38
<i>Vol. water content at 15 bar</i>	0.09	0.15	0.18	0.26
<i>AWHC / unit depth [mm/m]</i>	156	144	156	118
<i>Data reliability</i>	highly reliable		interpolated from elsew.	

We have used this soil characterization to set up corresponding parameters for HYBRID as follows. Given that the thickness of the A-horizon is roughly similar to HYBRID's upper-layer thickness and that no further information about the geological sub-layers under the solum is available, we have directly assigned properties for both horizons to the respective HYBRID soil layers. The soil's thermal conductivity λ is strongly dependent on composition, porosity, and water content. A well-known model computes λ as a weighted mean over the thermal conductivities of each constituent (de Vries (1975) in Camillo, Gurney, and Schmugge (1983)), i.e.:

$$\lambda = \frac{f_w \lambda_w + k_d f_d \lambda_d + k_a f_a (\lambda_a + \lambda_v)}{f_w + k_d f_d + k_a f_a} \quad (4.26)$$

with the respective volumetric fractions f of liquid water (w), dry soil (d) and air (a), respectively. However, this model requires as additional parameters the soil's porosity $\varepsilon = f_w + f_a = 1 - f_d$, soil and air factors $k_{d,a}$, and the volumetric soil moisture $\theta = f_w$ to be expressed as a ratio to porosity rather than fc. HYBRID originally used a conductivity expressed in analogy to equation (32) in Hansen et al. (1983), as the inverse of the serial coupling of resistances due to dry soil, snow cover (if present) and soil moisture. We have changed the bulk layer thermal conductivity dependency on water content to an estimation through a parallel resistance ($r = z/\lambda$) coupling between the dry soil matrix and the soil water content. Within the units-framework of HYBRID, i.e. $\lambda [Wm^{-1}K^{-1}]$, we thus get for the upper layer of thickness z_1 :

$$r_1 = \left(\frac{1}{r_{d1}} + \frac{1}{r_{w1}} \right)^{-1} + r_{snow} = \frac{1}{\lambda_{d1}/z_1 + (w_1 \lambda_w)/z_1} + \frac{z_{snow}}{\lambda_{snow}} \quad (4.27)$$

which includes a hypothetical snow cover with conductivity λ_{snow} and of thickness z_{snow} , and with the conductivity of water replaced by that of ice for frozen soils. Other

authors have proposed more complicated parameterizations, often based on empirical relationships incorporating further soil characteristics. Our relationship produces a linear dependency on volumetric water content, which approximately holds in the expected range of ratios of water content to field capacity (w_1) used in the model, i.e. typically between 0.3 and 1.0, except in relatively dry soils (see e.g. Yang and Koike (2005)). Note that values of w_1 below 0.3 are generally below the wilting point and cause instabilities within HYBRID. Dry soil conductivity λ_d cannot easily be estimated from its components since pore space air acts as an insulator, and we retained a rough approximate as a function of dry soil bulk density ρ_d [g cm⁻³] as given in Yang and Koike (2005):

$$\lambda_d = (135\rho_d + 64.7) / (2700 - 947\rho_d) \quad (4.28)$$

For estimating the volumetric heat capacity of dry soil, we have assumed that both quartz and clay minerals have an average density of $2.7 \cdot 10^3$ kgm⁻³ and mineral heat capacities of $2 \cdot 10^6$ Jm⁻³K⁻¹. Further, we stipulated that they were the only components contributing to the dry soil volumetric heat capacity c_{bsoil} , which we estimated in terms of the mineral fraction $a_{mineral}$ as:

$$c_{bsoil} \cong a_{mineral} \cdot c_{mineral} \cong \frac{\rho_{bsoil}}{\rho_{mineral}} \cdot c_{mineral} \quad (4.29)$$

The volumetric water content after an application of a matrix suction pressure of 0.1 bar/0.01 MPa corresponds approximately to the value at field capacity θ_{fc} (T. J. Marshall, Holmes, and Rose (1996)). Since the measured values in Table 3 match those found in the literature well (cf. T. J. Marshall, Holmes, and Rose (1996)), we used them directly. For the hydrosol's water holding capacity, we estimated porosity in wet light clays as an average between a surface soil of wet clay (0.58) and one of loam texture (0.52) for the upper layer, and used the lower limit of the characteristic range for clays for the uncompacted subsoil lower layer. The soil water diffusion constant is difficult to estimate from hydraulic conductivity, which is why we retained the original value used in HYBRID, corresponding to a diffusion time of 2 days. Finally, soil moisture at field capacity ($w_1 = \theta_1 / \theta_{fc} = 1$) is typically reached after 2-3 days of rainfall or irrigation. With a monthly mean November rainfall of 140 mm, and given the observed and measured precipitation events over Tiwi during the days preceding the simulation, we may assume that the soil water content should be near fc . In order to permit an interactive surface response to rainfall during the simulation, we uniformly initialized moisture at 90% of θ_{fc} . The final set of soil parameters selected for our study is shown in Table 4.

Table 4 HYBRID soil model parameters estimated from measured values, and ingested as single value defaults in *buildsurface*

	Layer 1	Layer 2
<i>Layer thickness z1 and z2 [m]</i>	0.10	4.00
<i>Soil thermal conductivity k_bsoil [Wm⁻¹K⁻¹]</i>	0.16	0.18
<i>Vol. heat capacity dry soil c_bsoil [Jm⁻³K⁻¹]</i>	9.60E+05	1.03E+06
<i>Soil water diffusion cst D_bsoil [s]</i>	1.70E+05	-
<i>Field capacity fc_bsoil [-]</i>	0.25	0.29
<i>Porosity wetland_por [-]</i>	0.55	0.40
<i>Ratio of water to fc wsoil_bsoil (θ_{fc}) [-]</i>	0.90	0.90

The soil's base temperature has been set to 27.85°C, the 2005 measured annual mean air temperature at the Point Fawcett station, thus reflecting the deep ground's thermal inertia. For the lower layer temperature, we took the average between the annual mean and the monthly mean (29.30°C), equal to 28.60°C, and we initialized the upper layer such that the resulting skin temperature from the quadratic extrapolation at model start was the same as the upper layer temperature, hence at 30.10°C (Fig 10(e)). This is close to the 30.8°C surface air temperature extrapolated downwards from the radiosounding used to initialize the atmosphere, and likely to be an appropriate value for an early morning simulation start. Daily-average SST was taken from the AVHRR-AMSR optimally interpolated (OI) SST dataset, a L4 bias-adjusted analysis produced daily at the NOAA National Climatic Data Centre from remote sensing, *in situ* ship and buoy data. After initial experiments using a spatial SST initialization, we chose to rather apply a domain average of 304.1 K homogeneously, to reduce lateral boundary inconsistencies and to better appreciate the interactive response of sea surface fluxes to the prevailing atmospheric forcing.

As in Friend (2010), climate data has been taken from the University of East Anglia's Climate Research Unit (CRU) TS3.0 dataset. We calculated an area-averaged monthly mean 24h minimum temperature of 24.2°C and maximum temperature of 34.87°C to set the vegetation phenology. Biomass distribution was prescribed heterogeneously from the standard MOD15 LAI product, revealing an average of 1.7 m²m⁻² over the islands. For the average grid-box shortwave albedo, the 16-days averaged spectral albedo from MERIS data at a spatial resolution of 0.05° has been transformed into broadband values as indicated by the data provider. Soil emissivity has been set to 0.90, water emissivity to 0.97. An illustration highlighting some of the initialized properties, as well as major features of Tiwi Islands, is presented in Fig 10.

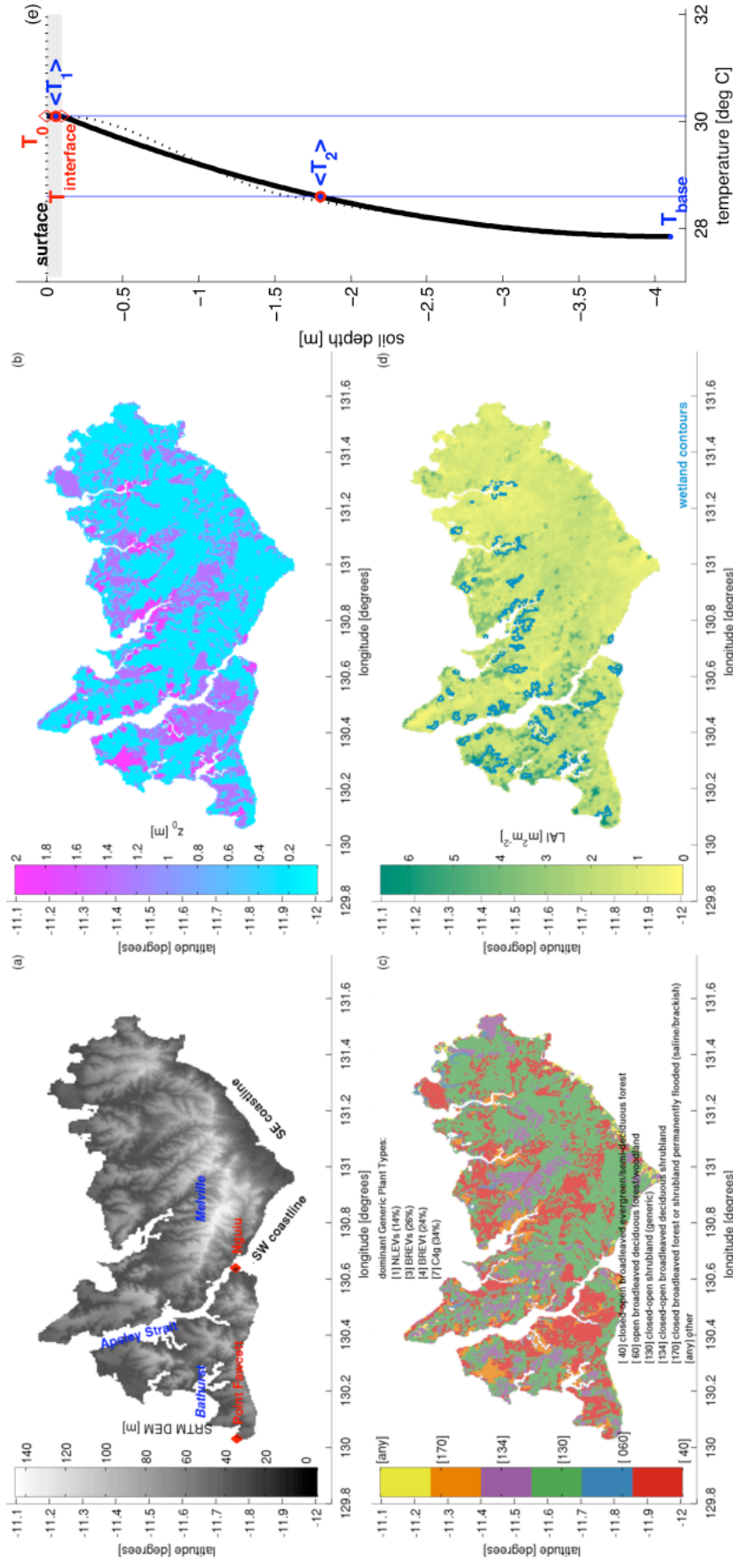


Fig 10 Tiwi Islands surface initialization for ATHAM-HYBRID: (a) topography from the SRTM DEM; only 3 levels are captured with ATHAM's vertical grid-spacing of 50 m; (b) average composite roughness length in each grid-box; (c) land cover map of the 5 dominant classes from GlobCover; (d) leaf area index and demarcation of wetland areas; (e) soil temperature profile. The 3 initialized values, i.e. the invariant T_{base} and the 2 mean layer temperatures (that determine the layers' prognostic heat content), are annotated in blue. The diagnostic skin temperature T_0 and interface temperature are depicted as red diamonds. The thick black line describes the quadratic temperature profile implemented in Gerken et al. (2012), the dotted line a more realistic profile (of similar heat content) used to qualitatively justify the initialization.

4.3 Simulating instrumental data for better model-observations intercomparison

Even if proper validation of complex Earth systems models running at very-high-resolutions is practically difficult to achieve at best, we try to cross-check our simulated results at least qualitatively through a direct comparison to data collected during an extensive observation campaign, and available from spaceborne remote sensing platforms.

For this purpose, and with the objective to facilitate future intercomparisons between convection-resolving simulations and observations, we have developed an ATHAM-tailored interface to the Cloud Feedback Model Intercomparison Project (CFMIP) Observation Simulator Package (COSP), version 1.3.2 (Bodas-Salcedo et al. (2011))¹⁹. COSP simulates observations from various passive and active satellite remote sensing instruments as a function of data produced by CRMs, NWP models and GCMs, emulating the observation process with as many known biases as possible. This forward-modelling approach of satellite measurements therefore permits comparisons between different model studies and to real data in observation space in a consistent fashion, at the expense of relying on variables that remain no longer trivially related to any single geophysical quantity (Bodas-Salcedo et al. (2011)). Since not all required modelled data fields are produced by ATHAM, we had to derive further quantities where necessary, in particular cloud radiative properties. The statistical downscaling from GCM grid-box mean values, producing sub-columns of similar size than an observed pixel, is not needed in our CRM context.

Instruments simulated with the interfaced version include CloudSat's Cloud Profiling Radar (CPR, Stephens et al. (2002)), CALIPSO's Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP, Winker et al. (2010), Chepfer et al. (2008)², no aerosols included), the Moderate Resolution Imaging Spectroradiometer (MODIS, King et al. (2003)), and the Multi-angle Imaging Spectroradiometer (MISR, Diner et al. (2005)). COSP also produces International Cloud Climatology Project (ISCCP, Rossow and Schiffer (1999)) cloud products. Many simulators are based on simplified concepts rather than on

¹⁹ The COSP source code package can be downloaded and updated via standard SVN commands from the project's repository, and the ATHAM interface from our own SVN server (atham/post/atham2cosp). The COSP directory needs to be stored on the same level as our atham2cosp directory, and the interface is built through an interlinked Makefile as *atham2cosp_pgrm*. COSP generates its CF-compliant output with Lawrence Livermore National Laboratory's (LLNL) Climate Model Output Rewriter (CMOR). A few minor changes had to be done to COSP source files to remove bugs and adapt them to ATHAM data, and these files are delivered as replacements with the interface. See also Appendix B.

detailed radiative transfer. For example, the MODIS simulator performs simple integration and extinction-weighted integration to determine the cloud optical depth and cloud top pressure, respectively (Bodas-Salcedo et al. (2011)). COSP can also be linked to the Radiative Transfer for TIROS Operational Vertical Sounder (RTTOV, R. Saunders, Matricardi, and Brunel (1999)) code, a fast radiative transfer algorithm that can be used to simulate clear-sky brightness temperatures for many past and current infrared sounders and passive microwave radiometers.

The CloudSat radar reflectivity signal is simulated using QuickBeam (Haynes et al. (2007)), which can also be configured to simulate Tropical Rainfall Measuring Mission (TRMM, Simpson, Adler, and North (1988), Z. Liu et al. (2012)) or vertically-pointing ground-based radar data for a large range of frequencies. Particle scattering follows Mie calculations (or look-up table values); the attenuation by gases is included. Any number of hydrometeors can be used (up to 50), quantified in terms of mixing ratios, matched to available statistical distributions (modified gamma, exponential, power-law, lognormal or monodisperse), and treated as spheres. Complex ice crystal shapes and multiple scattering, relevant for heavy precipitation events, are as yet not available.

We use the microphysical settings and effective radii from ATHAM within COSP²⁰. Since all hydrometeorological species are available as mixing ratios (or specific concentrations assumed identical to mixing ratios), and since COSP is run in cloud-resolving mode²¹, the conversion from the diagnostic precipitation fluxes generally provided by large-scale models to mixing ratios, as outlined in Bodas-Salcedo (2010), is unnecessary. We adapted the *HCLASS* table (Table 5), defining the microphysical assumptions used by QuickBeam, to reflect ATHAM's hydrometeor distributions. Values are assigned to the large-scale (i.e. resolved) quantities only; the convective (i.e. parameterized) ones do not need to be defined. The hydrometeor distribution parameters describe defaults that are ignored if effective radii from the model are available.

²⁰ By putting *use_reff=.true.*

²¹ *Ncolumns=1*, where *Ncolumns* is the number of downscaled subgrid columns

Table 5 Hydrometeor class settings used in the QuickBeam radar simulator

variable name	description	cloud water (q_l)	cloud ice (q_i)	rain (q_r)	graupel (q_g)
HCLASS_TYPE	<i>distribution type</i>	monodisperse	monodisperse	exponential	exponential
HCLASS_COL	<i>not used</i>	1	2	3	9
HCLASS_PHASE	<i>thermodynamic phase</i>	liquid	ice	liquid	ice
HCLASS_CP	<i>not used in COSP</i>	0	0	0	0
HCLASS_DMIN⁽¹⁾	<i>minimum drop size [μm]</i>	-1	-1	-1	-1
HCLASS_DMAX⁽¹⁾	<i>maximum drop size [μm]</i>	-1	-1	-1	-1
HCLASS_APM⁽²⁾	<i>α_m [$\text{kg m}^{-6\text{m}}$]</i>	-1	-1	-1	-1
HCLASS_BPM⁽²⁾	<i>β_m</i>	-1	-1	-1	-1
HCLASS_RHO⁽³⁾	<i>hydrometeor density [kg m^{-3}]</i>	1000	917	1000	700
HCLASS_P1⁽⁴⁾	<i>distribution parameter 1</i>	10.64	100.00	1.00E+07	1.21E+04
HCLASS_P2⁽⁴⁾	<i>distribution parameter 2</i>	0	0	-1	-1
HCLASS_P3⁽⁴⁾	<i>distribution parameter 3</i>	0	0	-1	-1

⁽¹⁾not used except for power law distribution, all other distributions vary from zero to infinity; ⁽²⁾as in the particle mass-diameter relationship $m(d) = \alpha_m d^{\beta_m}$, not used if density ρ is specified; ⁽³⁾used to calculate ice refractive index, chosen from ATHAM input data; ⁽⁴⁾for an exponential distribution ($N(d) = N_0 \exp(-\lambda d)$), **P1** is the constant intercept parameter N_0 [m^{-4}], **P2** is the slope parameter λ [μm] and **P3=2** indicates a temperature-dependent λ , only one parameter must be defined; for a monodisperse distribution ($N = N_0$), **P1** is the constant diameter d_0 [μm], **P2** and **P3** are set to 0 (Haynes (2007))

A particular issue consists in the fact that COSP is built for a terrain-following grid and not for the Cartesian reference system in which ATHAM data are generated. Further, it does not recognize the undefined values below the orography in ATHAM and replaces these by zeros during a sanity check, which produces runtime issues due to undefined mathematical functions. Given the stretched vertical axis in ATHAM and the particular implementation of the data structures in COSP, undefined sub-surface grid-points in ATHAM could not simply be cut off without further interpolation steps of the data fields. To avoid conflicts with COSP's internal sanity checks, several of the undefined variables were replaced by very small values, and the sub-orography pressure field was set to an infinitesimally small value. This results for such grid-points in a quasi-zero density and therefore optical depth, such that forward radiative transfer for passive or active sensors should be unaffected by the missing data in sub-surface columns. We tested this approach for several of the simulators and found negligible errors, but cannot confirm that it is applicable universally across the simulator package. Since the geometric effects, i.e. the inverse-range dependency, of active instruments seem not to be accounted for in the simulators, this approach should hold for the simulated radar and lidar signals as well. A potential issue also remains when choosing model tops at low heights, since this removes a significant residual optical depth that can no longer attenuate the transmission of the signal on its path towards a spaceborne platform.

In terms of estimating cloud radiative properties, we have emulated the implementation in ATHAM where possible. The effective radius is defined as

$r_e = \int r^3 N(r) dr / \int r^2 N(r) dr$, where $N(r)$ corresponds to a cloud drop size distribution. It is a good predictor for cloud radiative forcing (see e.g. Hu and Stamnes (1993) for water clouds). The volume mean radius is given as $r_{\mu_v} = \left(\int r^3 N(r) dr / \int N(r) dr \right)^{1/3}$. For historic reasons, the volume mean rather than the effective radius had been used in ATHAM. In what follows, we refer to r_e for our parameterizations but are actually using r_{μ_v} . Without a prognostic or an *a priori* size distribution of cloud particles, the effective radius of cloud droplets has been hardwired in ATHAM's shortwave radiation code (and in COSP) to $r_{el} = 5.32 \mu\text{m}$ (see Briegleb (1992)), and that of ice crystals to $r_{ei} = 50 \mu\text{m}$ ²². The effective (or rather volume mean) radii of rain and graupel are derived from corresponding specific concentrations via the Marshall-Palmer (exponential) distribution (J. S. Marshall and Palmer (1948)), as described in Herzog et al. (1998). They are passed to COSP for the radar radiative transfer, but are not used to define cloud optical depth or emissivity. The cloud shortwave optical depth required for COSP at 670 nm has been aligned with a corresponding estimate in ATHAM for the 350-700 nm shortwave broadband region, where extinction is calculated for cloud droplets and ice crystals only. Correspondingly, cloud droplet optical depth follows Slingo (1989) as:

$$\tau_{swl} = LWP(a_{sw} + b_{sw}/r_{el}) \quad (4.30)$$

The liquid water path (LWP) is computed as a function of the cloud droplets' specific concentration q_l , the local density of air ρ , and the grid-box height dz , $LWP = q_l \cdot \rho \cdot dz$, and $a_{sw} = 2.817 \cdot 10^{-2} \text{ m}^2 \text{g}^{-1}$, $b_{sw} = 1.305 \text{ m}^2 \text{g}^{-1} \mu\text{m}$. Cloud ice optical depth similarly follows Chou, Lee, and Yang (2002) as:

$$\tau_{swi} = IWP(a_{0sw}/d_{ei}) \quad (4.31)$$

with an analogous ice water path (IWP) and where $a_{0sw} = 3.276 \text{ m}^2 \text{g}^{-1} \mu\text{m}$.

Since the parameterization of cloud grey-body emissivity in RRTM (Mlawer et al. (1997)), the longwave radiative transfer model used in our study, could not be retrieved from the source code, we aligned emissivity with the method used in the NCAR Community Atmosphere Model (CAM2, Collins et al. (2003), following Ebert and Curry (1992)). Therein, it is a function of cloud phase, given in terms of the cloud ice fraction (f_{ice}), of the condensed water path ($CWP = LWP + IWP$ [gm^{-2}]) and of the effective radius of

²² This ice effective radius actually (and inconsistently) represents an effective size/diameter d_{ei} over a range of ice crystal shapes/habits in the following equation (4.31), see Chou, Lee, and Yang (2002), independently of different values used in the single-moment microphysics scheme. Consistent updating of ATHAM's radiation schemes and the COSP interface will be necessary, once a new two-moment microphysics scheme is available that will be capable of predicting r_e , particularly if applied to cloud radiative forcing studies.

ice particles (r_{ei} [μm]). Cloud emissivity is then defined through cloud longwave transmittance as:

$$\epsilon_{cld} = 1 - e^{-D\kappa_{abs}CWP} \quad (4.32)$$

where D is a diffusivity factor set to 1.66 and κ_{abs} [m^2g^{-1}] is a longwave mass absorption coefficient defined as:

$$\kappa_{abs} = \kappa_l(1 - f_{ice}) + \kappa_i f_{ice} \quad (4.33)$$

The absorption coefficient for liquid water (κ_l) has been set to 0.090361 and that for ice water (κ_i) has been related to the ice effective radius through $\kappa_i = 0.005 + 1/r_{ei}$, following a broadband conversion of the relationship presented in Ebert and Curry (1992). Again, only fixed-size suspended cloud particles intervene, such that the last relationship is actually irrelevant.

Best insights from a simulation-observation intercomparison of a highly transient and heterogeneous phenomenon such as the evolution of a deep convective cloud system require highly-resolved four-dimensional measurement data. Given the scale of the domain and the very large optical depths of convective clouds, the only currently available technology providing such data is a traditional rain radar. For the Hector storm, gridded attenuation-corrected (Bringi, Keenan, and Chandrasekar (2001)) reflectivity and hydroclassification data fields are available from the BMRC/NCAR C-band polarimetric (hereafter, C-POL) research radar system, located roughly 100 km off Tiwi Islands at Gunn Point near Darwin (Keenan et al. (1998)). It produces complete volume scans every 10 minutes. The C-band 5.5 cm-wave transmitter operates at a frequency of 5625 MHz. The low-noise receiver records signals down to -115 dBm, which translates into a minimum detectable reflectivity at 10 km with no path attenuation of -29 dBZ (0 dBZ at the 150 km maximum range). The fuzzy-logic microphysical classification into 10 different classes is described in May and Keenan (2005). Large difficulties in evaluating the retrieval's reliability are associated with similar species, overlapping in the phase-space hypervolume. This is of lesser concern for our purposes, since some of the various overlapping species have to be combined to match the two hydrometeor classes, rain and graupel, simulated by ATHAM. Data from the volume scans with 300 m sampling resolution have been interpolated to a $2.5 \times 2.5 \times 0.5 \text{ km}^3$ Cartesian grid.

We have adjusted the COSP-QuickBeam radar parameters to reflect CPOL's 5.6 GHz frequency and ground-based location. QuickBeam then assumes a zenith-looking instrument, and any direct intercomparison with data from a scanning system will be limited by the differing viewing geometry and path attenuation, reflected in the effective (i.e. attenuated, dBZe in Haynes (2007)) reflectivity factor returned by the COSP interface. A flare echo for example, such as described by May and Keenan (2005), will not be

simulated by QuickBeam; first, because of the geometry, and more importantly, because of the neglect of multiple scattering in the simulator. This will particularly affect intense precipitation detection and the comparison of reflectivity histograms between observations and simulations.

We have calculated a ‘statistical coverage product’ as outlined in May and Lane (2009), to evaluate the simulated results with respect to radar data, preserving height and time information, in addition to a qualitative inspection involving data slices at a given moment to compare the storm structure. These more quantitative statistical metrics rely on a calculation of the grid fraction as a function of height and time covered by certain reflectivity thresholds and microphysical classes, as well as profiles of maximum reflectivity across the analysis domain. All analysis has been performed on a 2° longitude by 1° latitude subdomain centred on Tiwi Islands.

High-resolution volume radar data is not always available. We therefore also used the MYD06_L2 cloud product derived from the 36-channel MODIS instrument on-board NASA’s LEO Aqua platform, with a local overpass at 05:20 UTC, to compare satellite-observed to simulated data. This operational level-2 geophysical data product is the only high-resolution satellite scene available for the Hector storm in its development phase, and combines data from the visible and infrared geo-referenced radiances and brightness temperatures to infer physical and radiative cloud properties. These include cloud top properties (temperature, pressure and effective emissivity) and particle thermodynamic phase at 5 km resolution. Cloud optical and microphysical properties (effective radius, optical thickness (τ), integrated water path and cirrus reflectance in the visible) are generated at 1 km resolution (Platnick et al. (2003), King et al. (2003)). It is important to note that the operational cloud products rely on prior identification of cloudy areas as given by a cloud mask product. The mask product has been designed with a bias towards high confidence in identifying clear sky pixels (clear sky conservative), and some problems with the cloud products due to false positives can hence be expected. Besides limits to instrumental accuracy, radiative transfer and decision-tree algorithms, higher-level retrievals rely on a range of ancillary data, often from operational re-analysis products with limited resolution and other observed data, as well as on numerous assumptions. Particular portions of the retrieval space are very sensitive to measurement and modelling errors, which is why the cloud products must not be considered as an absolute reference. Our intercomparison should thus be interpreted as a cross-validation rather than a unique validation of the simulation results. In this analysis, we only retained τ and cloud top pressure, as other products are either further derived (and hence biased) quantities, provide little further insight, merely reflect parametric choices in ATHAM and/or COSP, or are simply not available from the COSP package output.

Confidence levels of the cloud properties retrieval and out-of-bounds pixels for τ have been accessed from the individual bit-flags in the Quality Assessment Science Data Set (SDS) included in the Hierarchical Data Format (HDF) orbital swath granule, as outlined in Hubanks et al. (2007). We only retained τ regions that were flagged at high or very high confidence. Optically thick deep convective clouds saturate the single-phase retrieval method. The valid range of the measurements is defined only up to an τ value of 100. We retained out-of-bounds regions in the scene as indicators of deep convective cores but marked them appropriately. An error in the retrieval code affecting all operational cloud τ products had been identified. This affects predominantly τ centred on a value of 11.5 for liquid water clouds and of 8.5 for ice clouds, producing underestimates in histogram counts, and should not be of further concern in this comparison.

The CO₂ slicing technique for cloud top pressure retrieval produced excessive high-level cloud coverage, maybe due to sub-visible cirrus decks not directly linked to the Hector storm. We therefore used the IR-window brightness temperature retrieval, usually applied to low clouds, which assigns a pressure level to the measured temperature using an NCEP Global Data Assimilation System (GDAS) temperature profile. Remaining excessive cloud in this 5 km product was removed with the 1 km interpolated cloud mask and the τ low confidence mask.

Equally at a resolution of 5 km, a one-hourly time sequence of snapshots over the course of the Hector's diurnal cycle has been retrieved from the visible channel of JMA's geostationary multifunctional transport satellite MTSAT-1R (Fig 11), replacing the previous GMS series²³. The corresponding 5 km cloud albedo product has been retrieved from the Atmospheric Radiation Measurement (ARM) programme's data archive to qualitatively assess the evolution of the simulated storm, in particular the timing and the spreading anvil.

²³ Because of an initial launch failure and a subsequent commissioning period, 1 km highest-resolution visible imagery is unavailable for the last few months of 2005.

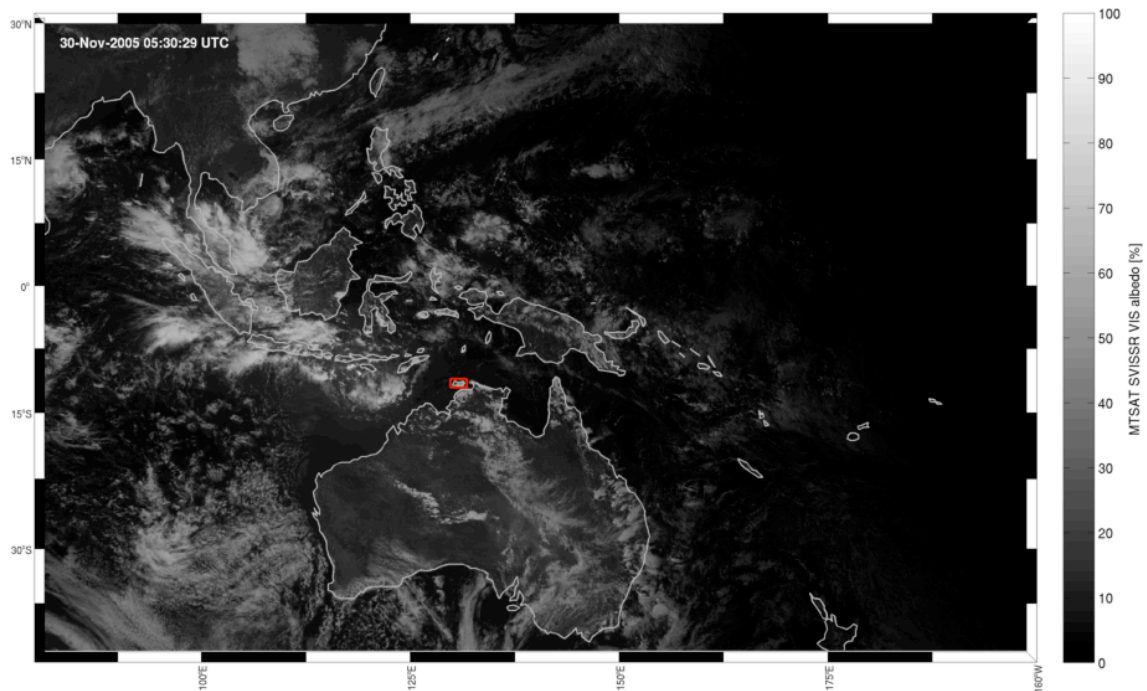


Fig 11 VISSR (geostationary MTSAT-1R) visible albedo from product twpmtsax1.a1.20051130.053029.hdf. At 05:30 UTC, the tilted terminator (twilight zone between day and night) approaches New Zealand from the east, affecting the retrieval of albedo from the visible channel. The scale of the Hector storm can be appreciated in comparison to the significantly larger MCSs over the Maritime Continent. The red bounding box surrounding Tiwi Islands delimits the area used for the observation-simulation inter-comparison, centred on 11.55S, 130.79E, with a 0.5 degrees NS and a 1.0 degree EW extension.

All remote sensing products, geo-referenced on non-uniform geographical grids, have been linearly interpolated from their original resolution to the higher-resolution ATHAM (and COSP) stretched grid, and used for some basic statistical analysis. This interpolation not only reduces the pixelated nature of the observations, but also produces some artificial smoothing with intermediate boundary values that have no physical meaning. In particular, this is the case where abrupt contours with largely different values previously existed, such as in the cloud top pressure of an anvil over otherwise low-level shallow clouds. Similarly, a simple 2D moving-average filter of similar window size as the relevant observational products has been applied to the COSP-simulated MODIS cloud optical thickness and ISCCP shortwave albedo. Fill values chosen to best represent unavailable observed or simulated data (e.g. a value of zero for cloud albedo and τ where cloud is absent) also produce interpolation artefacts, and quality assessment flags are similarly affected. Nevertheless, this interpolation facilitates the intercomparison at the expense of accuracy. A more advanced procedure would resample COSP data fields to the observational grids using kernels emulating the effect of discrete field-of-views on radiative transfer and subsequent processing for geophysical retrieval. Since COSP has been designed for climate model output, modelled fields are usually of lower resolution

than observations, and a major feature of the simulator is a facility for statistical downscaling, rather than the opposite that is required here.

4.4 Model atmosphere configuration, setup and initialization

A new ATHAM configuration for simulating deep convection and the Hector storm had initially been introduced by White (2008), who performed a pilot study and the starting point for this investigation. We have done a large number of optimization runs to find a model setup suited for the phenomena under investigation and optimized for our baseline and sensitivity runs. The model surface was initialized from preprocessed files as outlined in section 4.2. We produced all our experiments using ATHAM version 3.0²⁴.

Kang and Davis (2008) suggest an appropriate grid-spacing for a large-eddy simulation given the following considerations. If the typical size of energy-containing turbulent eddies l within the PBL is stipulated at about $1.5z_i$, and given an effective eddy resolution of 6Δ , the maximum grid-spacing (Δ) should be chosen at $\Delta \leq 0.25z_i$. This corresponds to values roughly between 100 and 500 m. From a turbulence perspective, a suitable grid-spacing for deep moist convection simulations is $O(100)$ m, for the assumptions in the design of the adopted LES-type closure schemes to be consistent with the modelled regimes (Bryan, Wyngaard, and Fritsch (2003)). They found persistent lack of grid-convergence in the statistics of the simulated properties of a squall line, even with grid-spacing between 125 and 250 m, the coarsest spacing that could be adopted for resolved eddies to reach into the Kolmogorov inertial subrange. They concluded that grid-spacing of $O(1)$ km should be avoided for control runs in resolution sensitivity studies. These failed to reproduce the correct spectral kinetic energy characteristics and associated turbulent fluxes, and they consequently advocate l/Δ ratios of the order of 100, with $l=10$ km chosen as the scale-height of the troposphere in deep convection studies. Kirshbaum (2011) therefore adopted a horizontal grid-spacing of 100 m for simulating convection over a mountain. To achieve convergence within the shallow convective PBL, finer grid-spacing would be required still; Sullivan and Patton (2011) mentioned a z_i/Δ ratio of 60 to ensure scale-separation between energy-containing eddies and the filter cut-off scale (in a homogeneous cloud-free PBL with no shear). Chemel et al. (2009) however found that besides fine-scale details in shallow convection and simulated rainfall

²⁴ Trunk at revision 513; see Appendix B. The parallel model used for 3D simulations was compiled on a Westmere architecture (running on an InfiniBand network) with the Westmere default openMPI communication library, using IFORT 11.1 with floating-point consistency and O2 optimization.

that better matched observations, refining the horizontal mesh from 1km to 250 m changed little to the lifetime and maximum height of a simulated Hector storm. KR06 found hardly any differences in the statistics of shallow and deep convection between two control simulations at 100 and 250 m. Khairoutdinov et al. (2009) simulated convergence in oceanic equilibrium deep convection statistical properties only at grid-spacing between 100 and 200 m. Qualitatively, and in terms of certain diagnostics, the evolution of convection remained similar up to grid-spacing of 1600 m, however. They speculated that convergence at finest grid-spacing might be due to resolving down to the inertial subrange. About 250 m (or rather a quarter of the subcloud-layer depth) were argued by Petch, Brown, and Gray (2002) to be an upper limit for simulating both shallow and deep convection, in particular to simulate moisture transport from the subcloud-layer into the free troposphere and to avoid delayed triggering of deep convection. Grabowski et al. (2006) judged 500 m sufficient to capture the essential processes associated with convective development in 3D. In the context of shallow convection simulations of open and closed cells, H. Wang and Feingold (2009) found that in spite of differences in the finer details of clouds and vertical velocity, the microphysical, morphological and optical differences between open and closed cells were well captured with both the coarser (300 m) and finer (100 m) horizontal grid-spacing adopted. The general patterns of structure were captured with both grid-spacing, and variations in the time-averaged cloud statistics varied between less than 5% for open cells and 20% for closed cells, even if the convective PBL was less vigorous and less well-mixed under coarser resolutions. As emphasized previously, the Monin-Obukhov similarity theory used for the flux transfer and coupling of the atmospheric and surface models is based on the assumption of stationary, homogeneous and averaged turbulence. This is obviously violated when resolving individual eddies, but no other theory currently exists that could be applied to LES simulations. Also, the assumption of the existence of thermal and dynamic equilibria between active tracers and their surrounding fluid theoretically limits the minimum (vertical) grid-spacing that should be adopted.

We found that a grid-spacing of 500 m in the horizontal and 50 m in the vertical reproduces well the features of deep convection, even if this spacing certainly limits details in the initial organization of shallow convection patterns. Nevertheless, this grid-spacing did capture shallow features such as open cells and horizontal convective rolls, although these might have been artificially enhanced by the model (see e.g. Tian, Parker, and Kilburn (2003), Gryschka and Raasch (2005)). Tian, Parker, and Kilburn (2003) for instance found a typical role spacing of 3-6 km at 1 km grid-spacing and of 2-3 km at 500 m. It is possible that this simulated spacing merely reflects the minimum number of grid-points to resolve the rotating velocity field of an eddy, although spacing (and orientation)

did not further increase (change) with finer grid-spacing down to 100 m. Lastly, our chosen grid-spacing also corresponds to an upper limit of what we can afford computationally. A 3D setup as outlined below clocks well over 30'000 CPUh (or about 10 times less as the 100 m benchmark run in Khairoutdinov et al. (2009)).

We used a 3D Cartesian grid with cyclic (double periodic) lateral boundary conditions²⁵. Cyclic boundaries applied to an isolated disturbance limit the length of the simulation to the time it takes to advect the effects of the disturbance across the boundaries. In our case, this is less than a day. Before any elements are noticeably recycled across the boundaries, the strength of the storm's cold pool gust front produces large-scale convergence and deepening of the outer-domain's PBL. This results in 'stratus' cloud condensation, and later increases the susceptibility to spurious deep convection triggering by reducing the convective inhibition. It is possible that this subtly contributed to an intensified storm propagation towards the end of our simulations. Below the upper boundary's rigid lid, a damping sponge layer is applied to the upper 5% of grid-points (roughly 5 km) to avoid gravity wave reflection. The selected sponge layer increases horizontal momentum diffusion by a step of 20 to a maximum value of 200, and further nudges tracers and horizontal wind to their original profile values; it does not increase vertical diffusion. The domain is centred on Tiwi Islands (130.79°E, 11.55°S), covers 360 km in longitude, 270 km in latitude and 35 km in altitude, (and is bordered by ocean grid-points only rather than continental Australia). We used 422x278x180 grid-points, with a constant horizontal grid-spacing of 500 m covering a rectangle encompassing all land masses and the nearby shoreline²⁶. The finest vertical grid-spacing of 50 m is applied over the depth of the PBL up to 2 km; it then increases monotonically to less than 350 m around the tropopause (17 km) and just over 630 m near the model top.

The simulations were started without a spin-up period at the time of the first available atmospheric sounding, on 30th November 2005 at 08:30:00 LT (+9.5h time zone). ATHAM's time-step is variable, following the Courant-Friedrichs-Lewy criterion (Courant, Friedrichs, and Lewy (1967)), where we use limits of 0.8 for advection and of 1

²⁵ The more natural choice for simulating a non-periodic phenomenon is open (no slip) lateral boundaries; however, these were found to lead to overall mass loss or gain, producing model instabilities.

²⁶ To this aim, 341x201 constant-spacing grid-points were selected in the x- and y-directions. This results in a stretched grid with 3 (in x), and 2 (in y) lines of constant symmetric boundary grid-points, respectively, at the coarsest grid-spacing of roughly 5 km. Grid stretching over 38 and 37 cells in x and in y is applied at a ratio of 1.065. The grid is distributed over 10x6 (in x and y) processing cores on a parallel architecture, an optimal configuration as deduced from a performance analysis. Besides giving approximately square sub-domains of 44x48 grid-points and making use of entire processing nodes of 12 cores each, we found 60 cores to lie around the upper limit of ATHAM scaling performance. With many more cores, any additional reduction in Wall Clock Time (WCT) is severely influenced by communication bottlenecks and results in highly increased cost (CPU time).

for diffusion. We further restrict the time-step between 0.01 and 20 s. General output is dumped every 10 min, and every minute for selected fields, which results in over half a TB of data per run, including the restart files.

In ATHAM version 3.0, additional momentum diffusion can be added to the solution in terms of a constant diffusion coefficient. Given the classical diffusion equation

for momentum, $\frac{\partial \rho u_j}{\partial t} = D_{mom} \frac{\partial^2 (\rho u_j)}{\partial x_i^2}$, the constant diffusion coefficient for momentum is

expressed as a function of a momentum diffusion time scale $\tau_{diff,mom}$ as:

$$D_{mom} = \Delta_{min}^2 / \tau_{diff,mom} \quad (4.34)$$

where Δ_{min} denotes the smallest grid-spacing in any direction anywhere on the grid. This produces less diffusion, (which is equivalent to a longer time scale), in the stretched portions of the grid, and significantly longer time scales in the horizontal as compared to the vertical direction. A more recent implementation replaces Δ_{min} by Δ_{xi} , the local grid-spacing, in equation (4.34), to maintain a constant diffusion time scale. We have set $\tau_{diff,mom}$ to 300 s, generating rather large amounts of additional momentum diffusion²⁷. We apply no divergence damping, no additional diffusion of turbulence, and no additional diffusion on the stretched grid (generally aimed at reducing wave reflection due to irregular grid-spacing). A detailed investigation into the influence of model grid-spacing and model dynamics parameters, in particular of $\tau_{diff,mom}$, on the evolution of a full diurnal convective cycle, performed in a 2D setting, is presented in section 5.4. This investigation also highlights further insights into detailed storm dynamics from a very-high-resolution simulation at 50 m grid-spacing.

With respect to the turbulent diffusion described in Herzog, Oberhuber, and Graf (2003) and briefly introduced in section 3.2, the empirical proportionality factor c_0 for the momentum turbulent diffusion coefficient K remains fixed to 0.32. The inverse turbulent Prandtl/Schmidt numbers $\alpha_X = \text{Pr}_{tx}^{-1}$ or Sc_{tx}^{-1} , giving the ratio between the turbulent diffusion coefficient for quantity X (heat/mass) and that for momentum, i.e. $K_X = \alpha_X \cdot K$, are determined as:

$$\alpha_X = 1 + \alpha_{X,p} \cdot \frac{\lambda}{\Delta_g} \quad (4.35)$$

where λ is the turbulent length scale and Δ_g the mean grid-spacing determined as an arithmetic mean between all three dimensions, (or $2/3$ of the distance of the grid-box

²⁷ This value has been determined offline as an optimum to reduce numeric noise, and to produce a smooth flow and vortices in idealized warm bubble experiments (Herzog, personal communication) aimed at reproducing the reference solutions in Robert (1993). In this context, future comparisons to a moist benchmark simulation (Bryan and Fritsch (2002)) might be particularly useful.

centre to the ground, whichever is smallest). The parameters $\alpha_{x,p}$ are set to 0.5 for heat, water vapour and passive tracers, such that α_x for heat and moisture tends towards 1.5 for fully developed equilibrium turbulence length scales ($\lambda = \lambda_0$), and towards 1 in very stable stratifications. For incompressible tracers (hydrometeors), this proportionality (inverse Schmidt number) is set to $\alpha_{it} = \alpha_{it,p} = 1.0$.

In order to maintain a constant synoptic flow and improve model stability, we nudge the pressure to the initial hydrostatic profile and the domain-averaged horizontal wind to the initial sounding profile, (assumed in geostrophic equilibrium above the PBL), with 1h time scales.

Kessler microphysics and short- and longwave radiation schemes are the same as presented in section 3.3. Perhaps in inconsistent treatment with the simplified broadband emissivity parameterization adopted for the COSP interface, based around Ebert and Curry (1992), the default longwave treatment of cloud liquid and ice optical properties in RRTM are computed following the more accurate descriptions in Hu and Stamnes (1993) and Q. Fu, Yang, and Sun (1998), respectively. We include the downward flux of additional tabled longwave radiation flux from above the model top, but not a preset splitting of solar input into direct and diffuse shortwave radiation, assumed negligible above 35 km. Note that this choice might produce an overestimation of the solar flux as the full solar constant is applied at the upper limit of the ozone layer where some absorption should already have reduced the flux. An ozone profile based on a McClatchey et al. (1972) mid-latitude summer atmosphere has been used. Since except for water, material fluxes between ATHAM and HYBRID have not yet been implemented, CO₂ concentrations, driving stomata aperture and hence water exchange, currently remain invariant across the domain and correspond to the single well-mixed value used for atmospheric radiative transfer, set to 380 ppm. The concentrations of all other radiatively active gases or radiation parameters have not been changed.

The atmosphere is initialized homogeneously from a radiosonde launched at 23 UTC (08:30 LT) from Darwin airport, 130.89°E and 12.42°S (Brunner et al. (2009)), and integrated into an initially hydrostatic profile upwards (see Fig 12 for thermodynamic plots of the 00Z operational sounding). The direction of the lower boundary layer wind is directly relevant for the location of deep convection triggering over Tiwi Islands (Carbone et al. (2000), J. W. Wilson et al. (2001)). For the February Monsoon break storms, a layer of surface westerlies a few hundred meters in depth is apparently not uncommon, and related to a heat low over Australia in this period (May et al. (2009)). This in turn leads to initial storm formation on the eastern parts of the islands where the sea breeze fronts steepen. A weak 700 hPa steering level easterly, typical for the transition period, was observed, predisposing the storm to move westward. The wind direction in the upper

troposphere centred around 200 hPa was westerly, governing the corresponding storm outflow at anvil-level. Higher up into the stratosphere, easterly winds gaining in strength were observed, due to the corresponding phase of the QBO (Brunner et al. (2009)); this is the level where stratospheric intrusions due to overshoots were measured with the M55 Geophysica aircraft. It was also pointed out that the operational Vaisälä sondes may be under-reading upper level humidity levels, which has an impact on the simulated storm development.

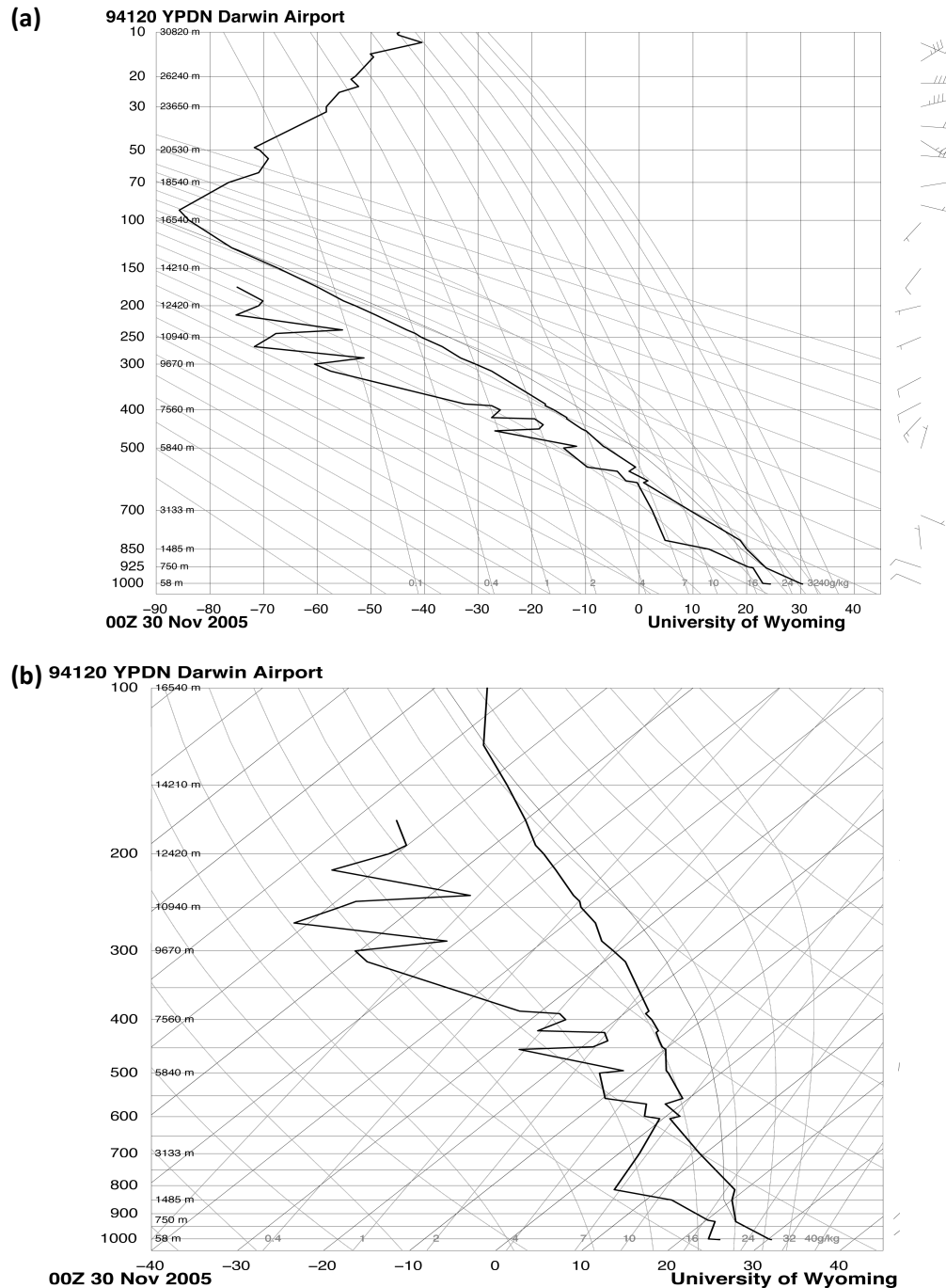


Fig 12 Operational radiosounding from Darwin airport on 30th November 2005 00Z, displayed as (a) Stuve to 10 hPa, and (b) Skew-T to 100 hPa

The initial PBL derived from the radiosounding has an inversion layer that is roughly 1100-1400 m thick. A straight potential temperature profile up to 700 m, which we define as the original inversion height z_i (Deardorff (1970)), is characteristic for a well-mixed convective PBL²⁸. The second inflection point is roughly located between 1800-2100 m, above which θ increases at a roughly steady rate of 2.6 K km⁻¹ (temperature lapse rate of 7.4 K km⁻¹). The initial lifting condensation level is roughly located between 800 and 1000 m, and the level of free convection at about 2.3 km. It is clear from this structure that shallow convective cumulus clouds will not form immediately and that a rather strong forced ascent is required to trigger deep convection.

²⁸ In what follows, we have often estimated z_i in simulated fields based on a procedure locating the maximum of the gradient of RH, θ_v , or a combination of both. Sensible upper and lower limits have been determined *a priori* based on visual inspection of the q_v field, as the gradient approach breaks down during cloud and precipitation formation. Corresponding undefined areas have been interpolated from nearest neighbours using inverse-distance weighting. A low-pass 2D FFT filter has then been applied to filter out high frequency variations from individual convective peaks at a cut-off wavenumber $k_\theta = 3.1 \cdot 10^{-3}$ (roughly 2 km wavelength). Finally, we removed the numeric waves produced by the filtering using a 7 grid-points-based 2D moving-average. Over Tiwi land masses, the inversion height estimates using RH and θ_v gradients are similar. Interestingly, large differences arise over downwind ocean regions. Here, the RH method picks up the islands' inversion layer as it is advected off the land surface, whilst the θ_v approach selects the much lower gradient at the top of the sea breeze current.

Chapter 5

Results and discussions

5.1 Comparison of the baseline simulation to cloud-top remote sensing observations

The simulated development of convective activity, and in particular the timing and propagation of Hector storm cells, corresponds well to that observed by geostationary satellite (Fig 13). Obviously, the low resolution from geostationary orbit does not capture the detailed structure in the initial shallow cloud fields, and it is difficult to compare it to the associated simulated fields. Sea breeze convergence appears in both observations and simulations, with a slightly more pronounced cloud albedo towards the southern, i.e. leeward, coastlines. The northern coastline of Melville, where the sea breeze further accelerates the existing flow, remains essentially cloud-free. At around 14:15 LT (04:45 UTC), ATHAM produces intensive convection which forms simultaneously along the two southern coastlines of Melville, whilst observations indicate dominant activity mainly towards the SE part of the island. Differences are possibly due to inconsistencies between the homogeneous wind field initialization and the real flow, leading to differences in the initial sea breeze penetration.

The simulated homogeneous cloud decks in the western corners are model artefacts, possibly due to periodic boundary conditions, which can generate large-scale convergence (and thus forced ascent) and divergence where it should not occur. Although observed and simulated snapshots are displayed at roughly the same time, we cannot exclude possible synchronization issues or discrepancies due to model spin-up time. After 15:15 LT (05:45 UTC), both observations and simulation reveal strongest convective activity approaching Bathurst and over the Apsley Strait, propagating essentially like a squall line westward and producing a large trailing anvil covering Melville. ATHAM generates a significantly larger anvil and convective cells are located slightly further north compared to observations. The seemingly reduced shortwave albedo at 17:15 LT (07:45 UTC) in the observations may be due to low sun elevation angles.

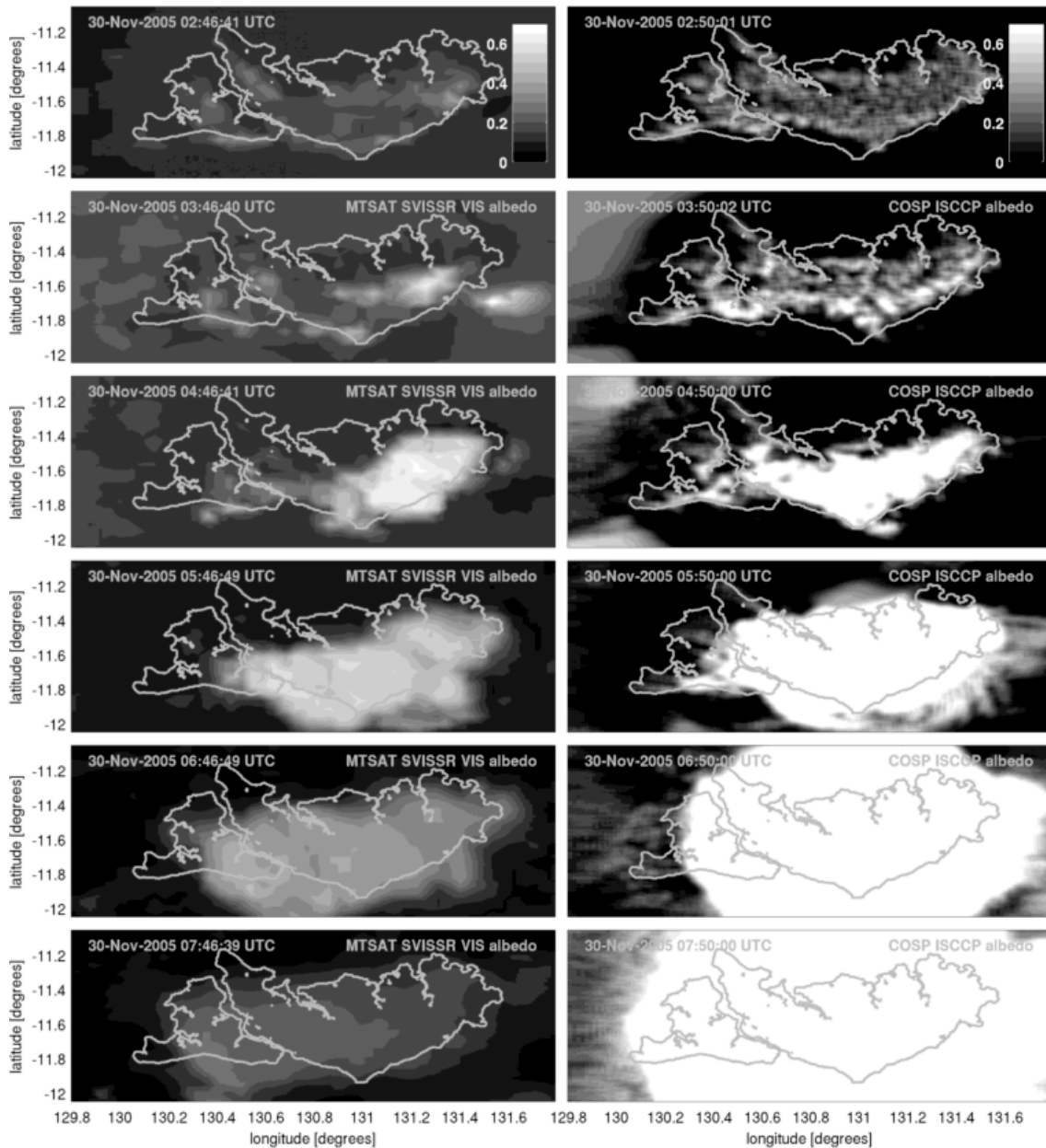


Fig 13 Time evolution of the Hector storm over Tiwi Islands. Visible channel albedo observations from the geostationary MTSAT-1R satellite, interpolated to the ATHAM-COSP grid, are in the left column. ATHAM simulations, converted to ISCCP albedo using COSP, and filtered through a 4.5 km 2D moving average are in the right column. The colour scale covers a range between 0 and 0.7; changing insolation conditions may have some impact on retrieved albedo values in the satellite imagery. The spinning VISSR instrument takes about 12-15 minutes to scan a full image; timings extracted here correspond to a mean pixel registration time over the depicted area.

At 14:50 LT (05:20 UTC), the Aqua platform passed over the area, providing some higher-resolution derived geophysical data. Discarding the obvious issues due to retrieval saturation, the morphology of the system seems somewhat different between observations and simulations (Fig 14(a) and (b)). It remains clear that ATHAM produces a more northerly line of convection, although the locations of simulated convective cores correspond reasonably well to those in the optical thickness product. As already pointed out, ATHAM generates a further line of strong convection along the SW Melville coastline,

which is heralded by a narrow NW-SE line of gust front clouds. Also, ATHAM produces the typical sea breeze convergence line clouds over narrow stretches of land that are often observed in reality, especially towards the west of Tiwi Islands, but are here absent in the satellite data. Simulated optical thickness values are much larger than those observed, and can exceed the latter by over an order of magnitude. τ in mixed-phase deep convective clouds cannot be estimated reliably from shortwave reflectance and IR radiance measurements. This is evident in the histogram counts, in which observed τ peaks at a value of 100, which corresponds to the highest valid measurement, whilst simulated τ pixels exist up to values of about 2000 (Fig 14(c)). The much higher simulated count of pixels with τ in the range of 1-10 is due to the artificial cloud layer mentioned previously.

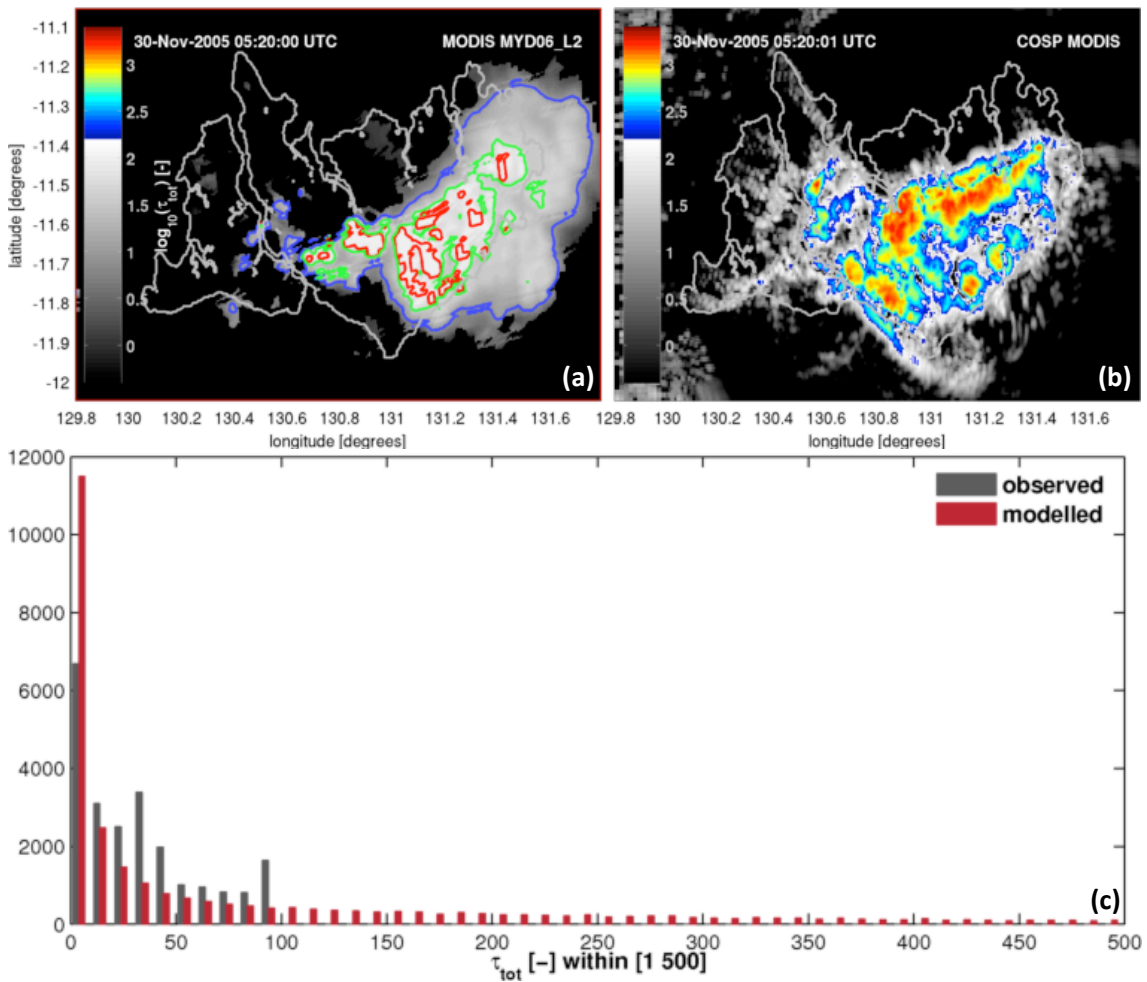


Fig 14 (a) optical thickness (τ) of the mature Hektor storm derived from MODIS observations during Aqua's PM overpass, interpolated to the ATHAM-COSP grid. To cover the large dynamic range of values between translucent, shallow and deep convective clouds, the base 10 logarithm of τ is displayed. Cloud-free pixels have been assigned a value close to 0 and are black, the colour range scales from τ of 0.5 to 2000. Two colourmaps are joined at an $\tau=150$, which defines the out-of-bounds retrieval limit for MODIS data (though practically, only values up to 100 fall within the data's valid range). Out-of-bounds regions, related to convective cores, are traced with red contours. Blue and green contours outline τ of 10 and 50, respectively; (b) simulated MODIS optical thickness using ATHAM-COSP. The original 500 m resolution data has been degraded using a 1.5 km 2D moving average; (c) histogram

counts for observed and modelled τ pixels, with bin-widths of 10, starting at 1. The modelled counts keep decreasing to a value of about 2000 but are only displayed up to 500.

Cloud top pressure is more useful to qualitatively assess and compare the intensity of convective draughts between observation and simulation (Fig 15). A large and seemingly homogeneous anvil has been remotely sensed, whilst the simulated cloud field at the same time consists of a number of individual convective cells, though the coarse resolution of the derived cloud top pressure product from radiance measurements (5 km) might have smoothed out a finer texture. This homogeneous anvil results in a much higher count of low cloud top pressure pixels in the observations (Fig 15(c)). The large amount of observed counts with cloud top pressure values between 500 and 300 hPa (Fig 15(c)) corresponds to the rim along the anvil (Fig 15(a)). This does not represent a mid-level anvil height but rather corresponds to an artefact from the interpolation procedure. The same is true for counts in bins going down to ground level (1000 hPa). ATHAM produces a much higher amount of low-level cloud, especially on the gust front, though part of it is due to the impact of the cyclic boundary conditions. Most importantly, both observation and simulation generate a maximum anvil height in the range of 100-75 hPa. ATHAM produces a further small overshoot in the range of 75-50 hPa, with a minimum at 66.5 hPa, which goes down to about 45 hPa during Hector's most intensive simulated updraughts at around 17:00 LT. Judging by the two modes, the simulated distribution seems to be shifted towards larger values by one bin-width (25 hPa). This suggests that the simulated anvil height may on average be lower than the observed one.

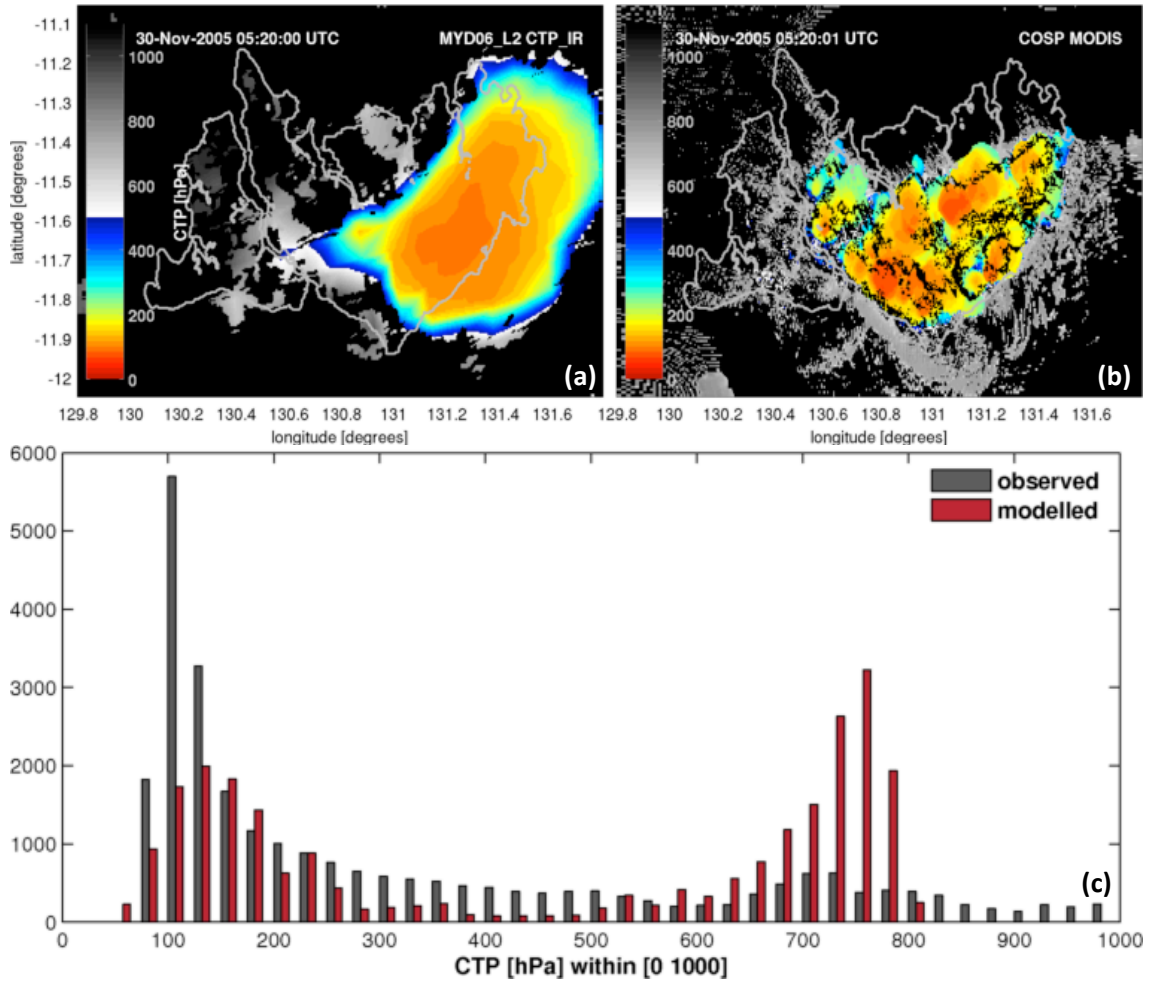


Fig 15 (a)–(c) same as Fig 14, but showing Cloud Top Pressure (CTP), with colours ranging from 1100 hPa (undefined value of a cloudless pixel) to 0 hPa. Colourmaps are joined at 500 hPa, the approximate pressure level for high clouds. The simulated MODIS cloud top pressure using ATHAM-COSP (b) has not been filtered and is displayed at original grid-spacing. Histogram counts in (c) have bin-widths of 25 hPa, starting at a value of 0.

At 16:15 LT (06:45 UTC), the Geophysica aircraft was flying over the most active region of the Hector storm, and its downward-pointing lidar MAL was recording a mean anvil deck at a height of 17 km, with overshoots up to 18 km and detached cirrus at the flight level of 18.5 km (Brunner et al. (2009) and Fig 13(b) therein). In ATHAM mean pressure levels, this corresponds approximately to 89 hPa, 73 hPa and 66 hPa, respectively. From Fig 16(a) and (b), it is clear that ATHAM underestimates the mean anvil height at this time, when the simulated mean cloud top pressure above 200 hPa lies around 120 hPa (or roughly 15.4 km). COSP also provides simulated CALIPSO spaceborne lidar output, for which simulated cloud top height is shown in Fig 16(c) and (d). Here, we have first estimated the background backscatter in the model's 30 grid-points within the stratosphere between 20 and 35 km. The background mean plus 3σ lies around $5 \cdot 10^{-7} \text{ m}^{-1}\text{sr}^{-1}$, and we have applied a conservative estimate of $10^{-6} \text{ m}^{-1}\text{sr}^{-1}$ to define the cloud backscatter threshold. Consequently, after applying the same threshold of 200 hPa (i.e. 12.2 km) to delimit the anvil's lower bound, we calculate the anvil's mean cloud top height

as detected from lidar to be around 15.5 km. Lowering the lidar backscatter threshold that defines cloud obviously raises the anvil's estimated mean height, as lower ice particle concentrations get accounted for as cloud. However, the algorithm then also starts to pick up a spurious signal concentrated in a thin isolated layer at 16.3 km (grid-point 140), covering large parts of the domain, and dominating the estimate of mean anvil height (this signal also appears as a small local maximum in Fig 16(d)). Since this layer is situated below the tropopause layer's cold point (roughly between 18 and 19 km), it is unlikely that the lidar return originates from a thin cold point detrainment and deposition cirrus layer. Whilst there are indeed very low ice specific concentration layers ($q_i \approx 5 \cdot 10^{-3} \text{ g kg}^{-1}$) at that model level and at others above, we attribute the 16.3 km signal to some unidentified artefact²⁹. In Fig 16(c), the uniform low-level lidar backscatter at around 5 km is likely due to molecular backscatter in the denser lower atmosphere.

The model produces more intensive (oscillating) overshoots than those observed, although the Geophysica flight level at 18.5 km limits the comparison. From Fig 16 and three-dimensional inspection of the data, it can be seen that the modelled convection penetrates up to and above 20 km, and generates a further small and flat detrainment layer at these heights, which coincides with a small local 'inversion layer' around 50 hPa in the original profile (Fig 12(a) and Fig 16(e)). The spread of the mean cloud top height within a $\pm 1\sigma$ interval (Fig 16(e)) is indicative mainly of the onset of deep convective development (after 12:00 LT) and the strong heterogeneity of cloud levels during the mature phase. The apparent rise of the anvil's mean cloud top height after 16:10 LT (06:40 UTC) is misleading: the stronger overshoots and detached cirrus formation at around 20 km bias the anvil's mean cloud top height towards larger values, whilst in reality, the main cloud deck is slowly subsiding. Unfortunately, it is difficult to say whether the strong overshoots and detrained cloud at highest altitudes, as indicated by the maximum cloud top height (CTH_{max}), is realistic; and increasing levels after 16:30 LT certainly are not. Due to a model upper boundary issue, model top temperature dramatically decays over time, gradually eroding the characteristic stratospheric temperature inversion over time. A capping layer remains throughout the entire simulation, but the tropopause cold point slowly rises over time, and so does the initial local 'inversion layer' mentioned above. It is thus well possible that overshoot-top detrainment, which coincides in height with the local temperature minimum, is indeed a model artefact, especially towards the late afternoon hours. Were convection to continue into the late evening, it would likely continue through the eroded stratosphere towards the model top.

²⁹ In section 3.5, we found the model's domain-averaged hydrostatic state to oscillate at a high frequency and with very low amplitude. This, or possibly gravity waves, could potentially generate pressure- or vertical displacement-induced transient ice deposition layers where the RH with respect to ice is near saturation.

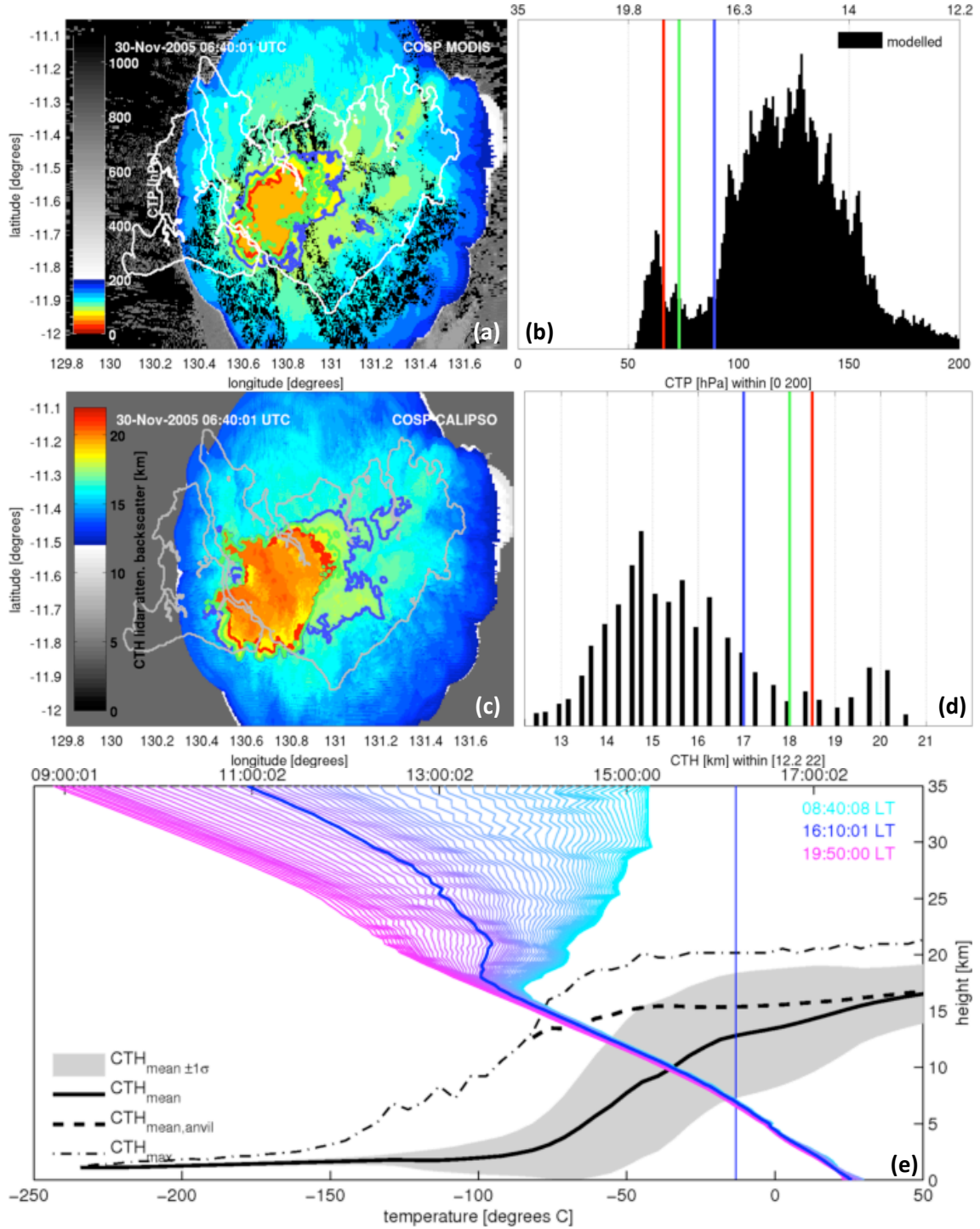


Fig 16 (a) ATHAM-COSP-derived MODIS cloud top pressure during Hector's most vigorous phase around 16:10 LT (06:40 UTC). The colourmaps are joined at 200 hPa to highlight details in the anvil, with levels spaced by 17 hPa; (b) corresponding histogram counts within the range 200 to 0 hPa, with 1 hPa bin-width. The height above ground level (upper axis [km]) is approximate, from matching the subdomain's mean pressure profile to ATHAM's vertical axis; (c) ATHAM-COSP-derived CALIPSO cloud top height, using a lidar attenuated total backscatter at 532 nm threshold of $10^{-6} \text{ m}^{-1} \text{ sr}^{-1}$; (d) corresponding histogram counts within the range 12.2 to 22 km, with 100 m bin-width. Empty bins are due to the coarser resolution. The red, green and blue isolines ((a), (c)) and lines ((b), (d)) correspond to the pressure levels ((a), (b)) and heights ((c), (d)) of the mean anvil deck, overshoot and detached cirrus, respectively, measured by the Geophysica aircraft during the SCOUT-03 campaign; (e) time evolution of the analysis subdomain's mean temperature profile between simulation start (cyan) and decay phase (pink). The blue profile is at the same time as the

other panels. The time evolution [LT] of the ATHAM-COSP CALIPSO cloud top height is also shown. To estimate mean, standard deviation, anvil mean and maximum cloud top height, a 5 times larger backscatter threshold is used at the expense of thin cloud detection aloft, to discriminate particle backscatter against the molecular backscatter in the dense troposphere (see text). The vertical blue line sets the time stamp of the blue profile at 16:10 LT.

5.2 Comparison of the baseline simulation to anvil in situ observations and some insights into convective dynamics, transport and overturning

The role of deep convective overturning and transport towards the upper troposphere-lower stratosphere (UTLS) and corresponding implications for climate and upper-air chemistry are not well-understood (see e.g. Brunner et al. (2009), Vaughan et al. (2008), May et al. (2008), Hoffmann et al. (2012) for some dedicated airborne and field campaigns and remote sensing mission proposals addressing this question). Evidence for UTLS hydration by the Hector storm, specifically concerning the event on 30th November 2005, has been reported and discussed by Corti et al. (2008), Schiller et al. (2009) and Chemel et al. (2009). Views on the effects of overshooting deep tropical convection are conflicting. Does it lead to dehydration, via ice precipitation in anvils or overshoots, detrainment of cloudy air above the neutral buoyancy height, followed by mixing of the adiabatically-cooled air masses from the cold overshoots with the warmer lower-stratospheric environment (Danielsen (1982), Sherwood and Dessler (2000))? Or, on the contrary, does it lead to hydration, via evaporation of detrained ice crystals? This question may critically depend on the existing air masses' RH with respect to ice. Schiller et al. (2009) argued that the major outflow of deep convection below the cold point leads to a moistening of the lower Tropical Tropopause Layer (TTL), without however transporting increased amounts of water into the lower stratosphere, due to the cold trap's freeze-drying effect. Above, episodic overshoots were deemed to provide water vapour and ice through strongly localized injections contributing to a moistening at subsaturated conditions, albeit of climatologically only moderate magnitude.

Here, we adopted the same thermal structure definition of the TTL as used by Chemel et al. (2009), using an *a priori* level of zero net radiative heating (355 K, at around 14.5 km, Sherwood and Dessler (2000)) and the cold point tropopause (roughly 372 K at around 17 km) as lower and upper limits. The TTL is a buffer region between the main convective outflow of deep tropical clouds and the cold point tropopause (Vaughan et al. (2008)), characterized by sharp gradients of tropospheric tracers and total water. This is obvious in Fig 17, wherein the evolution of UTLS water and boundary layer air is depicted

as a function of time. Note that ice and boundary layer air only appear after the onset of deep convection (Fig 17(b) and (c)), and that the vertical distribution of both is virtually identical (if displayed with identical axis scaling, not shown), as both define the extent of the anvil. Towards the early evening (pink lines), the TTL and lower stratospheric increase in ice and PBL air specific concentrations is accelerating. This is possibly due to the tropopause inversion layer erosion and not to invigorated convective activity (though invigorated it actually is), and we consequently delimit further analysis to a time period before this effect (16:50 LT, blue line). This artefact is most noticeable in the water vapour profiles (Fig 17(a)), where the lowest mean specific concentration (hygropause) decreases and rises vertically over time, before disappearing altogether. In our analysis, we have maintained a static (and initial) cold point height to define the TTL and refrain from a biased interpretation of the tracer evolution in the lower stratosphere. Even if the water vapour values around the cold point are becoming less reliable over time, it is nonetheless clear that the entire TTL (predominantly the lower region) and upper troposphere are being hydrated over time, partially towards saturation.

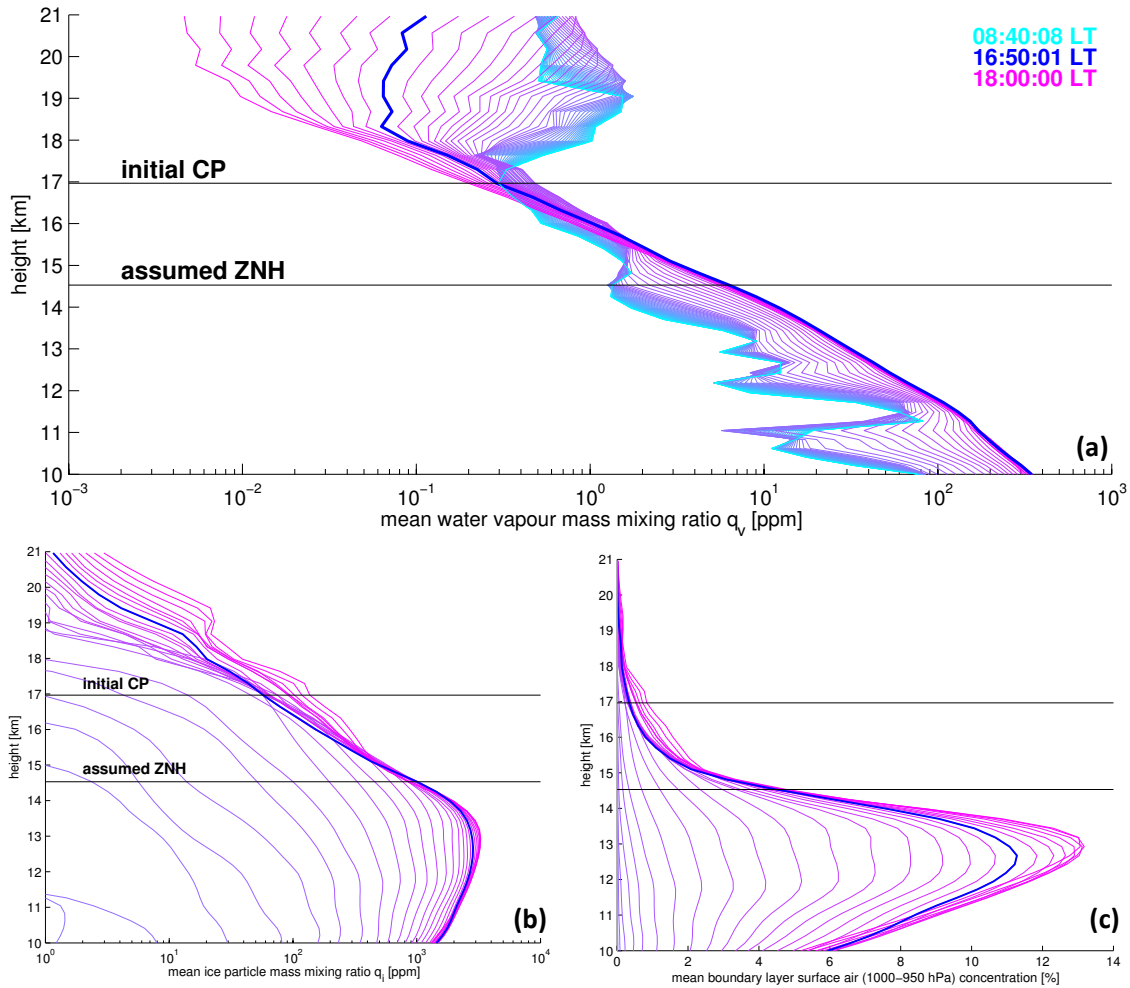


Fig 17 UTLS profiles of analysis-subdomain mean (a) specific humidity, (b) ice particle specific concentration, and (c) PBL passive tracer concentration. The ice particle specific concentration (b) has a very similar vertical distribution as the PBL passive tracer (c),

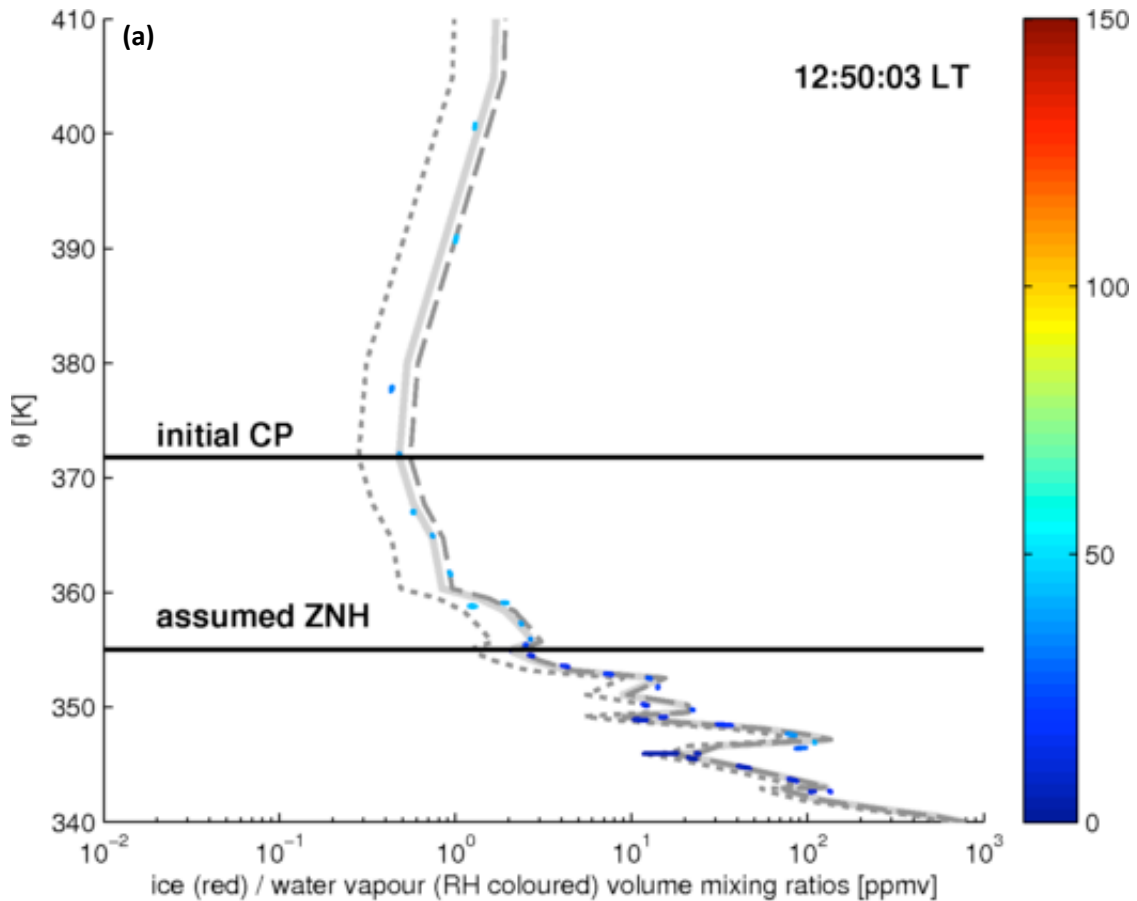
characterized by an exponential decrease within the TTL, and so do the other low- to mid-tropospheric passive tracers. The TTL definition is given in the text, and goes from the level of zero net radiative heating (ZNH) to the cold point tropopause. These levels have been retrieved from the initial profile, before the stratospheric temperature erosion artefact. The blue profile is retrieved at 16:50 LT (07:20 UTC), the estimated peak in convective activity, after which further stratospheric intrusions (Fig 19(b)) are probably ever more due to the erosion of the cold point inversion.

This can be better appreciated in Fig 18, which depicts ice particle and water vapour approximate volume mixing ratios (assuming specific concentrations are roughly equal to mass mixing ratios) as a function of collocated potential temperature, and which emulates Fig 2 in Schiller et al. (2009) and Fig 10 in Chemel et al. (2009) for the same storm. A few particularities need pointing out. As discussed before, the stratospheric temperature erosion manifests itself again by a strong upper-level decrease of specific humidity, as it displaces water into an excessive ice phase. In fact, the water vapour profile in the lower stratosphere should coincide with the line of highest ice clustering in Fig 18(c). Very large ice specific concentrations remain towards the end of the simulation, since ice in ATHAM is parameterized without a fall velocity and hence does not sediment. It will henceforth necessarily sublime eventually – which incidentally limits any conclusions on hydration versus dehydration of the stratosphere based on our model runs. The existence of continuously decreasing ice volume mixing ratios to very low values (towards the left of the original profile) is due to the implicit matrix solver used in ATHAM and thus a numerical artefact. The discrete lines and elements in the figure are due to the discrete and coarser vertical grid-spacing aloft. No ice is present before the onset of deep convection (12:50 LT, Fig 18(a)) and most θ - H_2O points remain clustered around their initialization values (thick grey line).

The lowest (initial) vapour volume mixing ratio of about 0.5 ppmv is by a factor of 5 smaller than the typical mean background over Tiwi Islands around the 380 K isentrope of about 2.5 ppmv (Chemel et al. (2009)), and that measured by the FISH hygrometer on 30th November (Schiller et al. (2009)). This very low humidity has been directly retrieved from the sounding's RH_{water} readings, and we confirmed the adequacy of ATHAM's conversion into specific humidities through a comparison with the parameterization implemented in the Weather Research and Forecasting (WRF) model (grey dashed line for RH_{water} and dotted line for $RH_{water,ice}$). It is possible that the sounding underestimates RH at lowest temperatures; measured values around the TTL were 10-15%. Because of the preceding model limitations and artefacts, we refrain from further comparison to FISH hygrometer data.

In spite of these limitations, we can still state that ice mixing ratios dramatically increase above the main outflow region, in the TTL and above. So does the water vapour mixing ratio, and a significant proportion of the region becomes more saturated, which is

normal given the extent of the anvil. Ice had indeed been observed up to a height of 18.8 km, embedded in subsaturated air, suggesting direct transport and detrainment by deep convective turrets (Corti et al. (2008)). The (green-yellow) bell-shaped elements in Fig 18(b) and (c) characterize the water vapour and RH_{ice} distribution as a function of potential temperature across the model levels. Given a horizontal cross-section through the overshoot, the strongest negative θ anomalies (5-10 K) are found within the adiabatically-cooled overshoot, characterized by high ice concentrations, low specific humidities but (super)saturated RH_{ice} (not shown). The other end of the base of the bell-shaped element is less straightforward. The area downwind of the overshoot turret is characterized by a detrained veil of lower concentrations of ice particles, high and (super)saturated vapour and positive θ and temperature anomalies. The lower RH_{ice} areas towards the centre of the distribution characterize the surrounding cloud-free regions of average θ and low specific humidity. At lower levels, active convective updraughts determine the high θ , high q_v , high RH_{ice} end of the distribution, whilst the lower temperature surrounding regions remain mostly drier and unsaturated.



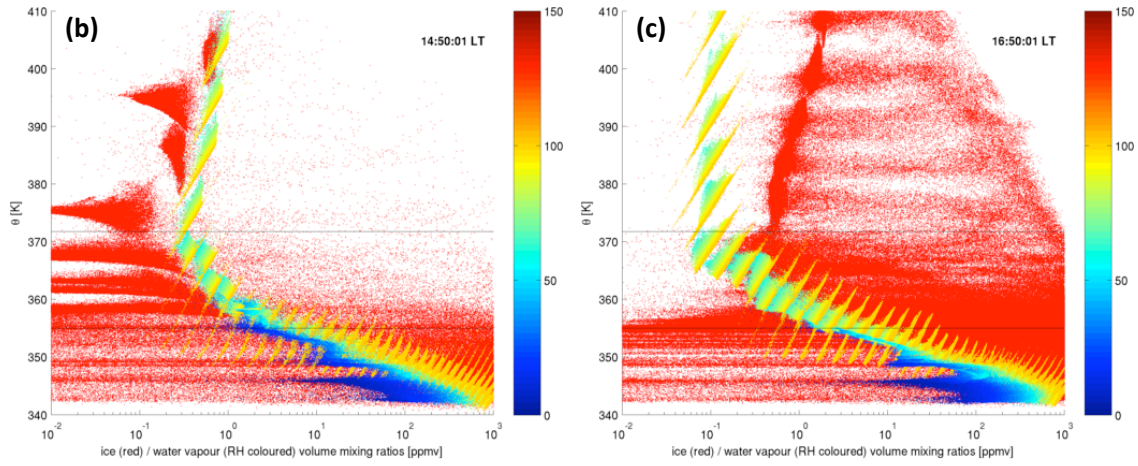


Fig 18 θ - H_2O scatterplots for approximate volume mixing ratios of water vapour and ice, at (a) 12:50 LT (03:20 UTC), (b) 14:50 LT (05:20 UTC) and (c) 16:50 LT (07:20 UTC). Vapour is coloured as a function of RH with respect to ice, as parameterized in ATHAM. The thick grey line in (a) traces the initial vapour mixing ratio as a function of potential temperature profile, as computed from RH in the sounding and parameterized in ATHAM. Mixing ratios estimated from RH with respect to water only (dashed grey line) and with respect to water and ice with a phase transition between 0 and -23 degrees C (dotted grey line), as parameterized in WRF, are plotted for comparison. Isentropes as vertical coordinates may provide erroneous data points later in the simulation, due to the stratospheric erosion.

It is surprising that specific humidity over time is increasing in the upper TTL up to slightly above the cold point-level, decreasing strongly just beyond that, and then increasing again above 19 km, during the first half of the simulation (Fig 17(a)), whilst temperatures steadily decrease over time (Fig 16(e)). This requires further investigation, but explains the slow initial rise of the TTL mean specific humidity in Fig 19(a), which is solely linked to an increase in the upper half of the TTL, confirmed by a similar increase at the upper limit (blue dotted curve). After the penetration of the first convective turrets, both the lower-limit (dash-dotted curve) and mean TTL water vapour and ice particle specific concentrations increase sharply. For reasons mentioned before, ice specific concentrations are much higher than those found in other studies, but are certainly linked to a direct injection into the TTL, as opposed to originating from condensation of vapour at much lower specific humidity levels. The final drop in vapour and rise in ice specific concentrations are again linked to the stratospheric artefact.

Since the anvil's extent can be characterized both in terms of ice and PBL air concentrations, it is interesting to determine the origin of the compositing air masses. Passive tracers implemented in ATHAM as markers of the original vertical distribution in pressure levels are particularly well fitted for this purpose³⁰. In Fig 19(b), we have plotted the mean TTL specific concentrations of 7 tropospheric passive tracers, illustrated as identically-shaded grey patches in the left side of the figure. As anticipated, tropospheric

³⁰ For a 3D visualization of passive tracer redistribution, we refer to the closing figure in the appendices.

air masses appear suddenly in the TTL with the penetration of convective turrets, levelling off during the mature phase of the storm, and experiencing an ultimate boost due to the stratospheric erosion. The two lowermost passive tracers have high concentrations in the TTL, whilst the two layers immediately above have much lower concentrations. This corresponds to the expected boundary layer origin of deep convection. The base of the inversion layer z_i effectively isolates the convective PBL from the free troposphere (coloured horizontal lines). During the initial dry and moist shallow convection phases, both the 1000-950 hPa and the 950-900 hPa passive tracers are well mixed by PBL turbulence. By the time z_i reaches the top of the 900-850 hPa layer, cumulus congestus clouds have appeared and broken through the inversion layer, and vertical displacements have replaced the shallow overturning. Less obvious is the large proportion of lower- to mid-tropospheric air in the TTL (650-500 hPa, and in particular 800-650 hPa), though the larger initial depth of these layers certainly contributes. To investigate possible reasons for this mid-level inflow into the convective towers, we have calculated the mean vertical mass flux over land areas and over time, $\overline{\langle \rho \vec{w} \rangle_{land}}$ (blue dashed curve), as well as its divergence, $\partial(\overline{\langle \rho \vec{w} \rangle_{land}})/\partial z$ (blue solid curve). Because of time averaging (over individual snapshots generated every 10 minutes), different dynamical phases are confounded within the same curves. In particular, the lowermost positive mass flux corresponds to the initial shallow convective updraughts (thermals). These partially compensate the following precipitation downdraughts that reach down to the surface, but in the averaged curve only appear between roughly 1 and 2.5 km. Convective updraughts during initial deep convection exist throughout the entire profile, but are strongest between 6 and 9 km. This is significantly above the freezing level, (linked to the small temperature inversion around 5 km), and probably due to some additional deposition, latent heat release and buoyancy production as adiabatic cooling continues to lower the saturation water pressure, limited Bergeron-Findeisen processes (not well represented in the model), and mostly due to the distance covered before peak acceleration translates into peak velocity. Most importantly, the maxima in mean vertical mass flux divergence are located near the surface layer, where convective thermals laterally draw in lower PBL air (see next section), and in the troposphere between 3 and 4 km. Here, the lateral air intake coincides with peak divergence, where on average precipitation downdraughts separate from convective updraughts. Partially, this air may end up in the descending rear inflow described in the classical squall line model (Houze et al. (1989)), but some of it contributes to the enhanced ingestion and upward transport at this level. The entrainment mechanism needs further process study and quantitative evaluation, but if confirmed experimentally,

such localized intake may warrant integration into deep convection parameterizations. A snapshot of the fate of 800-650 hPa passive tracers at 16:50 LT is shown in Fig 19(c).

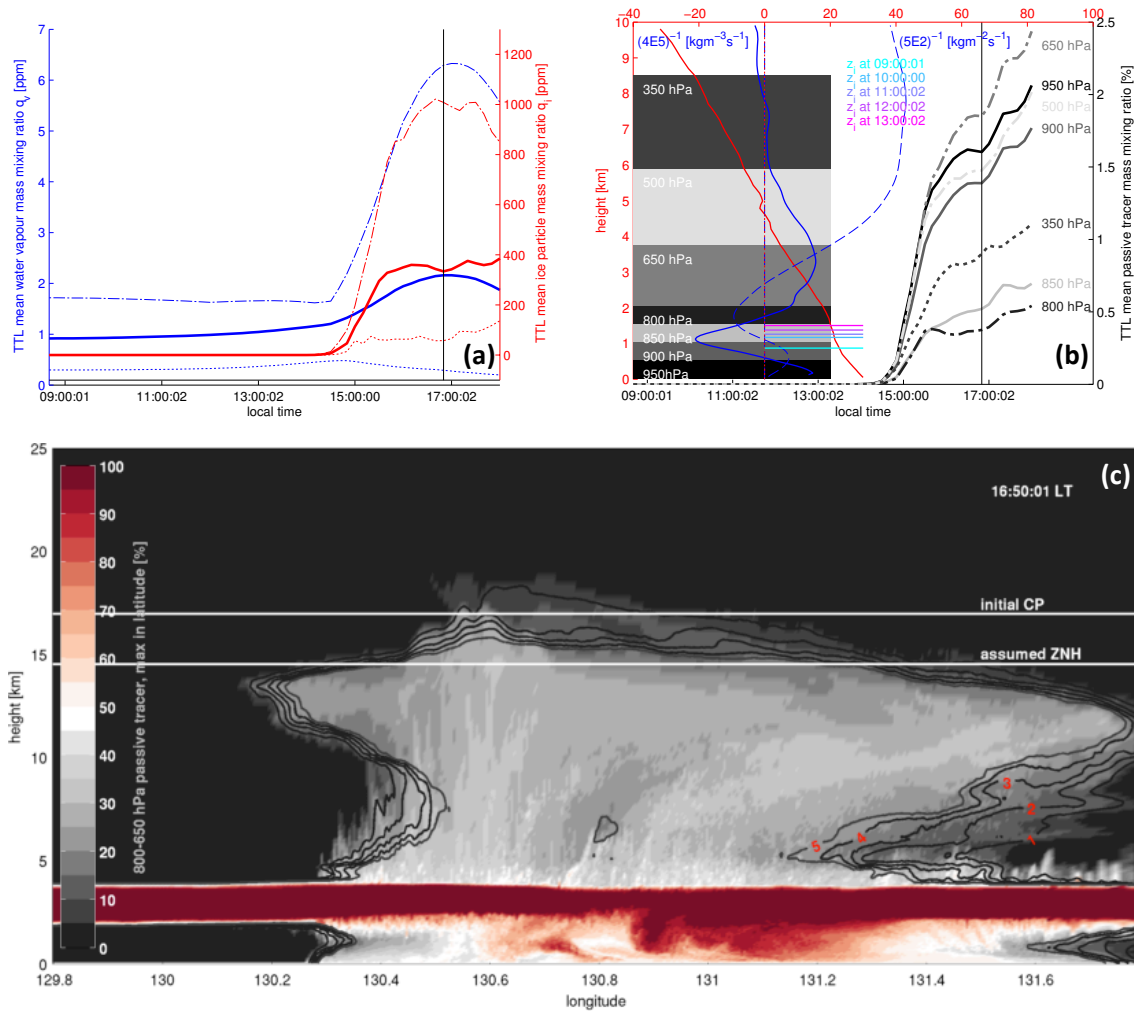


Fig 19 Storm outflow of lower-level air masses and water within the TTL: (a) analysis subdomain mean (thick solid), minimum (dotted) and maximum (dash-dotted) water vapour (blue) and ice (red) specific concentrations as a function of time. Minimum values are found at the top and maximum values at the bottom of the TTL (see Fig 17); (b) same as (a), but for passive tracers defining tropospheric air masses of different vertical origins (grey lines, right axis). The initial distribution of these passive tracers (identified by the pressure level of their upper limit) is shown as patches with identical shades of grey on the left. The red profile is the initial temperature profile ($^{\circ}\text{C}$, upper axis) of the sounding, where the vertical line indicates the freezing level. The five coloured horizontal lines correspond to the average PBL inversion height z_i (from the RH gradient) over land at the times (LT) given in the figure. The dashed blue line corresponds to the mean vertical mass flux, averaged over land areas and over time from the simulation start to 18:00 LT, the solid blue line is its vertical divergence. These profiles are drawn within the upper figure axis multiplied by the corresponding factor given in the figure; (c) lower tropospheric (800-650 hPa) passive tracer distribution at 16:50 LT (07:20 UTC). The longitude-height colour section depicts the maximum value across the latitude dimension. The 5 contours give the mean value in latitude at 1-5%.

With the aim of getting a better qualitative impression of the convective dynamics and turbulent diffusion processes that govern the entrainment of air masses from different height levels into the simulated cloud field at a particular snapshot in time,

roughly during the mature system's peak convective activity, we have plotted a series of streamlines released from various heights and locations within the storm environment (Fig 20). At 16:50 LT, the main axis of storm propagation is roughly zonal (east-west), such that streamlines released cylindrically around the main core provide little further insight with respect to a release limited to an XZ plane. Note that streamlines must not be mistaken for particle trajectories. Whilst the latter would be preferable in the highly transient and dynamic environment of deep convection, they require an advanced model for computation. Further, the streamlines may cross thermodynamic boundaries if residual velocity fields exist, and they unrealistically continue to rise into the stratosphere.

Nonetheless, they illustrate particularly well the lofting of PBL air by the cold pool density current front ahead of the storm, with successive ingestion into the cloud system and transport aloft. The rear inflow of a squall line is well represented, with a clear separation into flow that rapidly descends in the precipitation downdraughts and other streamlines that end up in strong updraughts just above. This separation occurs at heights between 4 and 5 km. Interestingly, streamlines released within the core rainfall region move forwards with the strong density current, before being lofted in the frontal region to move back and up into the updraught cores. We cannot tell from this representation whether such recycling actually occurs in reality or whether the cold high-density air masses would remain trapped within the density current. Mid-tropospheric air ahead of the storm gets invariably ingested into the updraughts, even if this shall not be considered as a direct turbulent entrainment mechanism into a single cumulonimbus tower. Once in the main updraught, most streamlines end up in the overshoot, where some separate and could be perceived as stratospheric 'fountain injections', whilst most oscillate laterally into the anvil. The radial velocity field created by the anvil produces an outward movement of streamlines released in the upper troposphere.

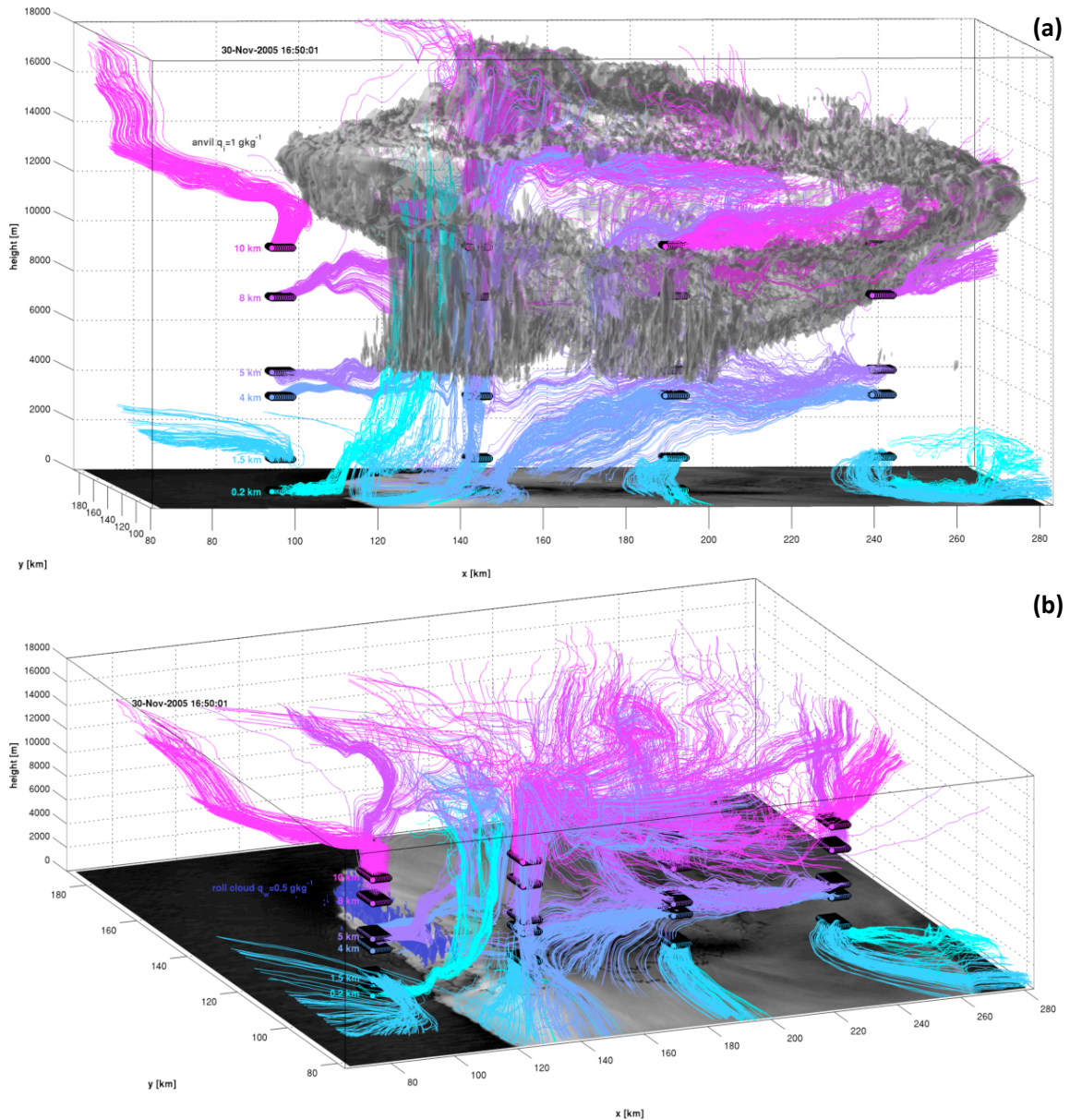


Fig 20 (a) streamlines for patches of 11x11 particles released at 6 different heights on the main axis of the storm (determined visually at $Y=112$ km in the Cartesian framework), within the main precipitation downdraught ($X=150$ km), 50 km in front as well as 50 and 100 km behind the core. The location of the release patches is also included in the following figures for clarity. The grey isosurface delimits ice water at $q_i=1$ g kg⁻¹. The surface shading represents the surface-level (lowest grid-box) wind speed, with brighter shadings indicating higher winds; (b) same as (a), but from a different perspective and without the ice. The blue isosurface delimits shallow cloud at a liquid water specific concentration of $q_l=0.5$ g kg⁻¹. For clarity, only a small box-subset of q_l has been extracted, delimited vertically to 3 km. The extract shows a section of the shallow clouds that form above the front of the cold pool density current (comparable to Fig 4 in Khairoutdinov et al. (2009)).

The overall 3D flow must be understood as the complex interaction between the original synoptic winds with which the model has been initialized and the velocity fields set up by the convective dynamics. From Fig 21, it is clear that even a small displacement of the particle release patches would have produced quite different streamlines, especially at certain critical heights. The very large cold pool generated by the simulated storm is obvious in the surface layer (0.2 km), with a thin line of updraughts along the convergence

lines, lifting PBL air. Air masses above the PBL (1.5 km) ahead of the storm largely remain unaffected and are deflected around the cold pool. In the lower-free troposphere (4km), the storm core constitutes a centre of convergence, with radial inflow both into the up- and the downdraught regions, whilst further up, the core seems to be a more isolated region that diverts the flow around it.

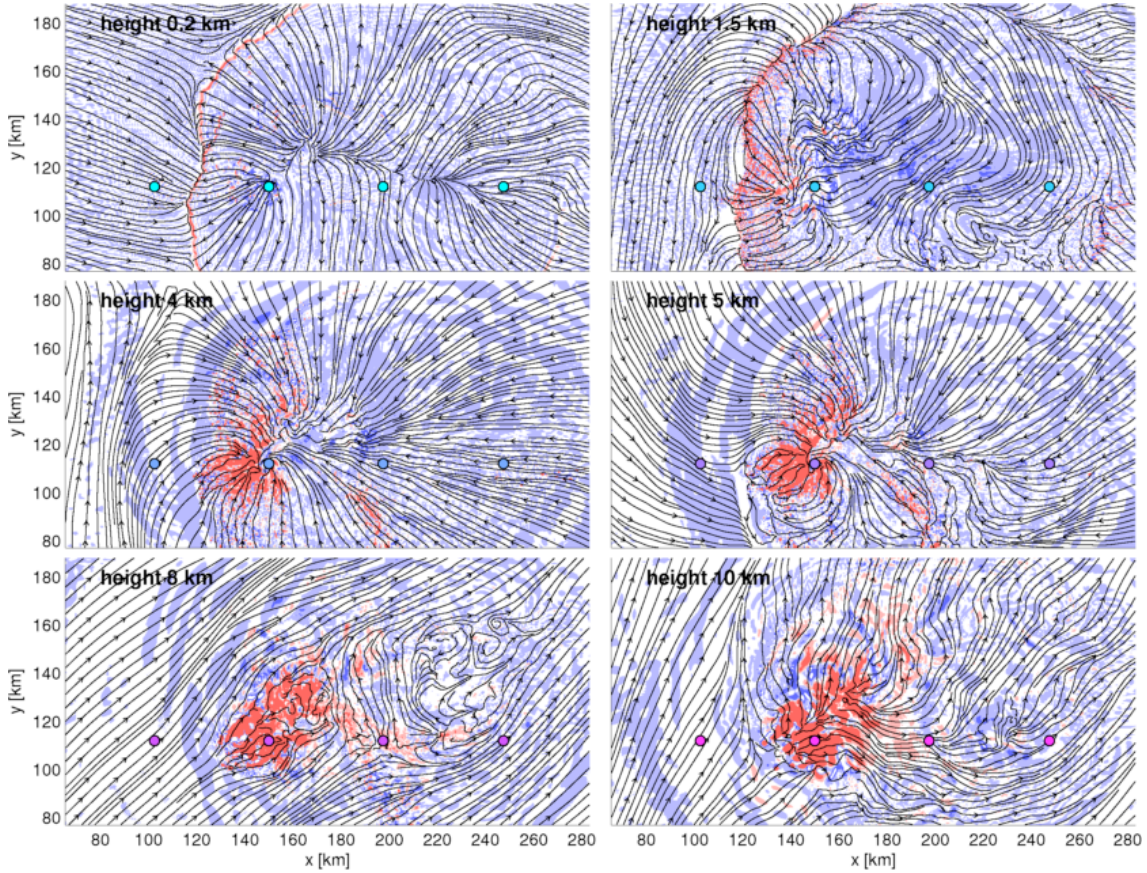


Fig 21 Horizontal stream slices through the storm at 16:50 LT, at the same heights as particle release in Fig 20, illustrating the complex flow in and around convective cores. The shading highlights areas of updraughts (red) and downdraughts (blue).

The region between $X=120-140$ km is not a single isolated deep convective tower, but a complex cloud field of newly triggered cells, starting around the gust front, and alternating with strong downdraughts (Fig 22). The mature core is located after $X=140$ km, whilst new cells develop ahead, growing to heights where some merge with the main anvil. Such cloud bridging is a common process, as is the merger with previously existing clouds and storms (e.g. Tao and Simpson (1984), Simpson et al. (1993), J. W. Wilson et al. (2001), D. Fu and Guo (2012)). This often leads to an explosive growth of Hector storms, but our relatively coarse resolution with 500 m grid-spacing certainly limits fine-structured details and blurs the boundaries. Thin downdraughts embrace rising convective cells. This region of strong vertical velocity gradients creates strong subgrid-scale vertical TKE and can be expected to be a region of strong mixing of cloud with

environmental air. The ingestion of up-storm streamlines from different heights into the main core is gradual and subjected to many alternating vertical directions. On average, this region of active triggering of new cells seems to act not unlike a stepwise conveyor belt bringing the lower-level air masses gradually to higher altitudes before they reach the mature core.

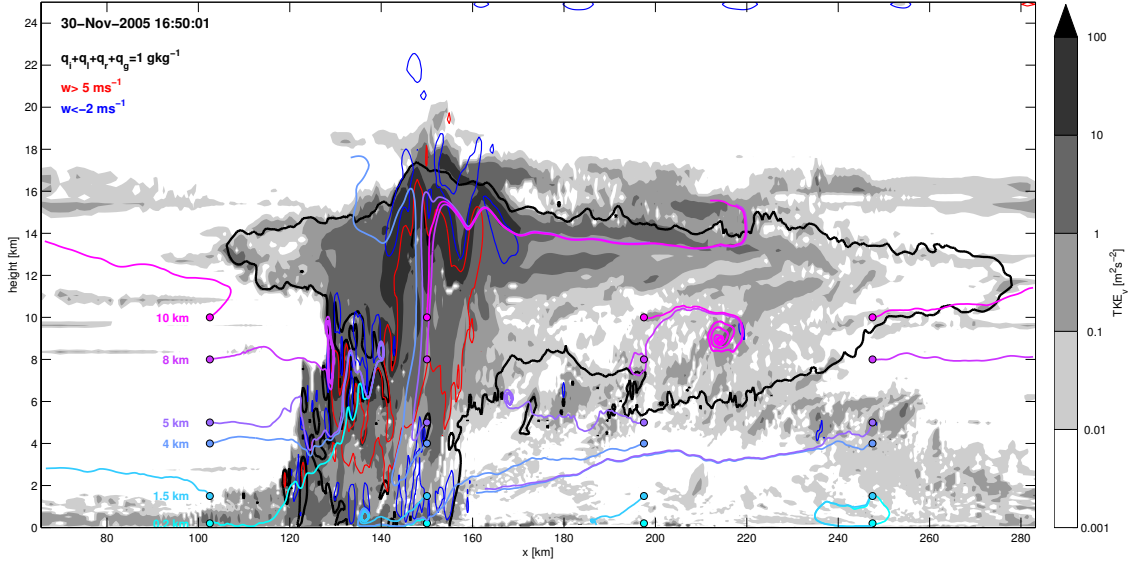


Fig 22 Zonal cross-section through the main axis of the storm ($Y=112$ km). The filled contours represent vertical subgrid-scale TKE in log-scale. The cloud is outlined by the solid black contour at a total water specific concentration of 1 gkg^{-1} . Strong updraughts (red contours, $w > 5 \text{ ms}^{-1}$), downdraughts (blue contours, $w < -2 \text{ ms}^{-1}$), as well as streamlines computed in the XZ-plane are also shown.

Simulated subgrid-scale turbulence is further highlighted in terms of the prognostic turbulence length scale λ , a characteristic scale of the unresolved eddies (Fig 23(a)), and the anisotropy γ between vertical and horizontal prognostic subgrid-scale TKE (Fig 23(b)), defined in Herzog, Oberhuber, and Graf (2003) as:

$$\gamma = 100 \cdot \frac{\frac{3}{2}TKE_h - 3TKE_v}{TKE_h + TKE_v} \quad (5.1)$$

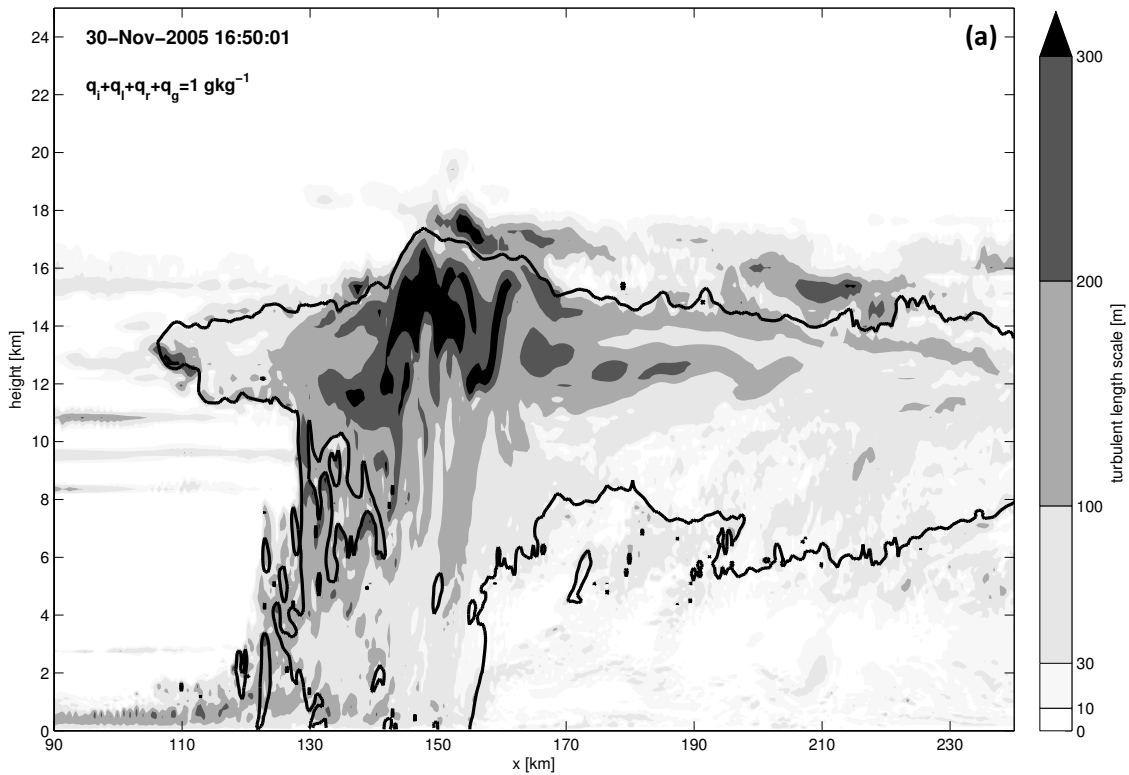
The effect of thermodynamic stratification due to the cold pool density current on parameterized turbulence is striking. From the gust front roughly around $X=120$ km to beyond the eastern figure limit, PBL subgrid-scale TKE is lower than in the up-storm convective PBL ahead of the gust front (Fig 22), except in the area affected by convective rainfall. More dramatically, the turbulent length scale (Fig 23(a)) is much smaller and even tends towards 0. This is essentially the result of nudging λ to a stable environment equilibrium length scale λ_0^* , expressed in terms of the Brunt-Vaisälä frequency N^2 as:

$$\lambda_0^* = 0.54 \sqrt{\frac{TKE}{N^2}} \quad (5.2)$$

Whilst this enhanced stability effectively limits the upward subgrid-scale turbulent diffusion within the PBL, surface heat fluxes may actually increase as a consequence of cool air masses spreading at high velocity over the ground, provided that soil heat content has not decreased excessively due to anvil shading.

Largest λ is simulated in the overshoot, presumably because of large subgrid-scale TKE, but also because vertical grid-spacing is coarser aloft. A further hotspot above the anvil around $X=210$ km is likely due to anvil turbulence. Overall, the simulated anvil (cloud) top seems to be a region of enhanced turbulence, which could lead to fast mixing with environmental air and cloud top detrainment. The region of convective rainfall and downdraughts seems to be the least turbulent of the main storm.

Deviation from turbulent isotropy in Fig 23(b) shows increased mixing due to vertical eddies (with respect to an isotropic limit) in the region we called the ‘conveyor belt’ previously, whilst the opposite holds for all the remaining regions.



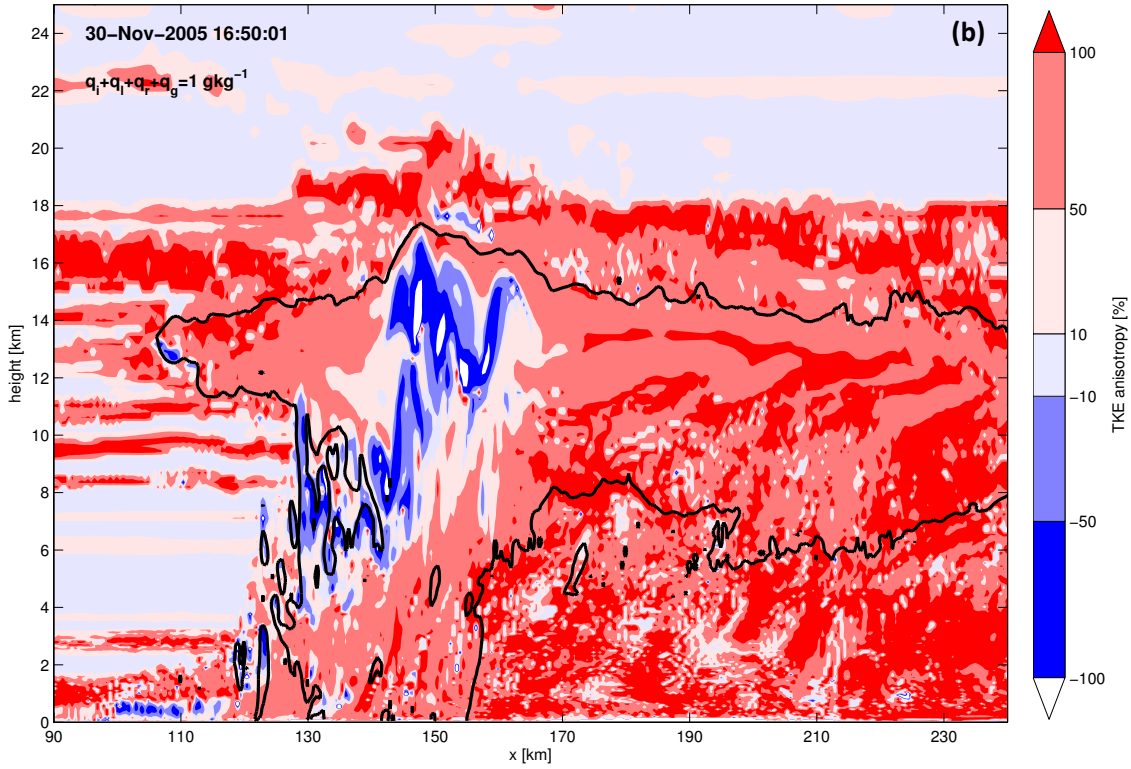


Fig 23 Same cross-section as Fig 22, showing (a) the subgrid-scale eddies' turbulent length scale λ (see equation (3.4)) and (b) the turbulence anisotropy (equation (5.1)). Vertical subgrid-scale TKE dominates in blue-shaded (negative) areas, horizontal TKE in red-shaded (positive) ones.

5.3 Comparison of the baseline simulation to radar observations

Lastly, an inspection into the 4D volume data provided by the C-POL radar and simulated by ATHAM-COSP-QuickBeam is given in Fig 24 in terms of reflectivity values. Horizontal cross-sections are plotted at the 2.5 km Constant Altitude Plan Position Indicator (CAPPI) after resampling the polar radar data into Cartesian coordinates. Further below this level, no observed data is available due to the minimum elevation of the scanning radar beam and the distance to Tiwi Islands. This makes it hard to retrieve rainfall reaching the surface, as a significant amount can be expected to re-evaporate below cloud base. Equally, at high elevation angles required for cloud top detection, the raw resolution is degraded and heterogeneous.

Still, simulated data from ATHAM-COSP-QuickBeam provides realistic reflectivities that match the range of observations well. This has to be considered within the limitations due to the different sensing geometries, the simple microphysics scheme in ATHAM, (with an assumed hydrometeor distribution prescribed for QuickBeam), and the absence of simulated snow or otherwise larger ice particles except for graupel. Also, simulated radiative transfer is based on Mie theory, although the larger wavelengths of the rain

radar, (compared to the CloudSat cloud radar for which the COSP interface to QuickBeam has been designed), may actually shift some scattering back into the Rayleigh regime. COSP does not output Rayleigh reflectivities ($do_ray = 0$, Bodas-Salcedo (2010)). Finally, C-POL reflectivities are corrected for attenuation, whilst COSP provides simulated effective reflectivities, reduced by gaseous and hydrometeor path-attenuation.

In terms of convective structure and evolution, some similarities and differences are noteworthy, and are best appreciated through an animation of the observed and simulated fields at the 2.5 km CAPPI (not shown). Initial isolated strong radar returns are apparent in both observations and simulation, especially around the centre of Melville's SE coastline stretch and towards Nguu in SE Bathurst. For the observed event, convective development then spreads zonally westward from the initial cells on Melville's SE coast, but predominantly southwest along the coast and sea breeze front towards the southernmost cape. This line then pivots again into a more zonal direction and the configuration shown in Fig 24(a), after merging with and ingesting the smaller cells over Bathurst and the Apsley Strait. This intensifies into a more compact system, which subsequently evolves into a line along the Strait (Fig 24(c)). Finally, this system propagates westward and rotates into the SSW-NNE-directed squall line mentioned previously, dissipating as parts of the line move over the ocean. The simulated field ends up in a similar, albeit larger squall line, as seen in Fig 24(g). Simulated convection seems however to develop strongly on gust fronts from multiple cold pools (Fig 24(e)), as well as on southern coastline sea breeze fronts. Individual cold pools seem to merge gradually into one big system, with dominant triggering of new cells on the westward-moving front. Convection decays on the northern edge, and the most intensive cells are located in the vicinity of Nguu.

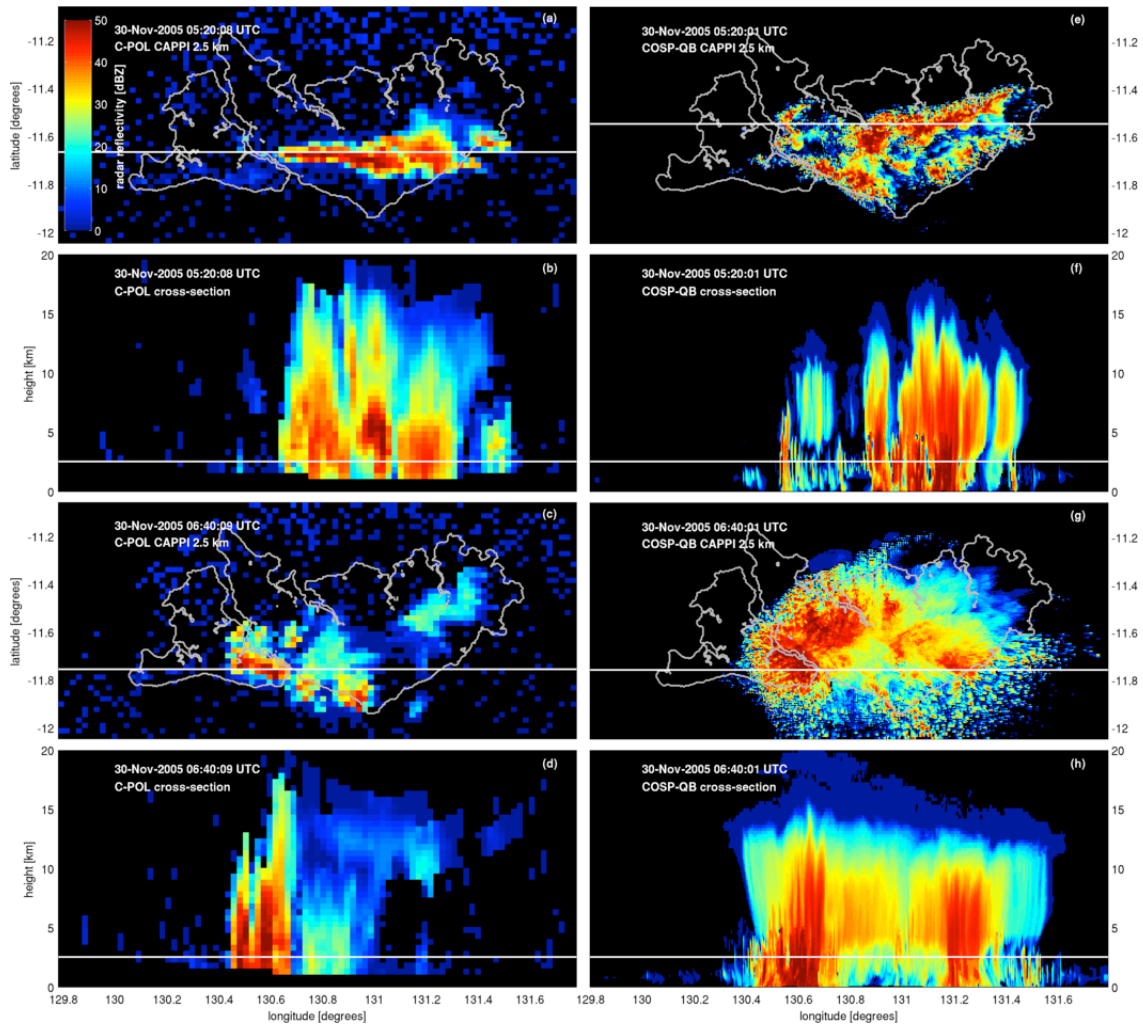


Fig 24 (a)-(d) C-POL measured attenuation-corrected rain radar reflectivities at the 2.5 km CAPPI (horizontal cross-section) at (a) 14:50 LT (05:20 UTC) and (c) 16:10 LT (06:40 UTC), corresponding to the timings in Fig 14/Fig 15 and Fig 16, respectively. The white lines mark the latitude at which the longitude-height cross-sections in (b) and (d) are shown, where the white lines in turn mark the height of the 2.5 CAPPI; (e)-(h) same as above, but for ATHAM data processed with the COSP-QuickBeam radar simulator to produce reflectivities. Simulated values below -40 dBZ have been discarded to remove homogeneous low reflectivity above 15 km. The zonal cross-section in the simulated field is 0.12° (10-15 km) further north than the one taken through the observed field.

In a more quantitative approach, the data have been compared using a Statistical Coverage Product (Fig 25). In spite of limitations to simulating reflectivities from model data, the statistical coverage product is best interpreted in terms of these. The comparison of hydrometeor classes strongly depends on the classification algorithm applied to the measured data, as well as on the reclassification of these to match fewer simulated hydrometeor species. Worse, delimiting fractional areas covered by simulated rain and graupel depends on the chosen specific concentration thresholds, which in the best case should emulate the criteria used in the classification algorithms for measured data, possibly in combination with simulated reflectivity values. In this respect, the excellent agreement between observations and simulation (Fig 25, last two rows) is strongly linked to our choice of a specific concentration threshold of 0.5 gkg^{-1} ; certainly a realistic value,

but chosen arbitrarily to give a best match. Setting this value to either 0.1 or 1 gkg^{-1} strongly reduces the agreement.

Statistical coverage products based on reflectivities (Fig 25, first five rows) imply that the model captures the timing of the convective cycle rather well, although with some delay and with an initial transition to deep convection between 12:30 and 14:00 LT that seems to be slightly more gradual than is observed. This is possibly linked to different triggering mechanisms. Observations do not show a noteworthy initial shallow convection field (Fig 25(a)), possibly because there was less cloud coverage (which agrees with visual inspection of the high-resolution visible MODIS data), but possibly also because these cumuli are too small and low to be captured by the radar beam. The maximum reflectivity anywhere in the area (Fig 25, fifth row) serves as a proxy for convective intensity (May and Lane (2009)). There seems to be a good match in range of values, but reflectivity is a function of the Drop Size Distribution (DSD) skewed towards larger particles. Missing effective radius variability in a one-moment microphysics scheme is certainly reflected in the simulated homogeneous time-height areas. There seems to be more intermittence of convective activity in the observations, particularly around 16:00, possibly suggesting separate Hector events. The same plots again confirm a higher maximum cloud top height in observations compared to the simulation. Conversely, the simulated domain has consistently more intense activity higher up, which hints at a larger area where intense cold microphysics governs convection. Large 10 dBZ fractional areas aloft (Fig 25, first row) are a proxy for the anvil. The detected anvil is fairly low in the radar data compared to *in situ* observations, and even lower than in the simulation, possibly because of smaller ice crystal radii (that are below the detection limit) aloft or because of the viewing geometry. The simulation has much larger mid- to upper-tropospheric fractional areas covered with hydrometeors producing medium to large reflectivities (Fig 25(b), (d), (f) and (h)). This is consistent with the generally much larger cloud areas simulated during the mature phase of the Hector storm (Fig 24(g) and (h)), and in part related to the absence of ice sedimentation in the model. The 40 dBZ fractional areas (Fig 25, fourth row) represent convective core areas, which are also significantly larger and reach higher levels in the simulations. Like in May and Lane (2009), anvil production follows the maximum in convective activity.

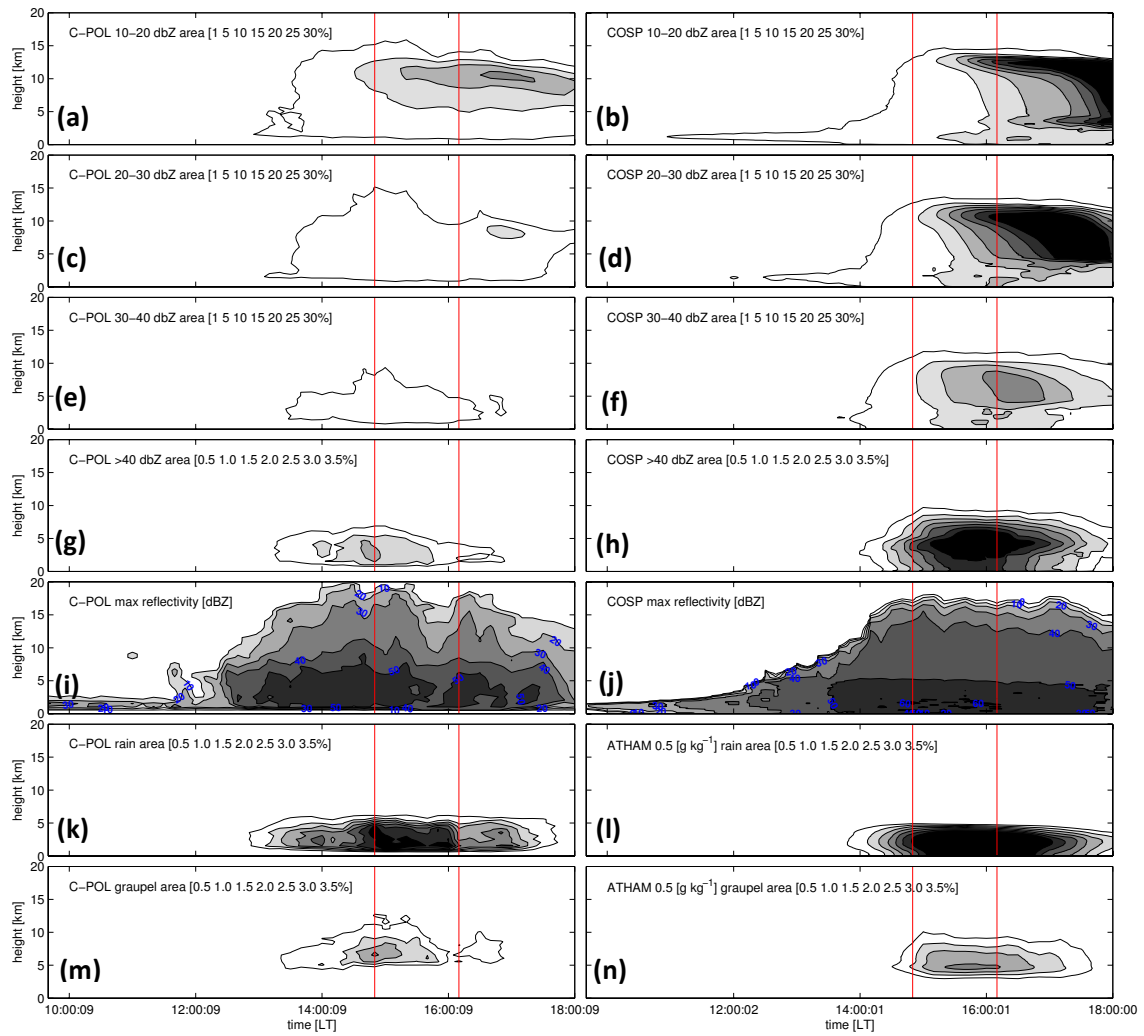


Fig 25 Statistical Coverage Product as described in May and Lane (2009), for C-POL measured and classified data (left column) and for ATHAM data processed with the COSP-QuickBeam radar simulator (right column, first 5 rows) or taken directly from model output (right column, last 2 rows). The fractional areas corresponding to the contour lines depicted in each figure are given between brackets. The vertical red lines mark the 14:50 and 16:10 LT at which the snapshots in Fig 24 are shown.

We can possibly attribute dissimilarities in the evolution between the simulated and actual storm to a predominant role of cold pool dynamics over sea breeze fronts in the simulation. Indeed, other model fields also hint at several strong radial density currents developing in the centre of the system depicted in Fig 24(e), with convective lines spreading radially outward. Our initial intercomparison with satellite data suggested a reasonably good match between the simulated storm and the actual event. The 4D data, however, possibly indicates that triggering and organization of deep convection may differ between the simulated and the real storm. Careful inspection of reflectivity snapshots indeed suggests stronger simulated storm cell regeneration due to forced ascent on extensive parts of cold pool gust fronts than can be gathered from radar observations or the storm documentation during the field campaign. The merger of multiple initial small density currents into one very large expanding cold pool will be illustrated in section 5.6 (see Fig 56). The following

analysis (section 5.4) from 2D sensitivity runs also confirms a possibly excessive cold pool density current, possibly linked to the coarse 500 m resolution. The surface forcing may be inadequate or outbalanced in our model, which could result in a misrepresented sea breeze. The evaluation of fluxes against field observations in section 5.6, however, suggests that at least bulk values seem appropriate. It is equally possible that the model's initialization, the absence of synoptic forcing, model dynamics and grid-spacing or other factors, including stochastic processes, are responsible for differences in the convective evolution.

In what follows, we will not further attempt to reproduce the actual Hector observed on 30th November 2005. We will rather explore the mechanisms behind the triggering and development of simulated convection and how surface fluxes, especially in various model configurations, may affect the latter, throughout the various phases of a full life cycle. In a first instance, we address these issues through a detailed analysis of the convective cycle and through a series of simulations run in 2D with different resolutions and model dynamics parameters.

5.4 From shallow boundary layer thermals to deep convective storm cells in 2D: insights and influence of diffusion and grid-spacing

Objectives, setup and simulations performed

We justified our initial choice of model dynamics parameters and grid-spacing purely on the basis of model behaviour in heavily idealized small-scale 2D reference simulations, similar studies found in the literature, and on the basis of *a priori* scales of turbulent eddies. To investigate the sensitivity of the simulated storm evolution on artificial momentum diffusion, expressed in terms of a momentum diffusion time scale ($\tau_{diff,mom}$, see equation (4.34)), and on grid-spacing, intimately linked to resolved turbulent mixing and subgrid-scale-induced turbulent diffusion, we performed a series of 2D simulations described in Table 6³¹. The sole difference in model configuration to the previous study is the use of a 2D domain, with possibly small differences in the interpolation of surface characteristics. We repeated the default 2D baseline run (tagged BL₀) with a second (longer runtime) simulation (tagged BL_r) to test the bit-wise reproducibility of an experiment. BL_r did not perfectly reproduce BL₀: if during the initial few hours of shallow convection, only very few grid-points presented relative differences

³¹ These runs were realized with source code at the same revision as that used for the previous 3D baseline simulation (ATHAM version 3.0), compiled with the same compiler and compilation flags, though executed on a different computing platform. The parallel version was used only for runs with refined grid-spacing.

in model fields larger than 0.1%, and these only for values near numeric 0, these differences grow exponentially to sizeable values with the development of deep convection, and explain the slightly diverging trajectory of integrated diagnostics in the following figures. The lack of reproducibility may have arisen because of a system upgrade; indeed, a later re-run of BL_r produced bit-wise identical output throughout the whole simulation.

For the particular case of the Hector storm occurring on 30th November 2005, 2D experiments should be reasonably well-suited to study the storm's behaviour, in spite of certain obvious shortcomings. As outlined in the previous sections, the storm system has been both observed and simulated to propagate mostly zonally, especially during the mature squall line-like phase in the late afternoon. When the dynamics in the third dimension are of lesser interest to those occurring in a vertical cross-section, the 2D slices may reveal deeper and more intuitive insights into relevant processes and interactions. Furthermore, a greater number of and significantly better-resolved simulations can be performed at affordable cost. Obviously, these advantages come hand-in-hand with potentially unrealistic convection and cloud dynamics, bulk diagnostics and timings, due to the negligence, mis- or underrepresentation of vertical and 3D vorticity and associated dynamics, of lateral turbulent entrainment along cylindrical cloud boundaries as well as of converging and diverging flows. Tiwi Islands are roughly elliptical and Hectors are often triggered (at least to some extent) by the latitudinal convergence of sea breezes along the minor axis; 2D longitudinal simulations are thus likely to initiate deep convection later than a 3D run. Also, the average shallow cumulus cloud cover is potentially higher in 2D than in 3D, significantly reducing the bulk radiative energy input to the surface.

Our aims are essentially threefold. First, we try to identify to what extent integrated diagnostics characterizing a major convective storm, some statistical properties of convective motions and cloud fields, as well as detailed features, remain robust across the various simulations. Second, we explore how relevant processes and local circulations, including turbulent eddies, are captured to various degrees of detail by these simulations, and how this may govern different trajectories of storm evolution. This includes a detailed analysis of surface-atmosphere interactions, particularly in terms of drivers and response, and some considerations about preferred location for deep convection triggering. Third, we would like to provide some food for thought regarding the complexity of deep convection dynamics in the context of parameterization development and some integrated energetics diagnostics for comparison.

We continue to concentrate our analysis of model output on data within a limited subdomain, to avoid artefacts arising close to lateral boundaries, and to exclude grid-points with excessive grid-stretching. As before, this subdomain is centred on Tiwi Islands

and covers a stretch of 2° in longitude, which includes well over 20 km of ocean grid-points on either side of the islands. Unless otherwise indicated, averages are computed without grid-box area weighting, which is a reasonable approximation over land masses and the nearby sea, where limited grid-stretching keeps the grid-box widths virtually constant.

Table 6 Experiment names and model parameters corresponding to 9 2D simulations run at different grid-spacing and with various degrees of additional momentum diffusion

	XP ID	n_x	n_{px}	$\Delta_{\min}$ (res) [m]	$\tau_{\text{diff},\text{mom}}$ [s]	$\tau_{\text{div},\text{damp},\text{high}}$ [s]
<i>r500mom0000div00</i>	xcontl_ms	422	1	500	- (0)	0
<i>r500mom0060div00</i>	xcontl_ns	422	1	500	60	0
<i>r500mom0300div00_BL0</i>	xcontl_os	422	1	500	300	0
<i>r500mom1800div00</i>	xcontl_ps	422	1	500	1800	0
<i>r500mom0300div60</i>	xcontl_qs	422	1	500	300	60
<i>r500mom0300div00_BLr</i>	xcontl_us	422	1	500	300	0
<i>r100mom0300div00</i>	xcontl_vp	2114	4	100	300	0
<i>r050mom0300div00</i>	xcontl_xp	4222	10	50	300	0
<i>r050mom0120div00</i>	xcontl_wp	4220	6	50	120	0

$\Delta_{\min}$, n_x , and n_{px} denote the lowest horizontal grid-spacing in the domain (constant over the islands), the number of grid-points and the number of processing cores in the x-direction, respectively. The momentum diffusion time scale $\tau_{\text{diff},\text{mom}}$ is defined in equation (4.34), $\tau_{\text{div},\text{damp},\text{high}}$ is the time scale for divergence damping acting exponentially with height and strongest towards the model top.

Integrated diagnostics

The most obvious integrated diagnostics that we can use to characterize the convective storm development, to estimate energy released and storm ‘intensity’, are total deposited precipitation (limited to the liquid phase only in our Hector studies) and an estimate of cloud top height, shown in Fig 26. From Fig 26(a) and (c), we stipulate that almost all the simulations were run beyond the storm’s mature phase into the onset of decay, assuming no further cells were triggered at significantly later times. Since BL₀ essentially follows the trajectory of BL_r, and given that the time scales for momentum diffusion ($\tau_{\text{diff},\text{mom}}$) and upper divergence damping ($\tau_{\text{div},\text{damp},\text{high}}$) in experiments *r500mom0060div00* (thin solid blue line) and *r500mom0300div60* (thin solid dark red line) hardly differ from those in the baseline, we will only discuss the latter where noteworthy deviations arise. The spatial distribution of rainfall (Fig 26(b)) is a first obvious exception, in as much as peak values of the simulation with additional upper divergence damping (*r500mom0300div60*) exceed the baseline by 50%. The location of peak rainfall in the simulation with slightly increased momentum diffusion (*r500mom0060div00*) is shifted westward by 15 km due to a delay in triggering. These significant differences for small changes of parameters and the much larger divergence of

the diagnostics across all our simulations allude to the potential difficulty in making accurate predictions of storm behaviour at very high resolutions, at least in 2D.

In general, the onset of precipitation occurs earlier in the higher-resolution runs (*r100mom0300div00*, *r050mom0300div00*, *r050mom0120div00*) and those with lower or no momentum diffusion (*r500mom1800div00*, *r500mom0000div00*), and is characterized by a more progressive increase over time (Fig 26(a)). For comparison, older studies (e.g. Petch, Brown, and Gray (2002) and references therein) also mostly document later (delayed) and more abrupt and stronger onset of precipitation at lower resolutions, which is in contrast to a more gradual transition to deep convection at coarser resolution in Khairoutdinov et al. (2009). The very-high-resolution baseline's (*r050mom0300div00*, thick dashed blue line, hereafter: r50) total accumulated rainfall follows the most intermittent trajectory, hinting at several separated intensive rainfall events as opposed to more continuous precipitation. Following grid-convergence arguments, we would have expected the simulation at intermediate resolution (*r100mom0300div00*, thin dashed black line, hereafter: r100) to lie in between BL_r and r50. Conversely, it evolves into a mature storm much earlier than both and decays rather quickly after only roughly half the accumulated precipitation of BL_r and 67% that of r50. Total accumulated precipitation varies by a factor of 6 between the highest and lowest simulated amounts. Additional momentum diffusion has opposite effects depending on resolution. Whilst at very high resolution (i.e. compared to r50), higher diffusion (*r050mom0120div00*) significantly hampers convective development, incidentally producing the least intensive convection of the series, at low resolution (i.e. compared to BL_r), lower or no diffusion produces a similarly dramatic abatement of convective precipitation.

The general pattern of spatial rainfall distribution (Fig 26(b)) follows the storm propagation discussed previously for the 3D baseline. With respect to the flow in the boundary layer, storms move westward upstream with newly generated cells on the upstream gust front. This results in a distribution that is typically skewed towards the location of initial triggering, with a long tail due to precipitation on the newly generated cells. As we will see later, r50 is the only simulation that has well reproduced two clearly distinct Hector storms. The early triggering and strong westward shift of the rainfall distribution from *r500mom1800div00* raises questions as to what triggered this event, given that sea breezes on the windward side (sea breeze in onshore flow) generally produce weaker sea breeze frontogenesis and are hence less likely to initiate deep convection, even if the direction of low-level wind shear may need further consideration in our study (see Moncrieff and Liu (1999)).

In this study, and for comparative purposes only, we have defined the maximum cloud top height on the basis of identifying the highest grid-point where cloud suspended

condensate exceeds an arbitrary specific concentration threshold of 0.01 gkg^{-1} (Fig 26(c)). This method should capture potential overshoots and gives a better feel for updraught strengths than comparing the height of main anvil outflow (Fig 26(d)). The latter should be similar to the neutral buoyancy height, and characterizes the average behaviour of the convective field in a more sensible manner; most simulations converge to a similar value. Given that the source region for all the buoyant plumes is the same, it is possible that less dilution due to decreased lateral entrainment maintained higher buoyancy and therefore produced higher neutral buoyancy heights in the lower-resolution runs. Comparing the initial progressive increase in accumulated precipitation from the higher-resolution runs with measures of cloud top height, it is clear that these simulations seem to capture a much broader transition period from shallow to deep, during which cumulus congestus clouds grow into precipitating cumulonimbi that precede the actual Hector storm. Their intermittency due to re-evaporation of the condensate is evident in the successive sharp drops of anvil neutral buoyancy height depicted in Fig 26(d). It is interesting that the simulation producing lowest rainfall (*r050mom0120div00*) has produced clouds that rapidly rise to levels higher than in the other high-resolution runs.

In terms of timings, the 2D simulations have an obvious lag roughly between 1.5 and 2.5 h with respect to the 3D baseline described previously (shown as a thick grey line in Fig 26(a)). This differs from Grabowski et al. (2006), who found a faster (or similar) transition from shallow to deep in 2D compared to 3D, with a more rapid increase in the surface precipitation rate. Since our 3D simulation was found to match the timing of the observations rather well, it is clear that triggering of the actual Hector storms is strongly delayed in 2D. Obviously, the 3D convergence pattern of the penetrating sea breezes, in particular in the narrower north-south axis of the island, is a likely candidate for an earlier triggering of deep convection. Surprisingly, the convective rainfall is also much less in 2D than in 3D. Note that during MCTEX, J. W. Wilson et al. (2001) observed a statistical time variation of only 2.5 h for the maximum extent of convection across the various events, and that within this set, there was no notable relationship between this timing and CAPE or maximum radar echo size. A weak correlation between morning CAPE or lowermost PBL q_v and maximum coverage size did exist; if 13:00 LT surface-layer q_v was taken as averaged over the island-interior only, this correlation was stronger. In Fig 26(b), we plotted the maximum value of deposited rain in latitude (y-direction) for each grid-point in longitude (x-direction) simulated with the 3D BL, for comparison to the 2D distributions (thick grey line). Even if compacting the 3D field by using maximum values necessarily results in an unrealistic distribution, the differences remain nonetheless striking. Peak accumulated rainfall reaches 115 mm in 3D compared to less than 42 mm (the maximum for *r500mom0060div00*) in 2D. The total accumulated rainwater amounts

to $1.33 \cdot 10^8 \text{ m}^3$ in the 3D BL. This exceeds the mean Hector rainfall production during the MCTEX campaign, estimated by Keenan et al. (2000) with considerable variability at about $7.6 \cdot 10^7 \text{ m}^3$, by 75%. In comparison, scaling up the 2D BL_r amount to a hypothetical convection width of 10 km produces only about $4.9 \cdot 10^6 \text{ m}^3$, i.e. over 10 times less.

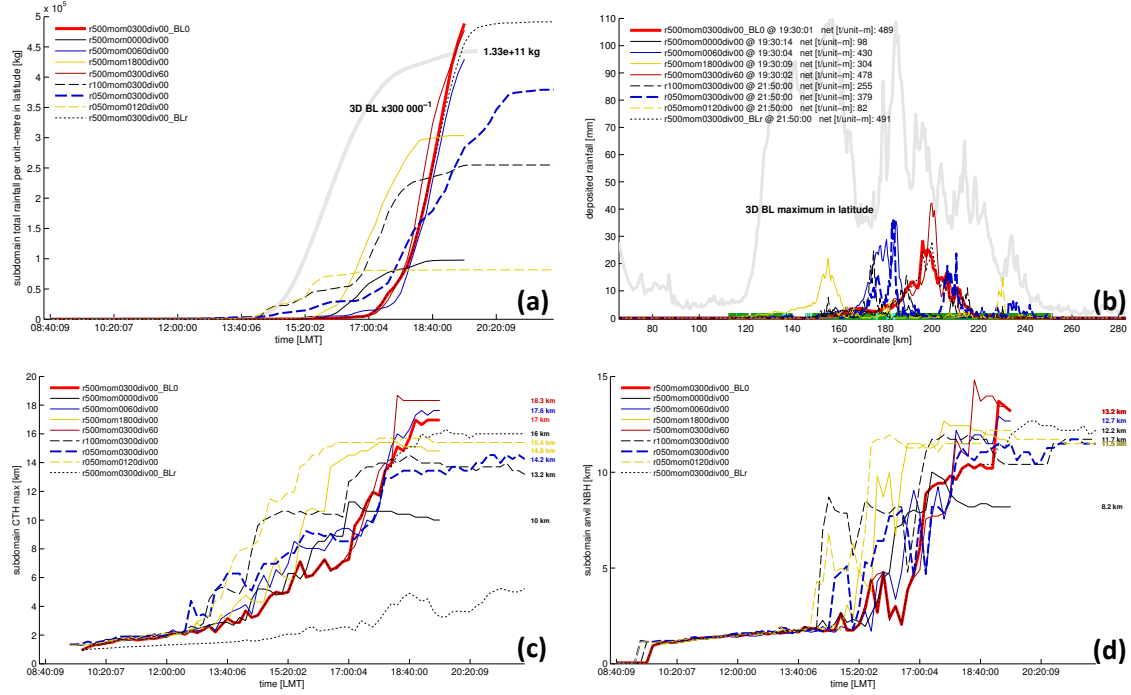


Fig 26 Time evolution and spatial distribution of the principal integrated model diagnostics for the simulations defined in Table 6. The thick red line corresponds to the 2D baseline simulation (BL₀) stopped at 19:30 LT, and performed with the same model configuration as the 3D baseline described in the previous section. The thin dotted grey line corresponds to a baseline re-run (BL_r) of BL₀, performed until 21:50 LT. Dashed lines correspond to simulations with finer grid-spacing than 500 m, the thick blue line is the very-high-resolution baseline equivalent (r50). The area-integrated total deposited rainfall in (a) has been calculated for a domain depth of a unit-metre. Also shown for comparison is the trajectory for the 3D baseline simulation, divided by a factor of 300'000 to fit within the axes (thick grey line); (b) spatial distribution of deposited rainfall at the end of each simulation. Island land areas are shown as a raised green line, with a slightly elevated profile to demark topography. Cyan land areas demark wetlands, water bodies correspond to the sea, the Apsley Strait and river cross-sections. The integrated total amount in tons or m³ per unit-metre is given in the legend; (c) trajectory of the domain-maximum Cloud Top Height identified as the highest grid-box with a suspended condensate (cloud drops or ice crystals) specific concentration larger than an arbitrary 0.01 gkg⁻¹. The lowermost thin grey line traces the subdomain-mean BL_r Cloud Base Height; (d) average cloud top height approximating the anvil's Neutral Buoyancy Height (NBH), calculated as the height of the grid-box with largest suspended condensate specific concentration from a subdomain-averaged profile.

To put the previous findings into a more insightful qualitative depiction of convective overturning, we have plotted the vertical redistribution of a boundary layer passive tracer towards the end of the simulations (Fig 27). All snapshots are taken at a time when the storms start to decay and the accumulated precipitation in Fig 26(a) is levelling off; r50 is therefore shown at a later point in time but at a similar stage in

convective development. Both *r500mom0300div60* and *r500mom0060div00* have a similar structure as BL_r (not shown). In a first instance, it is tempting to attribute the ‘strength’ of deep convection to that of the cold pool, since tracer concentrations aloft seem to be most abundant where a clear cold pool connected to the mid-troposphere is visible (Fig 27(a), (b) and (e)). Run r50 has 2 distinct albeit connected anvils and the remnants of a decaying cold pool under the decaying anvil around 250-260 km. Run r100 similarly seems to have several distinct weak cold pools. Cold pool gust front lifting is well pronounced in BL_r, in r50, and to some extent in r100. In Fig 27(b), the spread of the density current covers almost the entire subdomain, probably since it has been generated at an earlier stage. Convective overshoots are not clearly visible, suggesting much weaker convective intensity as compared to the 3D BL. The tracer is less diluted in the higher-resolution boundary layer as it is in that of the default 500 m runs. Overall, these snapshots seem to indicate that the cold pool plays a particularly important role in the evolution of the storm, which is, of course, not surprising, given the abundant literature on the topic. Note, also, that KR06 attributed the actual transition between shallow and deep convection to cold pool effects, albeit over a homogeneous land area.

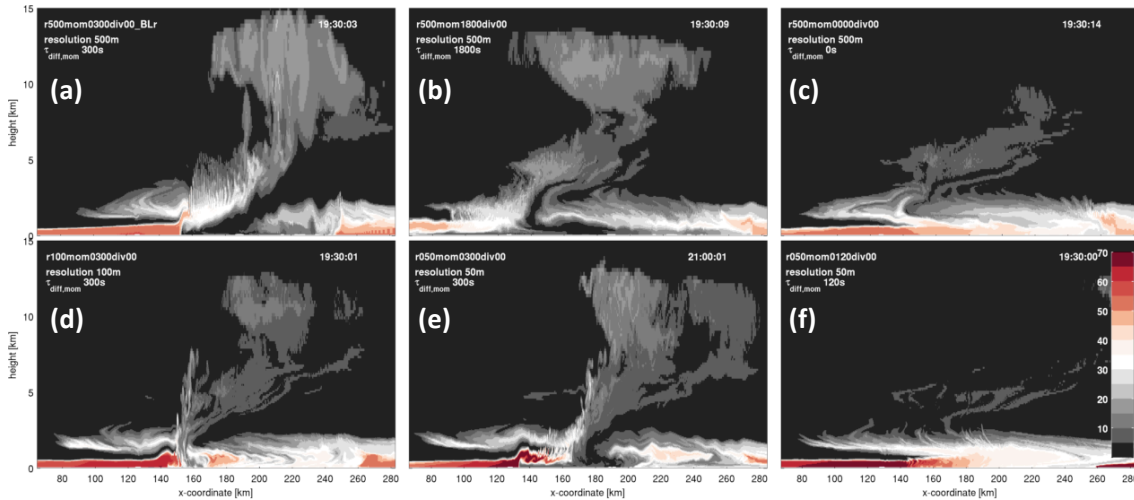


Fig 27 Snapshots of the spatial distribution of a boundary layer passive tracer (at concentrations between 0% (black) and 70% (dark red)), taken for the 6 most distinctive simulations at 19:30 LT. Higher-resolution runs are in the bottom row. Since *r050mom0300div00* was still in a mature phase at 19:30 (see Fig 26(a)), a snapshot at 21:00 is displayed instead.

Given the interactive coupling between surface layer atmospheric properties and the lower boundary, we expect a strong response of the surface physics to the cold pool density current, due to changing dynamics and thermodynamics, besides the more obvious radiative coupling through cloud shading. Conversely, modified surface fluxes may exert a potentially strong feedback on convection-driven atmospheric dynamics. To investigate the net variation in surface fluxes to the combined effects of a different surface

layer meteorology across the various simulations, as well as to a varying degree of turbulence captured by the model with increasing resolution, we plot the subdomain-averaged sensible and latent heat fluxes as a function of time in Fig 28, separately for land areas and water bodies.

Over land areas, modelled by HYBRID, both sensible and latent heat fluxes remain essentially invariant across the various simulations during the initial morning phase of clear sky and dry shallow convection. The average fluxes in 2D also match those of the 3D BL, displayed as the thick grey line for comparison. However, all the 2D runs are faster at generating shallow cumulus cloud than the 3D run, producing a growing cloud cover from 10:00 LT onwards. It is not surprising that fractional cloud cover due to dispersed cumulus elements is larger in a 2D than in a 3D environment, and the average sensible heat (f_h) released peaks at roughly 50-60 Wm^{-2} less in 2D due to reduced solar shortwave input. It is possible that this average difference contributed to faster erosion of the boundary layer inversion and faster triggering of Hector in the 3D BL. The effect of the impressive anvil generated in the 3D simulation results in strongly reduced and decaying heat fluxes in the early to mid-afternoon. Less dramatically, higher-resolution 2D runs also produce less of an average shallow cloud cover than their 500 m counterparts, because of larger cloud-free gaps between individual cumulus elements (see following figures). This is reflected in generally slightly higher sensible heat fluxes from 10:20 LT onwards; lower fluxes earlier on are due to an earlier onset of cloud formation. In the early and mid-afternoon, the higher-resolution simulation fluxes regress to lower values, due to a pronounced progressive transition phase to deep convection, as seen in the rising cloud cover and earlier drop in incoming shortwave radiation in Fig 29. The picture is not much different for the averaged latent heat (f_e) fluxes (Fig 28(b)); however, it is surprising that the divergence between the 2D and 3D average flux at 10:00 LT does not exist. We hypothesize that evapotranspiration in the late morning hours reaches a saturation level which is rather dependent on prevailing atmospheric humidity and soil moisture (or heat) conditions, as well as on biophysical processes, than on incoming shortwave radiation.

Over water bodies, where surface fluxes are modelled by COARE, f_h is low, virtually constant over time, (since SST is fixed, and diurnal warm layer processes are switched off), and hardly different across the various experiments (Fig 28(c)). The sharp rise in fluxes is provoked by the passage of the cold pool density current, arriving earliest in the 3D run, followed by *r500mom1800div00*, (which is triggered closest to the western coastline), then BL_r and last *r50*. The *r100* simulation does not produce a noticeable cold pool current that sweeps over the ocean. The situation is slightly more revealing for sea surface evaporation (Fig 28(d)), since fluxes are spread over a wider scale. Here, up to about 40 Wm^{-2} of a difference exists for f_e across the various experiments. Most noticeably, f_e

decreases over time for the run with highest momentum diffusion (*r500mom0060div00*) with respect to the other simulations, whilst it increases over time for higher-resolution runs. These variations are predominantly due to similar changes in the surface layer wind field (not shown), driving the fluxes.

It thus seems that averaged over a large domain, land surface fluxes respond predominantly and fastest to the shortwave radiative energy input, whilst sea surface fluxes, due to the much larger thermal inertia (modelled here through a largely invariant SST), are much more sensitive to the surface layer meteorology.

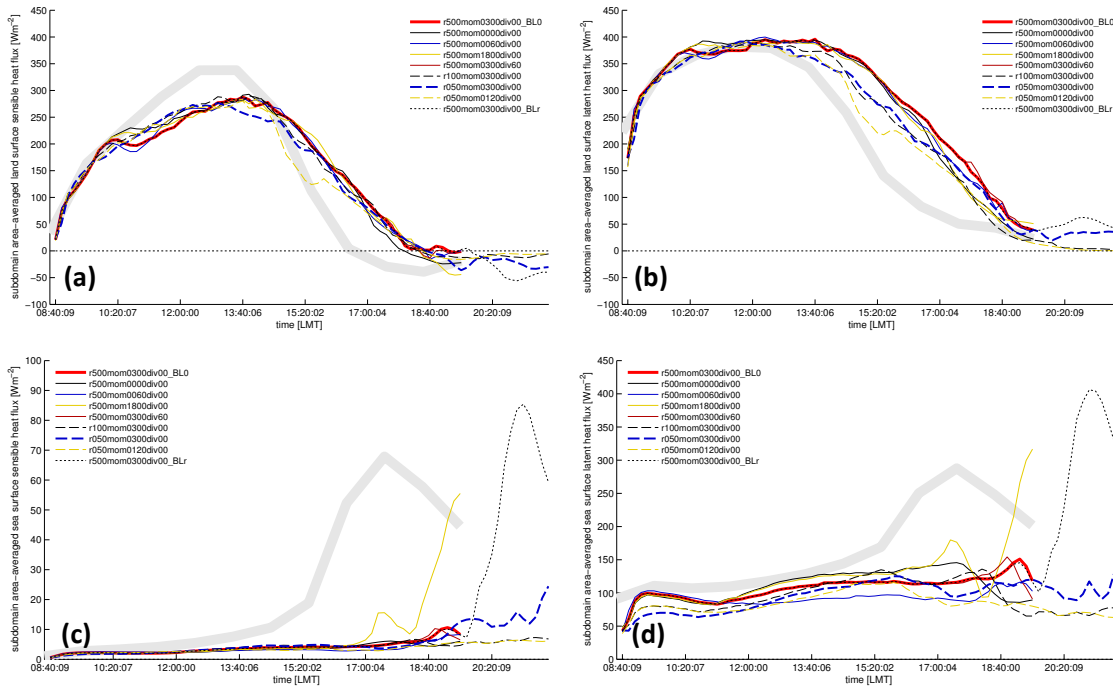


Fig 28 Subdomain area-weighted averages of sensible heat (first column) and latent heat (second column) fluxes over land (first row) and over sea (second row). The thick grey lines show the fluxes averaged over the 3D baseline simulation (not area-weighted and averaged over the whole simulation domain).

In order to get a more synthetic view of the evolving cloud fields and the triggering of deep convection, we have plotted Hovmöller diagrams of the condensed/cloud water path, including cloud droplets, ice crystals, rain drops and graupel, for the 6 most characteristic runs (Fig 29). Adjacent to each diagram, we have plotted fractional cloud cover (*cc*) over land areas and subdomain average total shortwave incoming radiation (R_s). Also, the onset of ‘significant’ precipitation (‘drizzle’ DRZ) and peak rainfall intensity (PRI) reaching the ground-level have been identified, following the method described in the figure caption.

Several common characteristics are straightforward. First, cloud formation is limited to land areas where sufficient sensible heat is released to drive the thermal updraughts that produce the first shallow cumulus clouds. The Apsley Strait separating

Bathurst and Melville islands (around 140 km) starts out cloud-free, and even remains that way in the higher-resolution simulations, in spite of advection. Second, fractional shallow cloud cover in the 500m runs quickly reaches a value of 0.5, characteristic of the single grid-point convection that we will discuss further at a later stage. The better resolved field is much more realistic here: single cloud elements are interspersed by a wider cloud-free gap in which air subsides; they also produce surface rainfall much earlier, using ‘drizzle’ (DRZ) as an indicator. Third, the intermediary transition phase between shallow and deep convection, already alluded to before, is clearly different between lower- and higher-resolution runs. Whilst in the former, cloud cover drops again from the 50% after an initial shallow convective phase before the final rise related to extensive anvil coverage, cloud cover in the latter consistently rises and produces successively deeper cloud cells, obvious from the increasing values of the condensed water path. This gradually rising cloud cover also results in a gradual decrease of R_s . The higher-resolution runs also produce seemingly stronger downstream-moving sea breeze convergence and deeper convection over Bathurst. By the time the Hector storms are triggered in most simulations, a lot of the shallow clouds will have evaporated (and pre-moistened the atmosphere), making a small dip in cloud cover an almost consistent feature. Fourth, all deep convective systems propagate westward (upstream with respect to the boundary layer flow, downstream with respect to the lower free-tropospheric flow or steering-level wind, defined as the average wind between 2 and 4 km and used as a surrogate for cell speed in J. W. Wilson et al. (2001)). This is clearly visible from the SSE-NNW³² tilted high-CWP lines; which initially trace the advection of cells reaching above the PBL. Where convection is deep enough, a clear anvil emanates from these lines, advected eastward in the upper-tropospheric westerly flow. The westward propagation speed is greatly amplified after the generation of a significantly strong cold pool density current, a feature that consistently appears as a strong line bounding the storm towards the West. The cold pool is most prominent in BL_r (Fig 29(a)), where the increasing slope indicates an increasing speed, or rather, a transition from advection to density current regeneration, eventually reaching an asymptotic value. The same current also clearly runs out the parent storm, with gradually less intensive cells triggered on its front. The typical westward propagation can be qualitatively compared to the composite Hovmöller plot in J. W. Wilson et al. (2001) (their Fig 4(a)); though note that they use radar reflectivity data at a low level to track cell propagation and produce their plots from 3D observations. Also, our synoptic (i.e. domain-averaged) wind profile is nudged towards the early morning sounding, which constrains the system-induced and externally-forced evolution of the

³² We adopt geographical directions for convenience. Obviously, north and south have to be read as the end (top) and beginning (bottom) of the time dimension.

large-scale wind. They estimated system propagation speeds between 6.4 and 10.3 ms^{-1} for MCTEX, which are higher than those one can extract from our Fig 29 (except if considering the gust front propagation alone). Our simulated propagation speeds are not too far off the easterly steering flow around 3 km ($3\text{-}4 \text{ ms}^{-1}$, see Fig 41(a)), similar to squall lines that were observed to translate at a speed similar to the 700 hPa easterly jet (Keenan and Carbone (1992)).

The cold pool's divergent flow on the surface obviously produces a radially spreading density current, modified by the surface-layer wind; in 2D, it spreads in the 2 opposite directions, the westward one upstream, the eastward one downstream. This forking out is difficult to discern in the simulations, since cells (if) generated on the downstream-moving current are likely covered by the spreading anvil generated by an event deep enough to produce the cold pool in the first place. Regeneration of new cells due to density current frontogenesis is potentially preferred on the upstream-moving current because of two reasons: more pronounced forced ascent on steeper fronts (though wind shear need also be considered, see Moncrieff and Liu (1999)), or potentially larger buoyancy of air parcels where sensible heat fluxes are stronger due to less anvil shading.

The branching out that is visible (e.g. in Fig 29(c) and (d) around $16:00 \text{ LT}$) is rather due to advection. Boundary layer winds are westerlies; this can easily be seen in the higher-resolution runs as SW-NE moving lines in the shallow cloud fields. Whilst moving eastward, these small cumuli are constantly evaporating and regenerating, moistening the inversion layer. At later times, lines in the opposite direction start to appear, especially for clouds with condensed water paths above several hundreds or thousands of gm^{-2} . These correspond to the first deep convective clouds that manage to break through the inversion layer and get transported westward by the easterlies in the lower free-troposphere (roughly between $2\text{-}4 \text{ km}$). When their updraughts are strong enough, they inject cloud content into the middle troposphere (around 8 km). Here westerlies advect the decaying ice cloud eastward again, explaining the lines of similar direction than the shallow boundary layer clouds. The most vigorous storms emerge out of these lines in the plots, raising the possibility that they develop predominantly in areas where the entire mid-troposphere has been previously pre-moistened, decreasing lateral dry air entrainment. That a (lower) free-troposphere with higher humidity should in general favour the development of deep convection has been shown in a convincing way through several CRM studies, e.g. in terms of integrated convective activity measured by surface precipitation and cloudy mass flux (Derbyshire et al. (2004)), in terms of earlier transition times to deep convection (C.-M. Wu, Stevens, and Arakawa (2009)), or through inspection of a succession of thermals (Kirshbaum (2011)). A positive feedback between convection and lower free-tropospheric moisture has also been emphasized by Tompkins

(2001a) for larger scales (1000 km), suggesting that it may contribute to convective organization and clustering. Tompkins (2001a) highlighted the supposedly dominant influence of dry lower free-tropospheric air on convection mediated through downdraughts, noting that the coarse grid-spacing (2 km) of his model might severely underestimate the effects on buoyancy related to entrainment. The previous studies looked into averaged environmental profiles, rather than into local effects (though clustering is, in essence, a local effect on a larger scale).

The cold pool density current manifests itself in terms of a ‘gradient-change’ in the SE-NW lines and emanates only when deep convection reaches highest condensed water paths, up to and above 10 kgm⁻². In the higher-resolution runs (Fig 29(b) and (d)), the corresponding timing coincides roughly with the peak rainfall intensity. In the 500 m runs producing significant deep convection (Fig 29(a) and (c)), peak rainfall intensity occurs later, potentially indicating that the cold pool density current actively regenerates, propagates and invigorates the parent storm, before outrunning it. We have described this squall line behaviour for the 500 m runs before, and it might explain why BL_r produces more accumulated rainfall than the other simulations. Squall line propagation is not evident in the higher-resolution runs, even if the cold pool gust front also contributes to the triggering of the second Hector storm in r50. None of the simulations generates convective clouds over the ocean until a gust front induces sufficient lifting. This agrees with findings in Khairoutdinov et al. (2009), where an artificial reduction of cold pools led to a significant reduction of low clouds over the ocean, especially given that convective inhibition is larger in our simulations.

The role of sea breeze current frontogenesis is difficult to discern. Convergence of the cloud field over time is clearly due to penetrating sea breezes, even if the sea breeze remains difficult to identify clearly and at all times in the simulations. In particular, the downstream-moving sea breeze on the windward (western) side of the islands is less clearly defined because of weak gradients in humidity, potential temperature and density fields. The upstream-moving sea breeze on the leeward (eastern) side of the islands conversely only slowly penetrates inland, if at all, and does so only in the lower-resolution runs (both for 500 m and 100 m grid-spacing). The single Hector storm in BL_r (Fig 29(a)) has most likely been initiated on the leeward sea breeze front, before propagating and intensifying on its own cold pool density current. The single Hector in *r500mom1800div00* (Fig 29(c)) has possibly been initiated on the windward sea breeze front, though the front location remains difficult to identify. Since many of the west-most deep convective lines emanate from a location close to 180 km around 14:00 LT in the 50 m runs (Fig 29(d) and (f)) and slightly later in the 500 m runs (Fig 29(a), (c) and (e)), this strengthens the

hypothesis of sea breeze front-generated initiation, assuming the sea breeze penetrates inland at a consistent speed across all simulations. Another hypothesis is presented later.

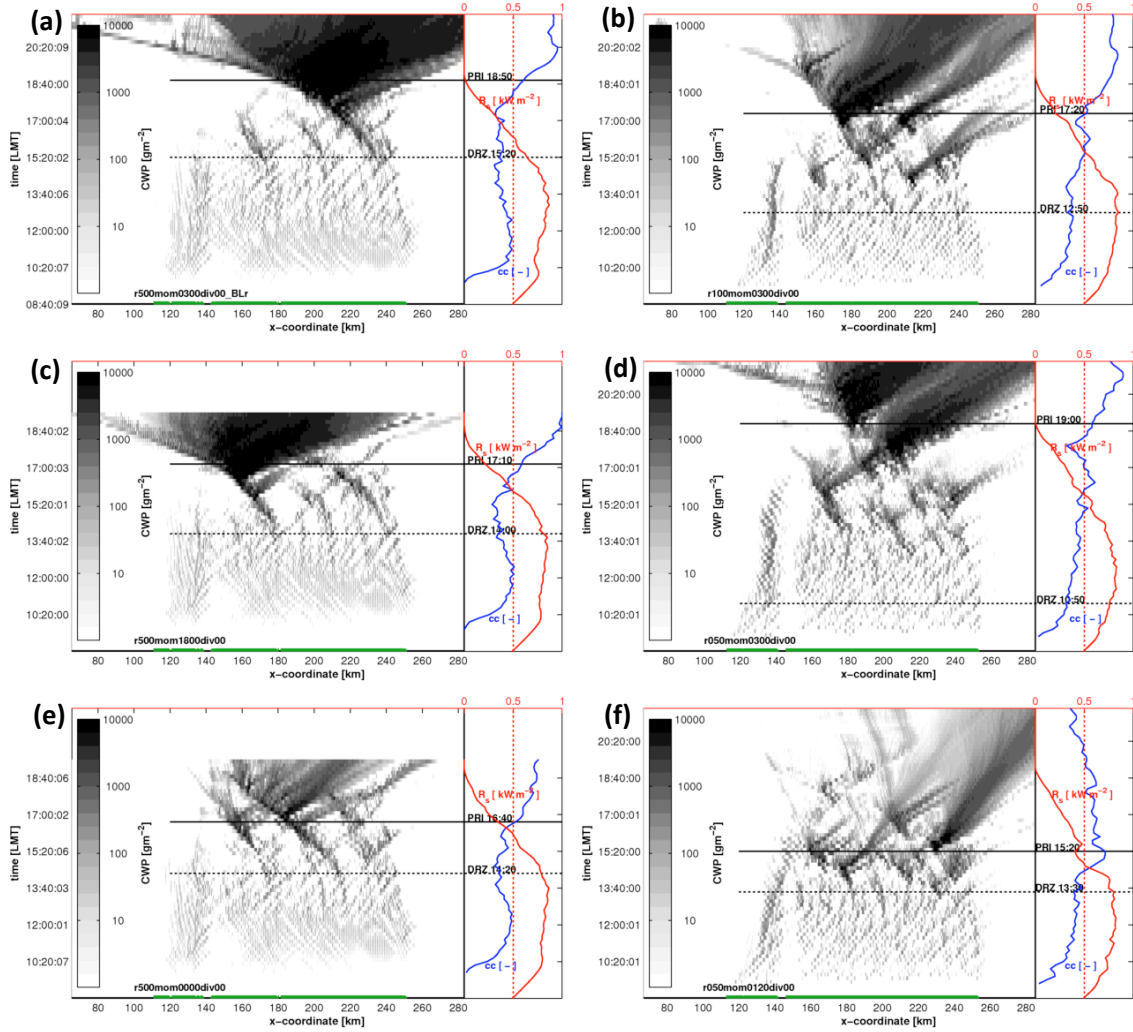


Fig 29 Cloud field Hovmöller plots corresponding to the same simulations as depicted in Fig 27 (transposed panel arrangement). The masked cloud condensed water path ($CWP = LWP + IWP$) is shown on a log-scale. The subdomain area-weighted average of total shortwave radiation reaching the land surface R_s is depicted as a red line. The land cloud cover (cc , blue line) is an area-weighted average over grid-columns for which a maximum cloud top height (as in Fig 26(c)) is defined (i.e. at least one grid-box is cloudy). The onset of subdomain-averaged 'significant' initial rainfall ('drizzle' DRZ) and the peak rainfall intensity (PRI) are determined from the rain rates [mmh^{-1}] derived from Fig 26(a). The peak rainfall intensity is straightforward; the DRZ timing is determined arbitrarily as the first peak above a certain threshold and within a 1h timeframe.

Shallow convection and updraught core statistics

The snapshots of potential temperature θ and of anomalies with respect to the initial conditions and a spatially-averaged profile, shown in Fig 30, provide a qualitative insight into the early phase of shallow convection, as captured by the model at different resolutions. Potential temperature at 11:00 LT in Fig 30(a) and (b) visualizes the fine structure in turbulent overturning and the upstream-moving sea breeze front around 252 km. The regular grid-point structure of up- and downdraughts is clearly visible in the BL_r

θ -field. All updraughts in Fig 30(a) are topped by cumulus clouds, except within a narrow coastal strip 5 km wide. This is reflected in the surface fluxes below, typically of the order of 100-200 Wm⁻² less at the base of each updraught due to shading. Run r50 has a much more ‘realistic’ field of irregular thermals, characterized by varying sizes, strengths and levels of maturity (Fig 30(b)). Due to a wind profile increasing with height to roughly 700 m before it decreases again, some of the thermals bulge over, but surprisingly, most remain essentially straight. A clear pattern between thermals and surface fluxes cannot easily be distinguished.

In spite of obvious differences in levels of detail and resolved circulations, the early convective PBL evolution is surprisingly similar between runs at 500 m and 50 m horizontal grid-spacing. Fig 30(c) and (d) display the θ -anomaly with respect to the initial conditions as well as subdomain-averaged profiles representing initial conditions and averages over land and sea at 11:00 LT. The averaged profile over the sea remains virtually the same as the initial conditions, with even a slight decrease of the surface-layer (potential) temperature. The heating of the PBL below the inversion layer (up to 700-800m) is comparable at both grid-spacing, as can be appreciated from the lighter shading in both snapshots and the averaged profile. Some individual thermals penetrate deeper into the inversion layer in r50, but the variability of penetration depths across the full spectrum of thermals is equally much higher. Thermals penetrating into the inversion layer entrain potentially cooler air into this stable stratification, thereby decreasing the temperature therein and destabilizing the layer. The erosion of the inversion is different between both runs. Whilst the lower-resolution simulation produces a deeper mixed-layer, it simultaneously strengthens the gradient in the compacted inversion above. This is the opposite in the higher-resolution run. Here, the strength of the inversion is hardly modified but the PBL has grown less deeply.

The distinct characteristics of the PBL thermals, cumulus clouds and inversion layer effects at different resolutions are shown in Fig 30(e) and (f), focusing on the narrow spatial band between the red dotted lines in the previous plots. Grid-point clouds in BL_r are not resolved, and are hardly penetrating into the inversion layer. They are separated by grid-point gaps. Larger areas of subsidence separate r50 clouds. As pointed out before, the lower cloud cover in high-resolution runs may increase total energy input at the surface, hence slightly increase sensible heat fluxes, which possibly contributes to earlier triggering. Well-resolved boundary layer clouds have a characteristic convex cloud base where they are fed by the underlying thermal and highest specific concentrations are concentrated around the cloud top. It seems that they are at least to some degree located over a positive θ -anomaly, generating the thermal updraught as expected. More relevant is the much more significant PBL entrainment heating due to the subsidence induced by

the large eddies driving the thermals, and the simultaneously stronger adiabatic cooling within thermals penetrating into the inversion layer. The negative in-cloud θ -anomalies come as a surprise. Nevertheless, from full ensembles of more idealized CRM experiments, C.-M. Wu, Stevens, and Arakawa (2009) found that in terms of mean virtual potential temperature profiles limited to cloudy grid-boxes, shallow clouds were on average thermodynamically colder than their environment, reflecting active entrainment and making them essentially stable. It makes sense that such entrainment and mixing is captured only at high enough a resolution. However, we might then expect the undiluted single grid-column updraughts in BL_r to trigger deep convection faster, which is not the case. The major negative θ -anomaly above the mature cloud in Fig 30(f) corresponds to the wake of another evaporated cloud now advected further downwind. The mature cloud itself is also decaying; cloud lifetime is typically of the order of 10-20 minutes. There is also some latent heat consumption due to sub-cloud evaporation of precipitation that only occurs in r50. Latent heat release and consumption due to cloud formation and re-evaporation are both slightly larger in magnitude and deeper throughout the capping layer in r50 as opposed to BL_r (not shown), but these processes tend to compensate. On average, therefore, most of these effects apparently cancel out spatially, which is why there seems to be no significantly higher entrainment warming in the r50 simulation compared to BL_r. On average, the specific humidity anomaly over land (green profile) is also similar, if bulged towards slightly larger heights in BL_r. The picture is very different if considering an individual cloud element alone (purple profile characterizing the cloud between the purple lines).

We can deal with the vertical convective motions in a statistically more relevant and quantitative sense by trying to compare some of their characteristics over the whole field. For this purpose, we have isolated updraught (downdraught) cores through masks bounding regions where the absolute vertical velocity exceeds the subdomain mean upward (downward) velocity plus twice its standard deviation. Mean and standard deviation have been computed as a function of time, and domain-wide oscillations in these quantities have been smoothed out by applying a half hour-wide (3 points in time) moving average. Thermal updraught core masks have been added to the first and last row of Fig 30 as black dotted and red solid contours, respectively. Updraughts above the PBL are visible in both simulations just near the shoreline; these are due to convergence of the offshore flow with the developing sea breeze. An alternative and more elaborate conditional sampling method such as that presented by Couvreux, Hourdin, and Rio (2009), using a (decaying) passive tracer, thermodynamic variables and w , is potentially worth exploring.

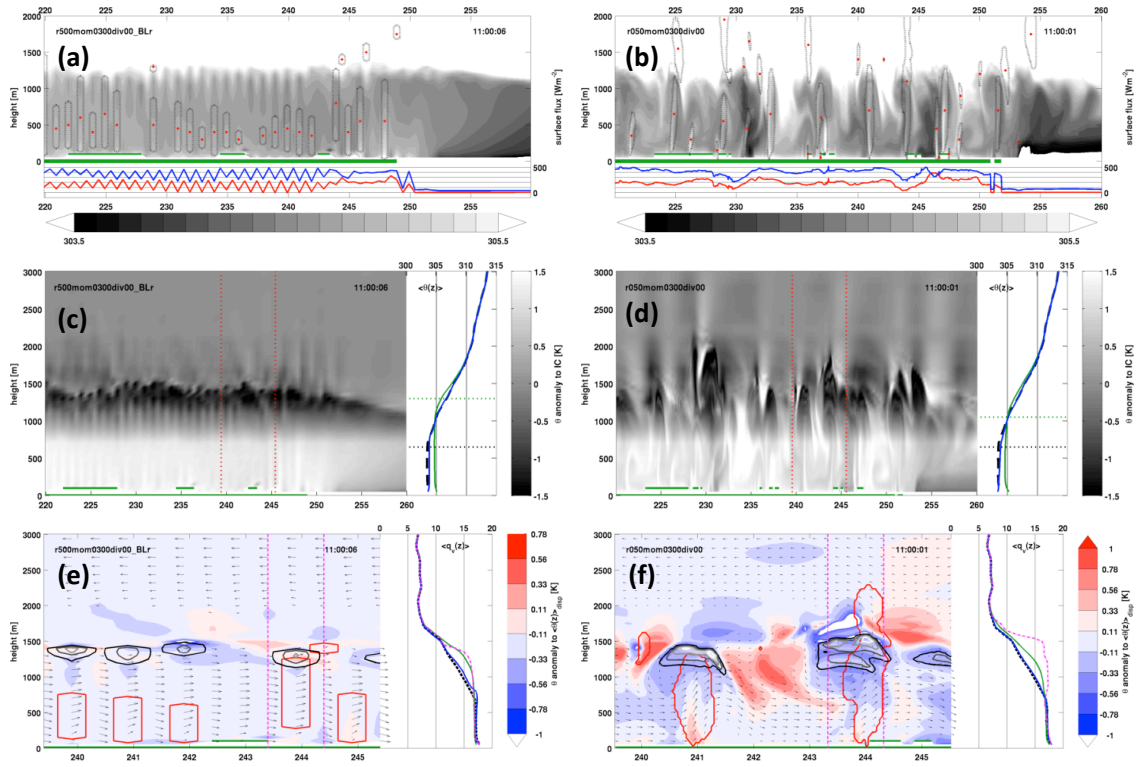
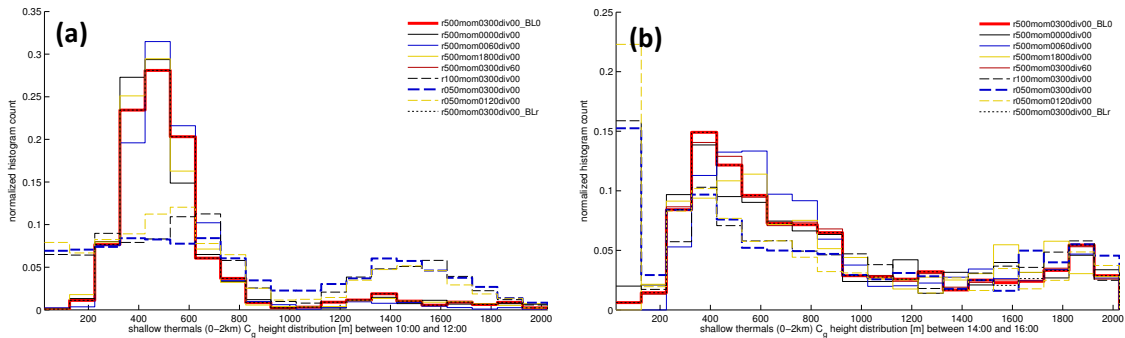


Fig 30 Shallow boundary layer convection at 11:00 LT near the eastern Melville coastline, at 500 m (first column) and 50 m (second column) horizontal grid-spacing. Land mask and topography are shown as green lines. A snapshot of the instantaneous potential temperature (θ [K]) is shown in the first row, together with surface sensible (f_h , red line) and latent (f_e , blue line) heat fluxes. Convective updraught cores (as defined in the text) are outlined by thin dotted grey lines, their centroids are indicated as red dots. The θ -anomaly with respect to the initial conditions is depicted in the second row. The thick dashed line is the initial θ profile; the green and blue lines represent subdomain-averaged profiles at 11:00 LT over land and sea surfaces, respectively. The bottom of the inversion layer z_i from the initial profile (black dotted line) and over land at 11:00 (green dotted line) is crudely estimated from the inflection point in the profile. The vertical red dotted lines delimit a focal region depicted as a θ -anomaly with respect to a spatially averaged profile over the same region and at the same time in the third row. Grey-shaded contour lines delimit cloud droplet specific concentrations at 0.1-1 gkg^{-1} . The same convective cores as in the first row are outlined with a thin red line. Arrows represent the flow field where local wind speed exceeds 1 ms^{-1} . Arrows are at different scales in the two plots. Specific humidity (q_v [gkg^{-1}]) profiles follow the preceding colour-coding. An additional profile (magenta) averages over a single cumulus cloud.

Next, we created individual objects out of the masked field based on contiguous pixels in a 4-connectivity framework (touching edges in 2D), using the Matlab® *regionprops* function. We have then computed statistical distributions of several properties of these convective core objects. No core area weighting has been applied. The vertical velocity-weighted core centroid heights have been added as red dots in the first row of Fig 30. Their distribution, limited to centroids within the lowest 2 km in altitude (i.e. shallow thermals), has been plotted for the initial shallow convection (Fig 31(a)) and the transition phase (Fig 31(b)). These distributions are not very different for simulations run at identical resolution; they differ nevertheless noticeably when changing grid-spacing. Typically, the centroids in the 500 m runs are initially mostly centred around the

mid-boundary layer height, where updraughts are strongest; few exist (or get picked up by the algorithm) within or above the inversion layer. At higher resolution, thermals at various stages of their evolution are well represented, and their centroid distribution within the PBL is pretty much even. As expected, few cores exist within the inversion layer itself, but there is a second mode between 1300 and 1600 m. This probably partially corresponds to oscillations within the inversion layer. Later in time, the initial peak at mid-PBL height for the 500 m runs weakens in favour of a flat distribution over the upper km. Note that deep convective cores have been excluded here, so this corresponds likely to first deep clouds growing through a weakened inversion. The higher-resolution runs follow a distribution that is not much different, apart from a second and highest mode in the surface layer. This corresponds to strong vertical velocities locked to the square profile topographic elements where they maintain continuity.

Core eccentricity (of the ellipse with same second-moments as the object), limited to the lowest 2 km for shallow convection including the transition phase (Fig 31(c)), and to all cores over the whole simulation excluding model spin-up (Fig 31(d)), is easier to interpret. The cluster around 0 is due to single grid-points, the one around 1 due to linear elements. What has been alluded to before is strikingly obvious in these plots: by far most updraught cores in the 500 m runs are (quasi-)linear in nature, predominantly because the largest number of objects correspond to the grid-point shallow updraughts. Refining grid-spacing shifts the distribution towards less elongated (and potentially more complex) shapes, more alike convective rising bubbles, which is likely to translate into different dynamics.



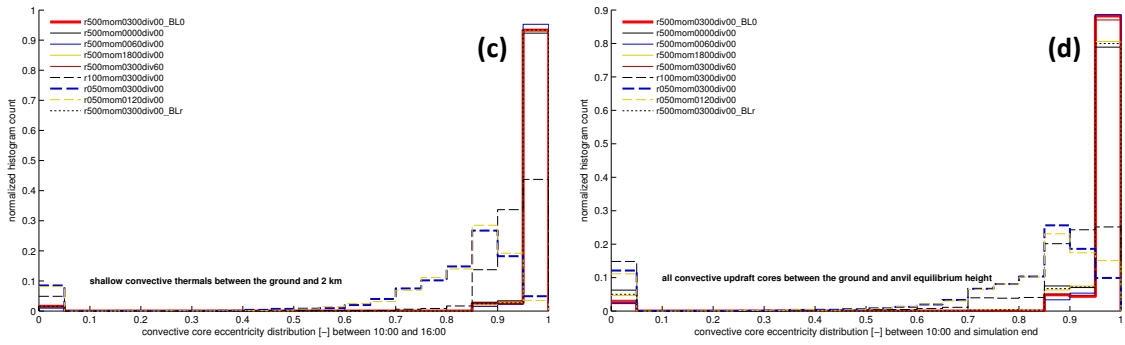


Fig 31 Statistical analysis of convective updraught cores: (a) centroid height distribution for shallow (below 2 km) thermals during initial non-precipitating convection, and (b) during the onset of deep convection triggering; (c) eccentricity distribution for all updraught cores during the shallow and transition phases and (d) over the whole simulation period, excluding spin-up time.

The number of updraught cores over time is given in Fig 32(a). After model spin-up, the number of cores is initially very similar for all the simulations; the larger spacing between thermals simulated at higher resolution is compensated for by a larger number at different heights. The strong drop in numbers at the onset of the Hector storms and during the transition phase are due to strong updraughts raising the mean and standard deviation of vertical velocity within the domain, such that the algorithm no longer picks up certain weaker objects from the previous model output. The slow decrease in the number of cores over time for the lower-resolution runs is consistent with the decrease in individual cumulus clouds described in Fig 29. Their number in high-resolution runs, more or less constant over time with a slight downward tendency, remains consistent with the more gradual transition towards deep convection. However, this decrease probably predominantly reflects the tendency of the updraughts to organize into fewer but stronger updraughts over the course of the day. The dramatic rise towards the end of the simulation occurs during the decay phase when the threshold for core selection is decreasing again. Also, besides the contribution of new cells triggered on the cold pool density current front, this significant increase may be partially explained by the inclusion of wave motions in the selection, particularly of those excited above the tropopause, as well as waves and turbulent eddies in the anvil.

We calculated the mean core updraught as a simple average over the vertical velocity field masked by the core outlines (Fig 32(b)). During the shallow phase, the mean core updraught velocity of r100 converges to that of the 50 m runs, and the cluster remains just about 1 ms^{-1} higher than the lower-resolution updraughts. The stronger updraughts in the higher-resolution runs, reaching velocities of around 2 ms^{-1} in the early afternoon, will be more efficient in breaking through the inversion layer. Mean core updraught velocity is obviously anti-correlated to the core number, with fewer cores of higher velocities. The existence of 2 different Hector storms is clearly visible for r50.

Mean updraught strength for the higher-resolutions runs during deep convection is much lower than that of the lower-resolution runs. Additional upper-divergence damping strongly boosts mean updraughts. The evolution of subdomain maximum updraughts (not shown) is similar to Fig 32(b), with considerably more variability. Early afternoon maximum velocities in the higher-resolution runs lie around 6 ms^{-1} , those in the 500 m run at slightly less than half this value. Maximum updraughts during the Hector storm are 27 ms^{-1} for BL_0 (21 ms^{-1} for BL_r), 22 ms^{-1} for r100, 20 ms^{-1} for r50 and largest for *r500mom0300div60* at 38 ms^{-1} . The picture is not much different for mean and maximum downdraught velocities (not shown), though the magnitudes and the relative difference between higher- and lower-resolution runs are lower. For the shallow convection phase, this is expected, as the cloud-free areas with compensating subsidence are larger when better resolved. Early afternoon mean downdraughts are around 1.3 and 1 ms^{-1} , for higher- and lower-resolution runs, respectively; maximum values are in the vicinity of 4 and 2 ms^{-1} . The noticeable difference is that maximum downdraughts at high-resolution actually are close to or exceed those at lower resolution, with peak values of 12 ms^{-1} for BL_0 (13 ms^{-1} for BL_r), 16 ms^{-1} for r100, 14 ms^{-1} for r50 and 18 ms^{-1} for *r500mom0300div60*.

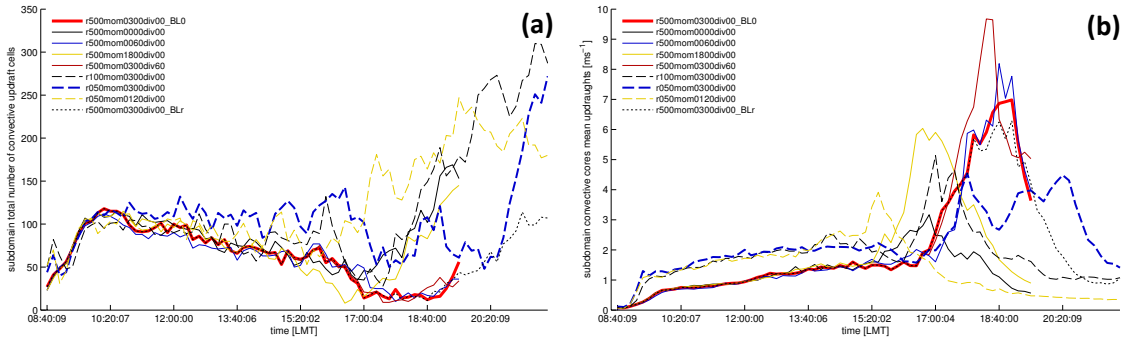


Fig 32 (a) time evolution of the subdomain total number of convective updraught cores; (b) mean updraught velocities within these cores.

Further to updraught core centroid and eccentricity distributions, we have plotted the median core width as a function of time and height, both in grid-point and in physical space and for the 3 different resolutions (Fig 33). The 3 simulations appear to have different convective growth rates: deep convection seems to develop exponentially in BL_r , almost instantaneously and in separate stages in r100, and linearly in r50, as is also apparent in Fig 26(c). Most of the shallow and transition phase cores in BL_r are represented by single grid-points or columns and only some of the later upper-level deep convective cores are resolved to a point where they can possibly capture internal circulations. Obviously, the finer the grid-spacing, the wider the updraughts in grid-point space (Fig 33, first column); to a point where most median cores in r50 are represented by 6-10 grid-points or more, enough to capture potential internal dynamics and circulations.

Median width in physical space (Fig 33, second column) suggests converging results between r100 and r50, whilst BL_r produces much wider updraughts, as expected from the limited resolution. The resulting mass flux in the BL_r shallow thermals is moderated by overall lower vertical velocities; during the deep convective phase, however, updraughts that are both wider and stronger end up in a strongly enhanced mass flux and convective overturning. Most convective cores simulated at high resolution do not exceed 1000 m in diameter, except in the mid-troposphere during a mature Hector³³. We can compare these results to probability density distributions (PDFs) of cloud size as a function of height from the 3D simulated fields at a horizontal grid-spacing of 100 m presented in KR06. Note that KR06 plot the mean rather than the median profiles, of clouds, rather than of convective cores, which we expect to be larger. The comparison fails especially for anvils, which are largest where cores in turn narrow down, as well as for large clouds with several embedded cores. More importantly, the statistics in KR06 refer to a distribution integrating to cloud fraction, whilst ours are over the core population. This means that, given the large amount of small-sized clouds/cores, our values will be systematically lower, especially for wide distributions. The PDFs in KR06 are rather narrow for the initial shallow field, and indeed their mean size estimate between 500 and 1000 m with a 1σ spread between 250 m and just above 1 km (their Fig 8(a)) compare well with the median values in our Fig 33(d). Obviously, our statistics, reduced here solely to a median value, cannot capture the size evolution of the largest clouds at cloud base, even if applying our method to that problem or in-cloud properties would be straightforward. Our core size is also in a very similar bulk range as simulated by Khairoutdinov et al. (2009) (their Fig 8(a)), even if their core selection follows different criteria and oceanic convection is generally less vigorous.

In BL_r, the height of the maximum updraught (red circles) consistently increases over time, with a few outliers around 10 km during the mature phase when strongest updraughts are roughly 2 km higher than in the higher-resolution runs. The higher-resolution runs are more intermittent, which may reflect successive convective bubbles rising over time and throughout the domain. The cluster of circles concentrated around the highest altitudes at the end of every simulation represents anvil dynamics and turbulence.

³³ Recall that these are median widths, the maximum core sizes are therefore potentially much larger.

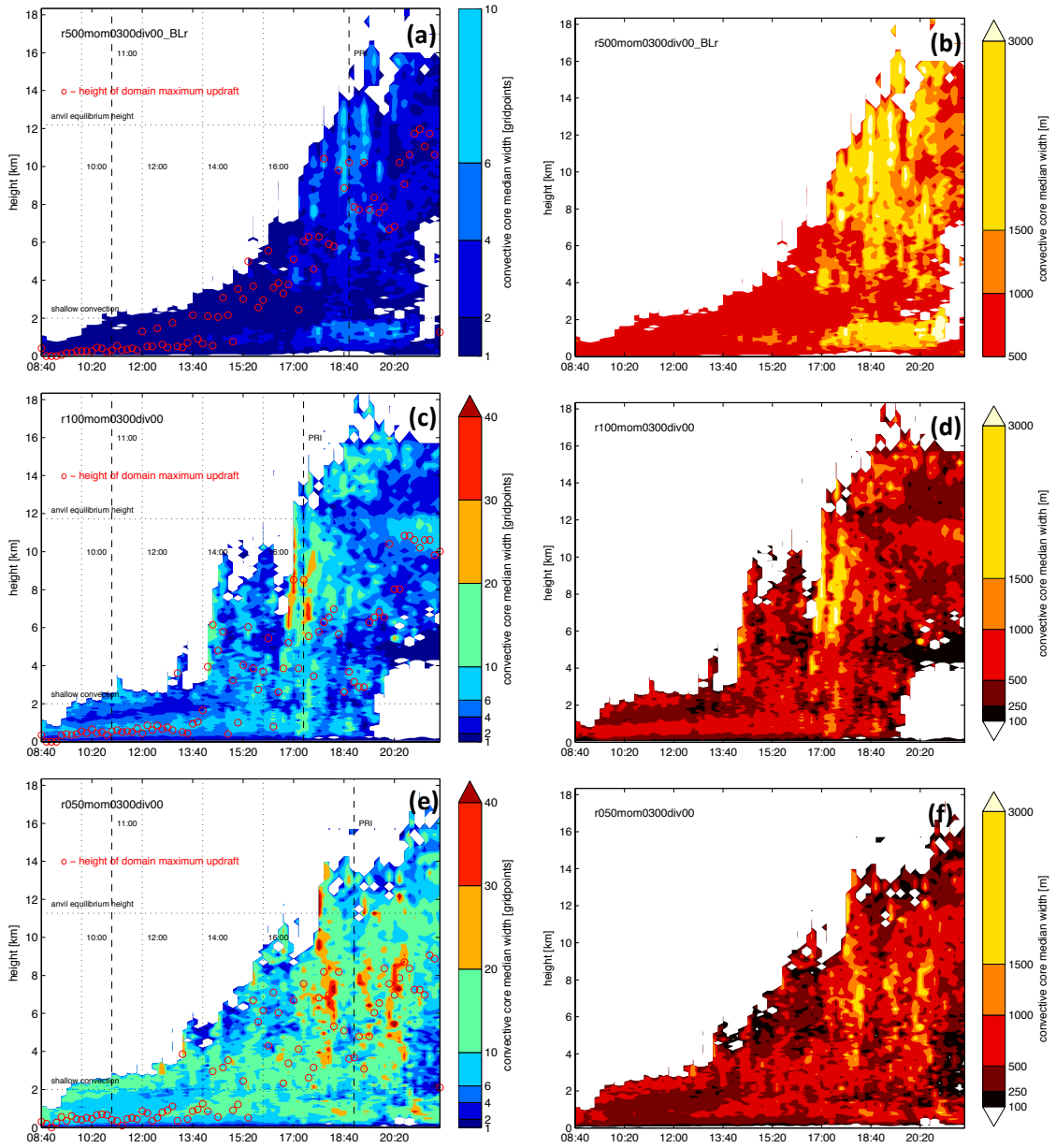


Fig 33 Time-height evolution of the subdomain-median width of convective updraught cores in grid-point space (first column) and in physical space (second column) for horizontal grid-spacing of 500 m (first row), 100 m (second row) and 50 m (third row). For comparison to Fig 29 and Fig 30, the 11:00 and peak rainfall intensity (PRI) times are emphasized; the arbitrary delimitation of shallow convection to 2 km and the space- and time-averaged anvil equilibrium height (as defined in Fig 26(d) for ice crystals only) are also indicated. The heights of the subdomain's grid-points with highest vertical velocity are given as red circles.

Deep convection and surface interactions

As for shallow convection, the previous results are easier to interpret in the light of a series of snapshots depicting the evolution of the storm system over time (Fig 34). The BL_r simulation only produced one single Hector storm, triggered around 17:00 and propagating westward. The outline of the cloud is given by the thin dotted grey line, representing faint precipitation at a specific concentration of 0.05 gkg⁻¹. The overall structure and dynamics of the storm are very much alike the squall line conceptual model (and referenced literature) described in (Houze (1994), chapter 9.2), in particular the

strong rear inflow entering the active convective region from the back. In our simulation, this inflow, an intensification of the prevailing lower free-tropospheric background wind, not only enhances convergence, but seems to provide a significant (if not the largest) proportion of mass flux ending up in the downdraught within the main convective precipitation area. This representative feature appears consistently in all our simulations and the ingested inflow enters at a level where precipitating downdraughts and core updraughts diverge. Equally, the conceptual model's general trend of upward motion from within the boundary layer near the gust front, stronger through the convective region and then more gently through the stratiform (or anvil) region, can be observed in the simulations. The upward trend in the convective region is stair-stepwise through the successive cores, as already described for the 3D baseline experiment. The streamlines visualized through the arrows seem to indicate an important return flow, from the rear inflow through the cold pool's density current within the lower boundary layer, up ahead towards the gust front, where the air masses converge with the boundary layer background wind, get lofted and seemingly re-ingested into the cloud system. This might suggest the possibility that a proportion of the air ending up aloft in the anvil may have originated in the lower free-troposphere behind the storm. This, however, seems to be a misconception, and all the rear inflow air masses remain within the density current, which would stagnate instead of propagating, were its air masses to be re-ingested into the cloud system. This is readily confirmed with snapshots of lower free-tropospheric passive tracers from various heights (only the 800-650 hPa tracer is shown), which reveal that the air originating in these layers and that gets entrained into new updraughts mostly comes from the up-storm side and is entrained laterally into the updraughts. Similarly, Y. Wang et al. (2003) had estimated from 2 km grid-spacing simulations of an oceanic squall line coupled to the COARE sea flux algorithm, that over 90% of the moisture taken up by the storm originated from surface fluxes within the clear air boundary layer ahead over the storm and its gust front, in spite of the fluxes being several times larger in the wake of the storm (presumably in its cold pool). We take note, nevertheless, of Tompkins (2001b)'s simulations over oceans, supporting the idea that within the gust front of a spreading cold pool density current resides a positive, albeit cold, moisture anomaly from the evaporation of initial rainfall penetrating into the subcloud layer. The author argues that these initially negatively buoyant air masses spawn new updraught cells once sufficiently warmed over a certain distance by surface fluxes, making the regeneration of cells thermodynamic, rather than dynamic, in nature. It is likely that the action of cold pools differs over land and ocean areas, where different surface responses and thermodynamic structures of the PBL prevail, and a larger sample of cold pools would be required to test his ideas over land in our simulations. The underlying idea that precipitating deep

convection regenerates (at least partially) its own moisture source for triggering new events on the gust front is similar to the one we initially considered, but then rejected for our own simulations.

Due to the very strong shear established by the rear inflow descending into the westward density current, the main convective precipitation streamers slope dramatically forward, establishing a slantwise upward motion feeding into the separate active updraught cells. This creates a circulation pattern that separates up- from downdraughts. There is little evidence in our model output of upper-level rain- or graupelshafts that might lead to the collapse of an existing updraught, the usual mechanism brought forward in the context of enhanced storm intensity under high wind shear. In other words, there are no peak upper-level downdraughts within regions of high condensate content. Within ATHAM's formulation, rain and graupel can however precipitate through regions characterized by net upward or zero vertical velocity of the total mixture: this entrails that the grid-box's gas phase is actually rising (faster) to compensate. Strong updraught cells in this simulation can be slightly sloped but remain essentially vertical. Strongest downdraughts occur on the edges of the ring-vortices marking the updraught's horizontally diverging top, besides the low-level rain- and graupelshafts where strongest precipitation leads to downdraughts due to drag and evaporative cooling, fed by the dry rear inflow. This inflow has been argued to supply the cold pool with the necessary dry air mass to uphold the positive pressure perturbation under the gust front head and to sustain the strength of the surface density current (Houze (1994), chapter 9.2).

Suspended condensate specific concentrations are largest within the updraught cores and upper parts of the anvil, often adopting inverted U-like distributions, which are easily broken up. Whilst the storm was initially moving westward, within the lower free-tropospheric steering flow and due to regeneration of new cells due to strong convergence on the upstream-moving gust front, the strongest updraughts eventually reach heights within the eastward background flow and start being advected back into the anvil. The pronounced cold pool fed by lower free-tropospheric air masses is best appreciated in the 18:30 LT snapshot. Eventually, the gust front outruns the parent storm, which dissipates (positive boundary relative cell speed, J. W. Wilson et al. (2001)). In spite of significant forced ascent, it is not capable of further triggering deep storm cells. Possibly, this may be due to the absence of sufficient pre-moistening of the mid-troposphere in regions ahead of the storm. Unlike a squall line's persistence over several and up to 10 hours, the storm simulated here lasts for less than 2h.

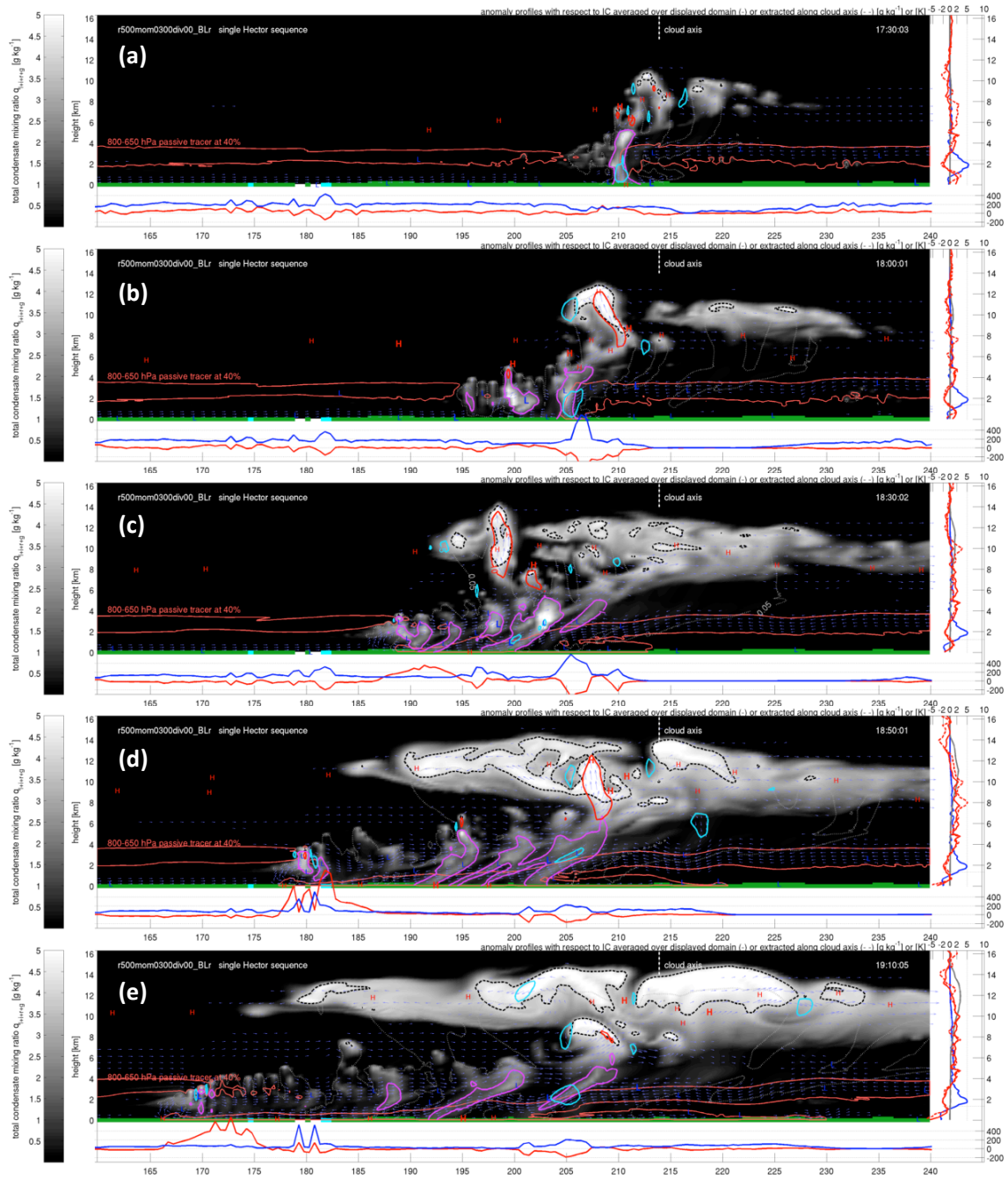


Fig 34 Sequence of snapshots of the total condensate specific concentration during the Hector storm propagation simulated at 500 m grid-spacing. The thick dashed black contours delimit suspended condensate at 4 g kg^{-1} , thick magenta solid contours precipitating condensate at 1 g kg^{-1} , thin grey dotted contours precipitating condensate at 0.05 g kg^{-1} . Strong updraught isotachs at 10 ms^{-1} are displayed as thick red solid lines, strong downdraught isotachs at -5 ms^{-1} as cyan-coloured ones. Land areas, topography and wetlands are coded as in the previous figures. The flow field is represented by evenly spaced arrows (every 500 m horizontally and 5 grid-points vertically) where local wind speed exceed 5 ms^{-1} ; further arrows at a higher density (every 250 m) are added where the vertical velocity alone exceeds 5 ms^{-1} (note that the visibility of arrows in clouds is mediocre at best). A 40% isoline of a passive tracer confined initially between 800 and 650 hPa (orange contour) visualizes lateral entrainment, especially into the rear inflow. Individual pressure perturbations (Highs and Lows, in red and blue letters) have been selected manually in the pressure perturbation field through inspection; these give subjective and relative anomalies with respect to the field at a given point in time and do not characterize the field completely. They have, however, been selected without considering other fields. The surface fluxes are drawn as in Fig 30. Anomaly profiles of quantities spatially averaged over the displayed domain at the given time with respect to the initial conditions are

depicted on the right-hand side: in blue for specific humidity, in grey for suspended condensate and in red for potential temperature. The red dashed line is computed from a single profile extracted along the indicated ‘cloud axis’ as opposed to from an area-average.

A much more intricate flow pattern can be observed in the better-resolved r50 simulation (Fig 35), which gives deeper insight into the associated dynamic and thermodynamic processes, even if the overall structure remains similar to that in BLr. The second Hector storm shown in this sequence seems to develop off a faint westward density current originating from the first Hector depicted in Fig 35(a). Keenan and Carbone (1992) discuss propagating, non-propagating and balanced squall lines, the morphology and dynamics of which (their Fig 16) bear some resemblance to the preceding figures, in particular at various times of the simulated storm evolution. The mechanisms behind the simulated propagation modes, and the way model grid-spacing influences the latter (given that the environmental wind profiles are the same), need further investigation.

A noteworthy feature of the r50 sequence is that it supports a conceptual model wherein convection is composed of individual successive rising bubbles, rather than of a vertical and ‘long-lived’ updraught core, not unlike the cells spawned off daughter clouds in the simulated squall-type multi-cellular storms described in Fovell and Tan (1998). These bubbles may get stretched into upward meandering streamers, particularly in an environment with background wind. The largest concentrations of suspended condensate remain consistently, as in all of our simulations, along the upper border of these streamers, whilst precipitating condensate is concentrated within fall streaks in the wake of the rising bubbles. The rising buoyant parcels are capped by local positive pressure perturbations (demarcated by the red letter H in the figures), where the bubble displaces ambient air. This environmental air gets accelerated downward on the edges in what are the strongest upper-air downdraughts, and engulfed into the vortices surrounding a strong rising bubble. These vortices entrain dry ambient air into the cloud. This suggests that cloud lateral entrainment may be predominantly vortical in nature and tied to the rising parcel, as opposed to driven by smaller-scale turbulent diffusion and mixing along the cloud lateral boundaries, which is driven by w -shear. The simulation results support a model of multiple parcels rising through a cloud, some diluted, others not, through discontinuous and inhomogeneous entrainment, as discussed in Houze (1994), chapter 7.3. The parcels themselves are very much alike (distorted) and capped Hill’s vortices (spherical vortices within an entraining buoyant bubble), as already suggested by Levine (1959) as a cumulus model. A similar entrainment pattern had also been simulated in 3D for elongated roll updraughts feeding into a squall line, orientated perpendicularly to the gust front (Bryan, Rotunno, and Fritsch (2007), their Fig 2).

The circulating streamers are embedded within the overall cloud system. If a real feature of clouds, they certainly will remain difficult to observe with cloud-penetrating rain radar systems, even those operating at very-high spatial resolutions. Indeed, the rising bubbles and the regions of highest suspended condensate content are not reflected in the synthetic radar reflectivity signal shown in Fig 36, which discriminates suspended condensate in favour of larger particles. The buoyant parcels (or rising bubbles) can be seen as positive potential temperature anomalies capping rising streamers in Fig 36, particularly on top of what would be identified as convective cells in the reflectivity field. Other such parcels get advected around in the flow. Obviously, if a large bubble rises close to the edge of the embedding cloud, it is more likely to entrain large amounts of environmental air (Fig 36(c)). Most positive θ anomalies in the mid-troposphere are capped by positive local pressure perturbations slightly higher up. It is difficult to dissociate source from response within these anomalies and perturbations. In the case of buoyant parcels, latent heat release will have produced a higher θ air mass, and the rising motion induces a dynamic pressure perturbation response. In other areas, local pressure perturbations may possibly induce subsidence and therefore adiabatic heating of underlying parcels. Many of the θ anomalies in the mid-troposphere, however, seem to originate within the cloud system and then to get transported outwards. Positive anomalies are partially due to latent heat release, partially generated adiabatically on the cloud edges where very vigorous downdraughts prevail. The large negative anomaly at a height of 8 km and at 178 km in Fig 36(a) for example is likely to be of adiabatic cooling origin, and is linked to the entrainment of environmental air and its forced ascent (and cooling) within the vortex on the cloud edge seen in Fig 35(c). Coincidentally, it is this vortex entrainment that has led to the break up of the original bubble in Fig 35(d) and in Fig 36(a), and to the more horizontal re-orientation of the rising streamer. The stretched slantwise downward θ anomaly just below the large negative one will provide a preferential guide or bridge to connect the developing convective tower ahead to the parent storm.

Other local positive pressure perturbations are found in the upstream-propagating cold pool density current (further discussed below) and at the surface under heavy rainfall. Local negative perturbations (demarcated by the blue letter L) characterize the strongly heated surface layer before a passing gust front, arise in the downstream-moving density current, as well as in any other (mostly lower free-tropospheric) region characterized by a strongly divergent flow. The deepest lows occur within strongly vortical circulations and are probably cyclostrophic pressure minima. Some of these are situated near the strongest lower-level downdraughts and the rear inflow (e.g. Fig 35(a), (d)), as well as within the gust front heads (e.g. Fig 35(b), (c), (d)). The downstream-

moving gust front's negative pressure perturbation at 187 km in Fig 35(d) (and in Fig 38 for close-up) corresponds to a strong rotor. Here, the radial pressure gradient $(1/\rho) \cdot (\partial p / \partial n)$ is roughly equal to 0.08 ms^{-2} , where n is a radial coordinate vector. The centrifugal acceleration, V_s^2 / r_s , with the tangential wind speed V_s at a distance r_s from the centre of rotation, is more difficult to estimate, given the very heterogeneous wind field. We have taken an 'average' V_s of 10 ms^{-1} over roughly 800 m, giving an acceleration of 0.13 ms^{-2} . Values are difficult to average in the model fields and other forces are obviously involved, but the rotor is not too far off from being in cyclostrophic balance (see Houze (1994), chapter 8.9).

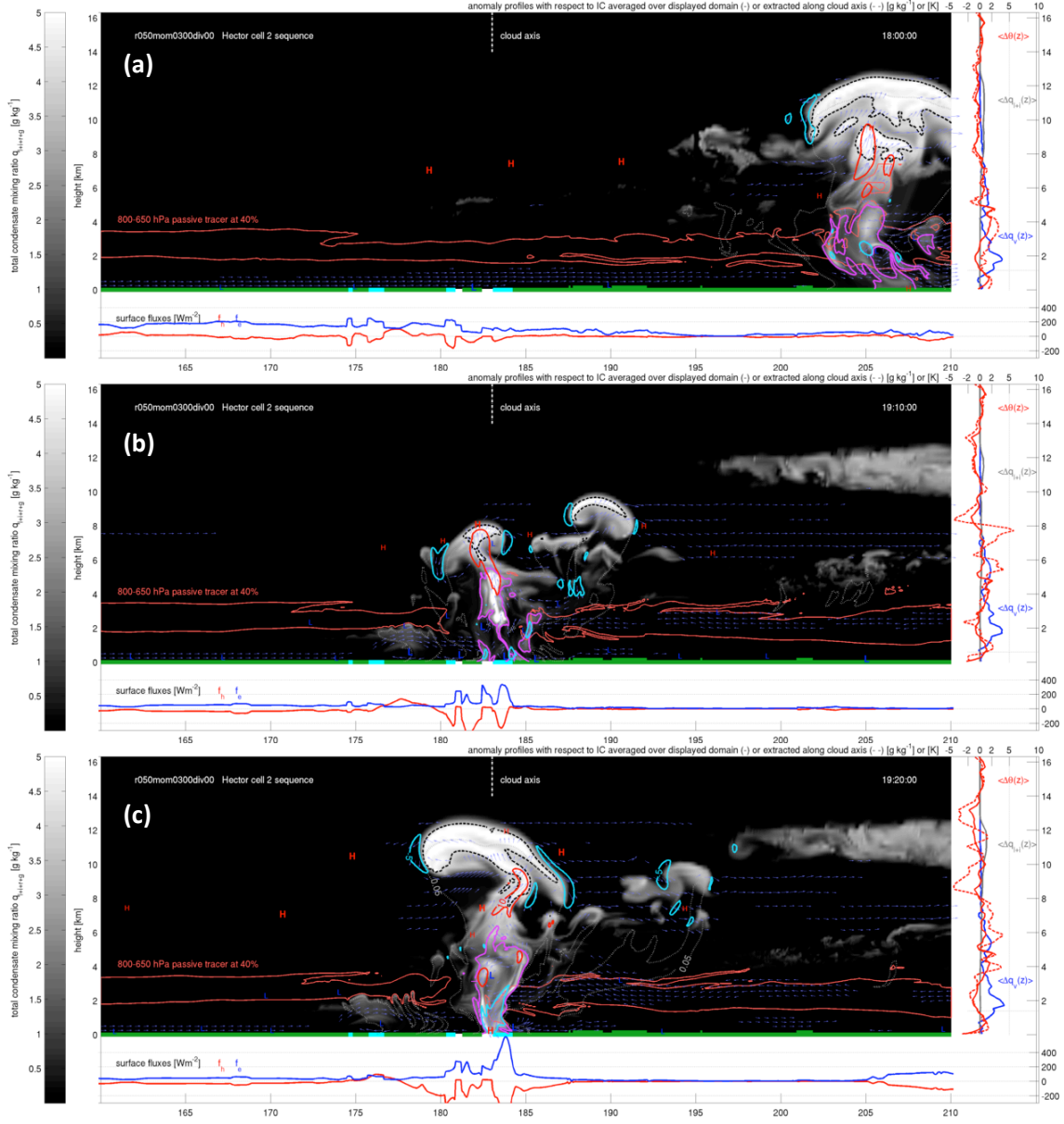
As in BL_r, there is still no evidence for upper-level precipitation shafts strong enough to generate major downdraughts of the mixture. Strong rotating circulations do however exist in the lower free-troposphere. The circulation located around 182 km in Fig 36(a) is potentially a region of significant raindrop recycling and growth, and an intense low-pressure perturbation has been generated in its centre. Interestingly, the rising branch of this vortex is characterized by a negative θ anomaly, perhaps because adiabatic cooling dominates over possible vapour deposition. That most of the air in the downstream-moving 'cold pool' density current seems in fact to be characterized by a strong positive θ anomaly (and to be positively buoyant from a density perturbation point-of-view, not shown) is most intriguing. The current that we continue to refer to as cold pool density current is thus likely to be driven at least to some extent by mass continuity rather than by negative buoyancy. Note that the rotor discussed above does not actually reside within the gust front's head but seems to sit just ahead of it, even if it is still composed to some extent of lower free-tropospheric air (Fig 38(e)). Given its buoyancy and strong vorticity, it seems that its air masses get re-inserted into the rear inflow stream, rather than travelling eastward with the density current. Only the divergence within the density current, which accelerates downstream with the prevailing wind, potentially impedes these buoyant air masses to produce as strong a new lifting mechanism as they possibly could under the stratiform region. A much more detailed analysis, including vorticity and shear considerations, along early and more recent ideas of e.g. Rotunno, Klemp, and Weisman (1988) and Weisman and Rotunno (2004), amongst others, might prove useful to substantiate any of the above, but is outside the scope of this dissertation. The positive θ anomaly within the rotor might be creating a positive pressure perturbation partially offsetting the centrifugal acceleration in the cyclostrophic balance above. Where does this warm air in the cold pool come from? We hypothesize that it is mostly lower free-tropospheric dry air from the rear inflow (and some from the up-storm environment) that has been forced downward due to precipitation drag and mass continuity during the strongest rainfall events, and which has warmed adiabatically.

Some of the adiabatic heating of the dry air would have been offset by evaporative cooling or mixing with cooled air within the downdraught. Indeed, a negative θ anomaly exists in the funnel-shaped region marking the inflow into the downdraught, which is likely due to evaporation. The temperature of the inflow taken at 3 km is roughly 11°C, that in the centre of the vortex roughly 29.5°C, i.e. 18.5 K warmer (not shown). Pure dry adiabatic heating from a vertical displacement of 2.5 km would have produced a warming of roughly 24.5 K, hence the evaporative cooling should be roughly 6 K. Humidity has increased roughly by between 2 and 5 gkg⁻¹ (not shown). Since the air in the downdraught is considerably drier than the surroundings, the gain in buoyancy due to a positive θ anomaly is partially offset. Still, the virtual θ_v anomaly also remains positive, in particular at the edges of the rainfall streak and in the rotor; and the density anomaly, which factors in additional effects of pressure perturbations and liquid water loading, also indicates a partially positively buoyant storm outflow and density current edge. At the onset of the density current, it seems that the rear inflow only feeds into the downstream-moving branch of the current (Fig 35(c) and (d), Fig 36(a), Fig 38(e)), revealed also by a very sharp interface in all the tracer fields to the west of the rainfall downdraught (not shown). Since a strong upstream-moving PBL current is nonetheless present west of the storm, this raises the question where the mass flux to sustain this current comes from. We tentatively speculate that this current, at least after an initial onset through precipitation and in its early phase, may actually be maintained as an indirect circulation by the up-storm boundary layer wind, lofted on top of 'its own' return flow, travelling towards the parent storm without being ingested into the storm itself and folding downward near the rain front. The rear inflow's downdraught is eventually lifted in the strong vortex mentioned previously (one instance of such vortical lifting is evident in Fig 35(f)), before collapsing under a new precipitating cloud and evolving into a consolidated upstream-moving current fed consistently with evaporatively cooled air from the new precipitating cells (Fig 35(e)).

Air masses ending up in the precipitation cold pool and in the boundary layer are unlikely to have come from very high up in the atmosphere. Their gain in buoyancy would be too large, unless dilution of saturated cloud air with dry environmental air from lateral or cloud top entrainment induces enough evaporative cooling to overcome the stable thermal stratification. Since a lot of cloud water has been removed through precipitation, such re-evaporation is presumably insufficient to support major downward motions. In other words, even though some of the precipitating particles may fall from much higher altitudes, the gas inflow to feed the cold pool probably needs to originate at a low altitude.

The newly generated clouds on the westward gust front in Fig 35(d) look like they are capped by Kelvin-Helmholtz billows. However, the local Richardson number is much

too large anywhere but at the top of the density current for Kelvin-Helmholtz waves to be generated, given the relatively low density stratification and limited shear within the convective PBL and the inversion layer. A more detailed investigation along the lines of e.g. Weckwerth and Wakimoto (1992) would be required to extract possible wave activity. A shelf cloud is generated on the westward gust front and seen as the low wedge-shaped arcus in Fig 35(b), (c) and (d), though it quickly detaches from the parent storm.



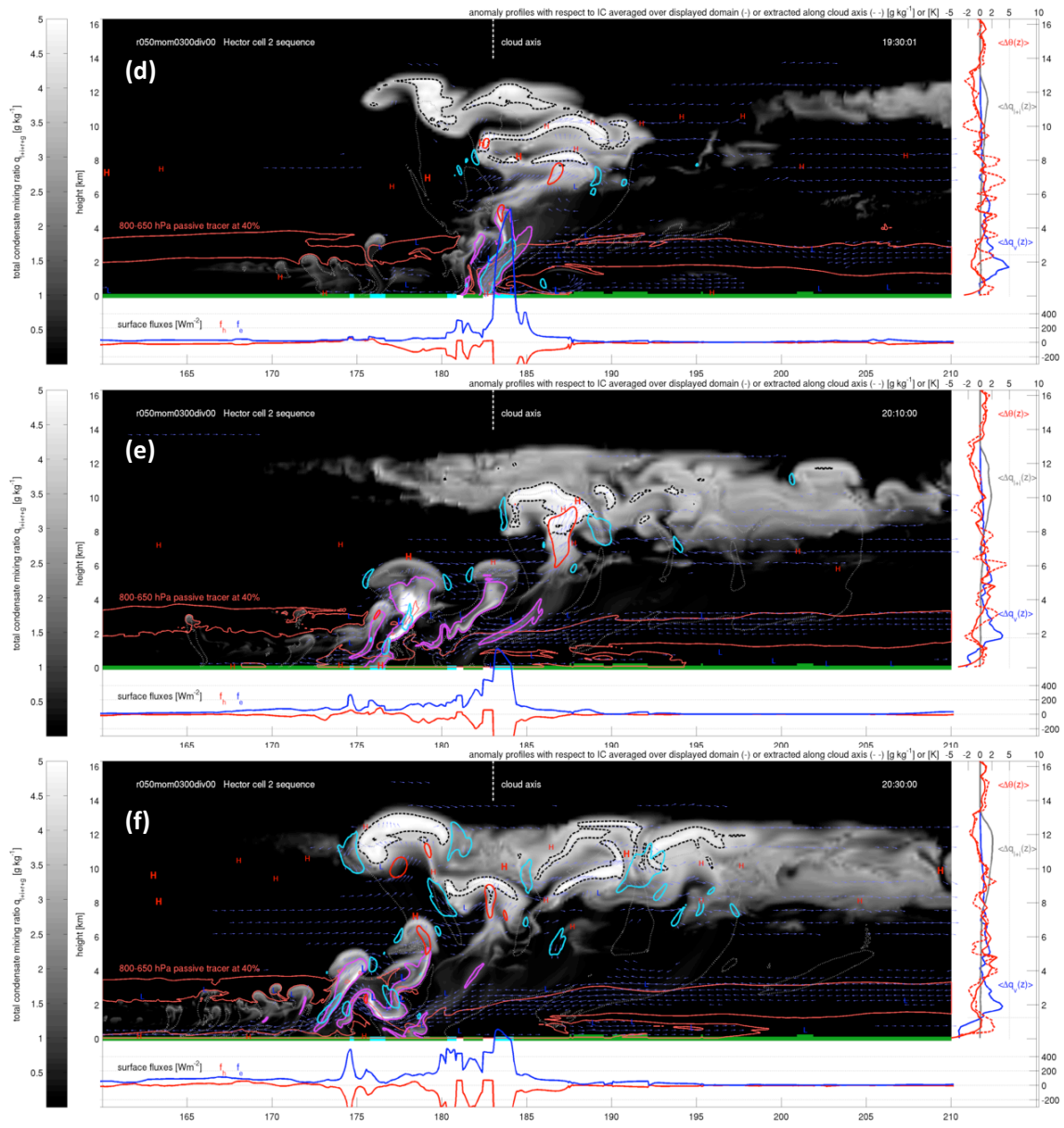


Fig 35 Same as Fig 34, but for the second Hector storm simulated at 50 m grid-spacing.

We have synthesized the effects of the previously described convective overturning on the mean atmospheric thermal stratification and moisture content by lateral spatial averaging and computing anomaly profiles with respect to the initial conditions (Fig 34 and Fig 35, right-hand profiles).

The most prominent and consistent feature in both BL_r and $r50$ remains, as already pointed out during the analysis of the shallow phase, the inversion layer moistening and its erosion over time. Between the top of the PBL (z_i , roughly around 800 m) and 3-4 km, $\langle \Delta q_v(z, t) \rangle$ has strongly increased over time, consistent with the formation of shallow cumulus clouds and their re-evaporation. This mechanism has transported significant amounts of moisture into the inversion layer and deepened the PBL. At the onset of a major deep convective event, the specific humidity slightly decreases, particularly near its peak at 2 km, as water is condensing and entrained into the deep convective updraughts.

This leads to an upward transport and release in the mid-troposphere, mostly between 4 and 7 km (Fig 35). Note, however, that q_v in the upper atmosphere only increases slightly in absolute terms (and even seems to decrease again). This reflects the redistribution over a deeper column and the much lower RH at lower temperatures. Another prominent feature is the strong drying of the lower PBL with the penetration of dry lower free-tropospheric air masses during the cold pool formation. Most of the depleted lower-level water vapour ends up in the condensed phase $\langle \Delta q_{l+i}(z,t) \rangle$, and particularly in the ice phase, as shown by the significant increase of condensed water in the anvil and stratiform region. Very little water remains in the liquid phase during deep convection in the model.

In terms of sensible heat changes, illustrated by the averaged potential temperature profiles $\langle \Delta \theta(z,t) \rangle$, the inversion layer erosion through the entrainment of adiabatically cooler air from below and shallow cloud-top radiative (and evaporative) cooling is clearly visible as a drop in θ over time. Around the level of z_i and just below, the opposite occurs through adiabatic heating by warmer air entrainment from aloft during the shallow convection phase. As soon as deep convection precipitates, the average lower PBL and its surface layer cool down strongly, (once a proper cold pool has developed), with the exception of short warming events just below cloud base and on the down-storm side (dashed profile, e.g. in Fig 35(d)), which are due to the downward forcing of higher- θ air within the precipitation drag.

Within the free troposphere, the sensible heating profile is not trivial. A direct transect through a cloud (dashed line) reveals sections of strong positive θ anomalies due to the presence of a rising convective bubble, heated through latent heat release (e.g. below 8 km in Fig 34(a) and in Fig 35(b) and (c)). Cloud-top cooling (e.g. above 13 km in Fig 34(d) and (e), above 8 km in Fig 35(b), above 12 km in Fig 35(c), (e) and (f)) may be partially due to dry adiabatic upward displacements, partially due to cloud-top radiative or evaporative cooling. Since the upward displacement seems to be negligible (or indeed reversed) in the cross-section of Fig 35(f), this suggests that cloud-top radiative or evaporative cooling play a significant role in at least some occasions. Adiabatic cooling due to lateral dry air entrainment in a vortex-circulation with a strong upward branch is present between 8 and 10 km in Fig 35(c), even if some of the cooling might be of diabatic nature due to simultaneous mixing with and evaporation of cloudy air. On average (solid lines), the free troposphere θ anomaly profile does not change dramatically, contrary to what we expected in terms of redistribution of heat due to deep convection. As a general pattern, the much stronger single Hector storm in the BL_r simulation has resulted in slight net sensible heating all throughout the column between 4 and 12 km, all effects (overturning, latent heating/cooling, radiation) combined. The r50 simulation, on the

other hand, produces most net sensible heating roughly between 4 and 7 km, and sensible cooling roughly between 10 and 13 km.

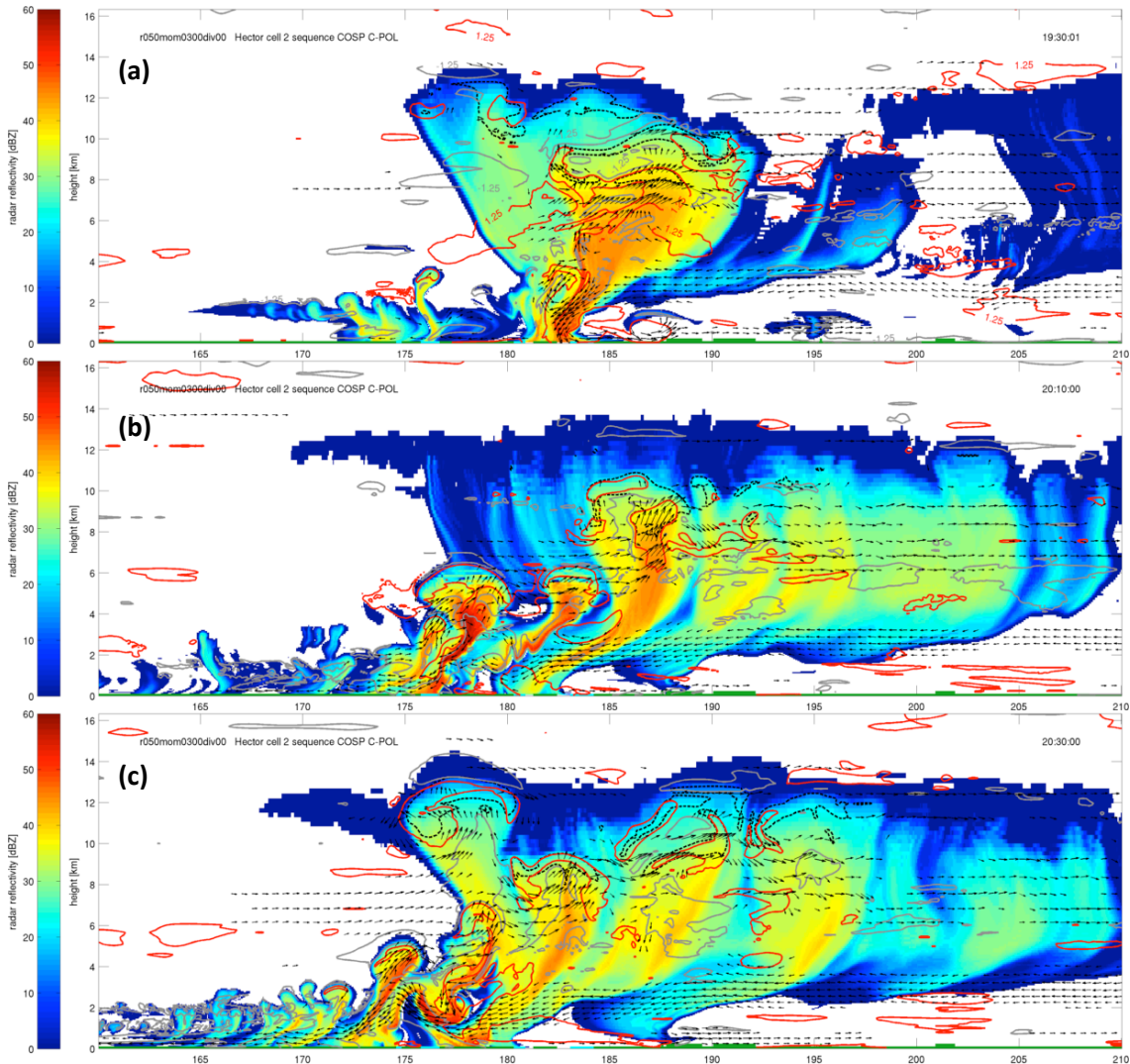


Fig 36 Same sequence of snapshots as in Fig 35(d)-(f), but showing a synthesized C-band radar reflectivity signal as described in section 5.3. A threshold of -40 dBZ is applied; the dark blue areas hence agglomerate any value between -40 and 0 dBZ. Flow vectors and the isolines of suspended condensate at 4 gkg^{-1} are the same as in the previous figures. The red contours show 1.25 K positive θ anomalies with respect to the local subdomain-averaged profile (as in the third row of Fig 30); the grey contours show equivalent negative anomalies. Buoyancy perturbations calculated in a similar way from the density field generally follow the θ anomalies pattern; note however that buoyancy is generally smaller, especially in the high-altitude bubbles with large condensate content.

We are tempted to argue that both simulations have led to a stabilization of the lower and mid-tropospheric profile and to a destabilization of the upper troposphere, even if magnitudes and altitudes separating stabilization from destabilization differ. It is not clear to what extent a destabilization of the upper troposphere actually matters, since it remains dry-adiabatically stable (or in the worst case, neutral), and moist convection is unlikely to be triggered at these heights. However, we raise the question whether it could lead to deeper and more vigorous convection during the next day's diurnal cycle, in the

absence of any other large-scale forcings. We could envisage that deep convection intensifies over several convective cycles until an extreme event stabilizes the entire profile up to the tropopause.

What is the effect of the (weak) moistening of the free troposphere on stability and convection during the next convective cycle? We speculate that a more humid environment will lead to a faster development due to reduced sensitivity to environmental air entrainment, similarly as we speculated on consecutively deeper cells developing in the wake of previous clouds. The lowermost free troposphere has been moistened most. Will this lead to a significantly earlier onset of deep convection the following day? In terms of equivalent potential temperature anomalies (not shown), by far the largest changes occur in the lowest 3 km of the profile: averaged over the whole analysis subdomain at the end of the simulation, $\langle \Delta \theta_e(z, t_{end}) \rangle$ is lowest in the surface layer (-8 K) and highest at 2 km of altitude (+9 K). The least we can say is that shallow and deep convection are intimately interlinked.

The possible effects on atmospheric stratification of the low ice fallout rate in ATHAM, through the formation of a correspondingly large stratiform cloud deck and detrained cirrus, are multiple and complex. First, we expect the re-evaporation of the large remaining ice cloud to consume an equally large amount of latent heat, contributing further to the cooling and destabilization of the upper layers, albeit slightly offset by the decrease in condensed water loading and the increase in buoyancy due to water vapour release. An unstable upper atmosphere increases buoyant turbulence throughout the anvil (as we do indeed observe towards the end of the simulation), which will increase mixing, dilution and evaporation. As already pointed out, cloud-top radiative cooling will also further enhance destabilization, though this depends on cloud thickness. Given estimated anvil emissivities >0.9 , Danielsen (1982) predicted large gradients in radiative heating, with cloud top cooling and cloud base warming, leading to further buoyancy production and convective instabilities in the anvil. Radiative cooling may even turn into greenhouse warming once sufficiently thin cirrus clouds are formed. At night, a thin cirrus upper cloud deck might thus contribute to the warming of the upper layers, stabilizing the profile throughout.

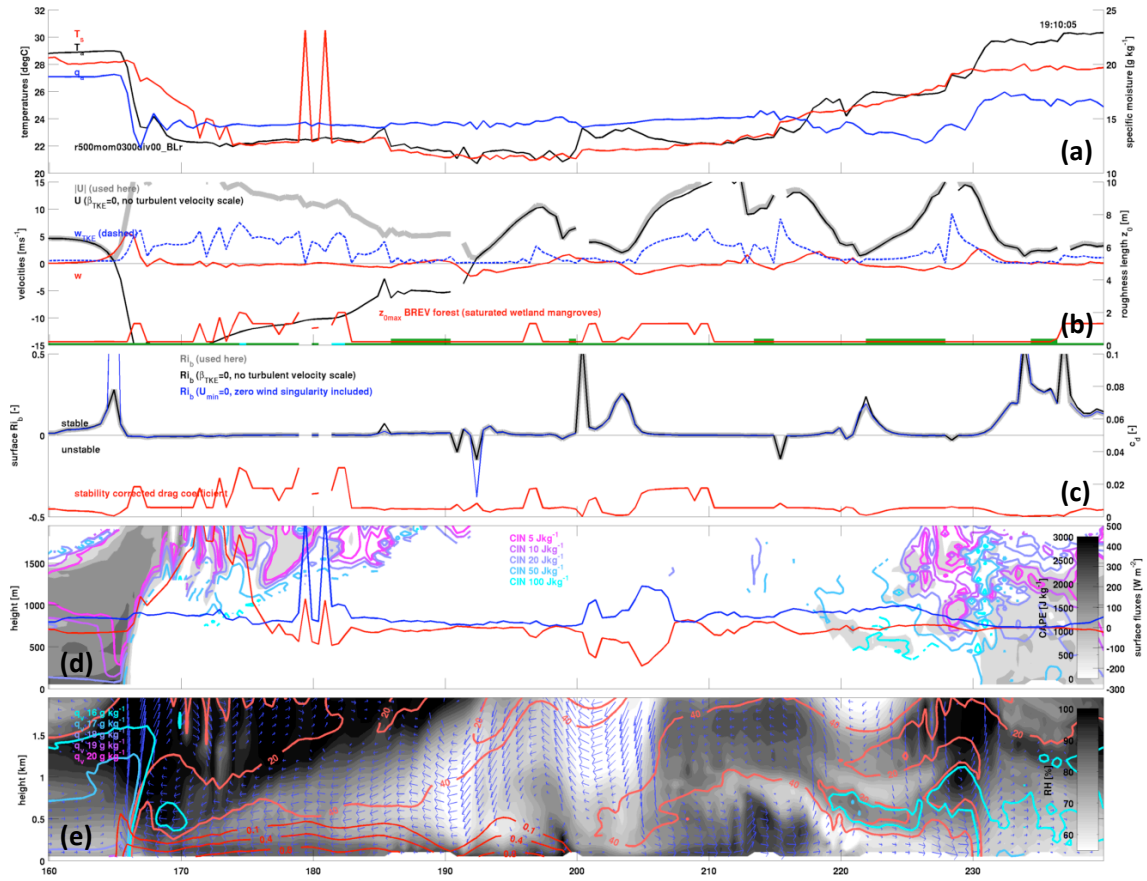


Fig 37 Detailed surface-atmosphere interactions and PBL properties below and ahead of the mature storm in Fig 34(e): (a) atmospheric temperature (T_a , black) and specific humidity (q_a , blue) in the surface layer, and surface skin temperature (T_s , red), intervening in the bulk transfer parameterizations (4.9); (b) wind speeds fed linearly into the flux transfer (equation (4.9)) and non-linearly into HYBRID's transfer coefficients C_d and C_h (equations (4.7)-(4.8)) through Ri_b in equation (4.5). The surface layer horizontal wind speed U is given as the thin black line, w (red dashed) is the vertical velocity, and w_{TKE} (blue dashed) is the turbulent velocity scale introduced in equation (4.2) to boost fluxes in those highly turbulent regions where the mean wind tends towards zero. The thick grey line represents $|U|$, the absolute wind speed including unresolved turbulence. The grid-box averaged roughness length z_0 is given as the red line at the bottom; (c) Ri_b calculated without removing the zero-wind singularity but with $\beta_{TKE}=1$ (thin blue line), after removing the zero-wind singularity by setting $U_{min}=1.5$ but with $\beta_{TKE}=0$ (thin black line), and by both setting $U_{min}=1.5$ and adding w_{TKE} with $\beta_{TKE}=1$ (thick grey line). The non-neutral drag coefficient C_d is in red; (d) cross-section through the PBL CAPE levels estimated from pseudo-adiabatic ascent using the lifted parcel model by D. Brunner (2000), translated from *calcsound* in Emanuel (1994), applied to each grid-box within the lowest 2 km in the PBL (shaded). CIN coloured contours correspond to the negative energy/area on a thermodynamic diagram and characterize the convective inhibition or strength of the barrier. The surface fluxes are the same as in Fig 34(e); (e) PBL RH (shaded) and specific humidity (coloured contours). The minimum speed for arrows representing the flow field is 2 ms^{-1} . 20% and 40% isolines of the same 800-650 hPa passive tracer as in Fig 34 (orange contours) visualize the cold pool density current fed by the rear inflow. Positive pressure perturbation (local highs) isobars of 0.1, 0.4 and 0.8 hPa are contoured in red.

Previously, we alluded to the possibility that initial deep convection triggering near the windward coastline may have occurred on a sea breeze front, even if the latter produces less pronounced convergence than the leeward-side sea breeze. This triggering region (between 175 and 185 km) coincides with a river, though, surrounded by mangrove wetlands, which constitute an area of low (mostly negative) sensible heat fluxes

but also of consistently high evapotranspiration (see Fig 34-Fig 38). The question naturally arises as to what extent triggering over this area happened fortuitously, and to what extent this particular surface configuration contributed to a preferential area for deep convection initiation and development. Before we can try to tackle this issue, we should assess how the model simulates surface-atmosphere interactions before and during a deep convective storm.

Surface fluxes of sensible and latent heat constitute the link between the surface and the overlying atmosphere, through changes in thermodynamic properties of the air. The simulated heterogeneity of surface fluxes in space and their variation in time over a realistic area can be appreciated in Fig 34 for BL_r. The particular response of the wetlands is obvious, even though the fact that the sequence is plotted towards the evening, where radiative energy inputs are limited, needs to be taken into account. Starting in Fig 34(c) around 190 km, enhanced sensible heat (f_h) fluxes around the gust front, probably due to strong winds sweeping with cold air over a warmer surface, can be seen ‘propagating’ westward. On the down-storm-side of the main rainfall region in Fig 34(b), there is a strong increase of latent heat (f_e) fluxes and a decrease of f_h , possibly because of the forced descent of dry warm air masses described before. As the storm progresses westward, these flux anomalies remain locked to this particular area, indicating that something else must influence the magnitude of the fluxes here. Disentangling dynamic storm effects from the influence of surface heterogeneity is more difficult in r50, where a more or less stationary second Hector cell has set up over the wetlands (Fig 35).

The detailed surface response at 19:10 LT of BL_r, corresponding to the storm snapshot in Fig 34(e), is shown in Fig 37. The 800-650 hPa passive tracer contours outline a textbook example of a cold pool density current. Within the atmospheric surface layer, in immediate contact with the ground (and here defined as the lowermost layer of grid-boxes), the air temperature T_a is significantly lower within the cold pool than in areas surrounding it, with the sharpest gradient on the upstream-moving gust front (Fig 37(a)), characterized also by a dynamic positive pressure perturbation where kinetic energy is converted into enthalpy (Fig 37(e)). The surface layer specific humidity (here denoted as $q_a = q_v(z = 25 \text{ m})$) is also significantly lower; both contribute to an increased density within the current. This is also reflected in the large positive hydrostatic pressure perturbations at the bottom of the current. The surface skin temperature T_s follows T_a closely, meaning that the flux response to the passing density current is very fast. Noteworthy exceptions are between coordinates 200 and 210 km, where we previously pointed out the adiabatically-heated warmer downdraught, and within the gust front head (165-174 km), where the surface did not yet have the time to respond by cooling through f_h . By model design, the water skin temperature remains constant in our simulations, as

seen in the 2 T_s peaks. A clear response of land T_s , an extrapolated diagnostic variable, to surface moistening is not present.

Surface fluxes depend both linearly on surface wind speed through equation (4.9), and non-linearly through the shear stress generation of turbulence term in the surface Ri_b number in equation (4.5) (over land areas, or in the Obukhov length L , equation (4.6), over water bodies), which intervenes as a measure of stability in the transfer coefficients in equations (4.7) and (4.8) (or similar for water bodies). The surface wind speed in BL_r (black line in Fig 37(b)) is straightforward; it is the sum of the weak PBL westerly and the density current. The main downdraught occurs between 190 and 210 km, and the density current is accelerating westward in the upstream-moving section until it reaches the strong convergence line around 165 km. Similarly, the downstream-moving section accelerates eastward, but convergence is less sharp and less intense on the downstream front. Here, wind speed is broken by strong decelerations ahead of topographic elements. The broken line in the plot is an artefact due to averaging with undefined velocity components below ground level. More importantly, though, this deceleration itself may be a model artefact, linked to the use of a Cartesian rather than a terrain-following coordinate system. The characteristic features of the vertical velocity w (red line) are the two frontal updraughts on either gust front. The turbulent velocity scale w_{TKE} (dashed blue line), defined in equation (4.2), is driven by the magnitude of the wind speed itself, and is tightly linked to both the surface roughness heterogeneity (solid red line at the bottom of the graph) and discontinuities in topography. Note that from the surface characterization, roughness is largest in the wetland areas, which correspond to tall mangrove forests with highest z_0 . The thick grey line traces U as defined in equation (4.2); given that it closely follows the non-modified wind speed, this alleviates previously raised concerns about departing from the theoretical framework by introducing w_{TKE} . However, as w_{TKE} tends towards 0 with the mean wind speed, in the absence of very strong free convective buoyant generation of turbulence, the merit of introducing it in the first place also vanishes; if anything, it creates a slightly more irregular wind forcing of surface fluxes.

Surface layer stability depends first and foremost on the sign of the temperature difference between T_a and T_s (by definition of Ri_b in the surface layer). Stratification in Fig 37(c) therefore oscillates between stable and unstable according to the respective evolution of T_a and T_s in Fig 37(a). At this time of day, the sun has already set and the air is mostly warmer than the underlying surface, installing stable surface layer stratification. The starkest difference is within the gust front head, where surface cooling lags behind. Here, the cold air in the density current sweeping over a warm surface locally creates a fairly unstable surface layer. Since Ri_b in equation (4.5) estimates the mechanical generation of turbulence through vertical wind shear, and given a no-slip lower boundary

condition, the denominator is forcefully large at moderate to high surface winds. In other words, with significant surface winds, turbulent transfer is generally estimated for near-neutral conditions (i.e. $Ri_b=0$). Also, at sufficiently high winds, imposing a minimum U_{min} of 1.5 ms^{-1} hardly impacts the stability calculations, but removes the zero-wind singularities ((near)-infinite Ri_b), occurring here around 165 km and 192 km. Similarly, adding w_{TKE} hardly makes a difference to the stability estimation; if anything, it brings it slightly closer to neutral conditions.

The neutral drag coefficient C_{dn} is a function of z_0 , and the stability-corrected transfer coefficients are linearly proportional to C_{dn} (see equations (4.7) and (4.8)). Taking C_d as a proxy for C_h and C_e in Fig 37(c), it is obvious that the value of z_0 will be of first-order relevance to the flux transfer in the coupled models, at least under the near-neutral conditions set up by moderate to high winds. Fluxes will be cut off quickly in stable conditions and enhanced in unstable ones. We pointed this already out from a theoretical perspective in section 4.1. Inspecting the surface fluxes in Fig 37(d) in terms of the various factors involved in their computation within a realistic situation is still a worthwhile exercise. Besides situations in which conditions are momentarily extreme, such as the large temperature difference and wind speed under the gust front head, and which can generate short-lived flux peaks; in our simulations, areas of consistently high fluxes seem predominantly locked to regions with strong surface roughness.

To what extent is the propagating storm system linked to its influence on surface f_h and f_e through variations in surface layer properties? This question is of course difficult to settle from the example in Fig 37 alone, but a careful analysis of the boundary layer evolution will provide first hints. Strong changes in fluxes are confined strictly to within the boundaries of the density current itself. Cold and dry, the current is inherently characterized by very low values of CAPE (Fig 37(d), shaded, or alternatively θ_e , not shown). In other words, no parcel lifted from within this current will ever reach free convection. In spite of relatively large (but short-lived) fluxes as the gust front sweeps over the surface, they are by far not enough to raise the (potential) buoyancy of these air masses, at least not in our simulations and at this time of day. This could to some extent have been expected; but the very low specific humidity in the current comes as a surprise, since it seems to indicate that re-evaporation of precipitation within the downdraught is not very high. Specific humidity remains highest in the lower PBL on either side of the density current (Fig 37(e), contoured), and it is forced aloft and over the current on the gust front. The region atop the current is where RH is highest (Fig 37(e), shaded). It is here that condensation takes place, and where instability and new triggering of deep cells are highest and most likely, as reflected in the low values of CIN (Fig 37(d), contoured).

The equivalent to Fig 37 for r50 at 19:30 LT, an early stage of cold pool development corresponding to the second Hector in Fig 35(d), is shown in Fig 38. This is mostly for reference, as the overall picture does not dramatically change with respect to BL_r , besides better-resolved and more detailed circulations. The surface configuration is slightly different at different resolutions; this is due to the design of the surface preprocessor. Because of the low winds and the sign of the temperature difference, the downstream surface layer is rather stable, translating into a very low C_d and hence virtually no surface fluxes. An extremely high f_e has momentarily appeared near 184 km. It is located straight over the wetland and linked to the very dry and relatively warm air blasting at very high wind speed over a moisture-saturated surface, further characterized by tall trees and thus high z_0 and C_d . Given the temperature difference, the surface layer should be very stable, but the high wind effectively draws stability towards neutral conditions. For the same reasons, f_h is very large, and negative, essentially describing a strong heat flux from the atmosphere to the ground. Whether any of these fluxes, and in particular f_h , are realistic is of course debatable but difficult to assess – in any case, the strong heterogeneity and non-stationarity of the turbulence conditions violate the theoretical framework on which flux transfer is based. The fluxes remain, however, consistent within our modelling framework adopted. Note that Keenan et al. (2000) described occasional point measurements of f_e in tidal mudflats in the northeast coast of Melville that reached values as high as 800 Wm^{-2} for short periods of time. Similarly dramatic flux enhancements over ocean surfaces have also been described from simulation results by Tompkins (2001b).

A noteworthy difference to BL_r is the possibly indirect nature of the upstream-propagating current mentioned before. Here, we see that this current seems to consist of two separate circulations, one between 171-176 and another between 176-181 km (Fig 38(d) and (e)). The main front near 171 km has a pocket of high specific humidity air at over 20 gkg^{-1} (contoured). It is located behind the dynamic pressure perturbation and hence originates from the downstream side. The large moisture convergence in this region likely originates at least partially in initially higher levels of surface layer specific humidity. Some of it may also have originated in the upstream surface layer, lofted over the front and recycled backwards within the surface layer current. This whole region is characterized by high RH at very low levels, forming what looks like shelf cloud(s) on said front(s). The up-storm-side boundary layer also has high levels of CAPE and low CIN, and new cells get triggered quickly within.

When we carefully inspect the propagation of the system over time, we realize that the surface return current between coordinates 172 and 182 km in Fig 38(e) may well have intensified due to the convergence of the boundary layer flow on the downdraught

front of the second Hector, but that it has actually been installed by prior convergence on that of the first Hector. As a matter of fact, it is very likely that this return circulation has triggered the second Hector when moving over the wetlands, possibly due to stronger moisture convergence and lifting related to surface roughness. The return current does not seem to be (but may have been reinforced by) a cold pool density current from the first Hector, as it does not have the typical defining low temperature and specific humidity; furthermore, no passive tracer from the lower free-troposphere is transported within the current. Consistent with Fig 29(d), and based on the full series of snapshots as given in Fig 35 and Fig 37, we propose the system to have evolved as follows: (1) at 14:00 LT, two major cumulus clouds form over or in immediate vicinity of the wetlands (177 and 182 km). The local PBL is characterized by relatively strong low-level wind convergence, possibly due to the penetrating western sea breeze and strong roughness heterogeneity. There is no particular local specific humidity or sensible heat anomaly, and another major cumulus forms at that time around 205 km, another region of wind convergence and z_0 heterogeneity. (2) 20 minutes later, these two separate systems have grown into precipitating cumulonimbi reaching 4 km in height. By 14:40, they have grown to about 7 km, broken up, and start to dissipate. There is still no major sensible or latent heat anomaly within the PBL. The broken up cloud elements get advected westward from the wetlands in the steering-level flow. (3) At 15:20, a new deep convective cloud gets triggered into the wake of these broken elements, around coordinate 171 km; possibly again due to convergence related to z_0 heterogeneity on either side, but this is difficult to say. (4) By 15:50, the rainfall downdraught of this cloud starts accelerating the PBL westerly, larger values of specific moisture in the lower PBL get transported eastward. Within the next 30 minutes, the cloud rises to almost 9 km, breaks up, and the parts above 6 km get advected eastward. In the meantime, PBL moisture is converging around coordinate 195 km, where a new major cumulus cloud begins to form in an area of high CAPE and low CIN at 16:30. (5) This grows into a new system with two strong rainfall streaks at 16:50; interestingly, a lot of the inflow comes from the rear lower free-troposphere. Deep convection does not develop for long, but merges with the advected upper-level anvil bits, concentrating even more water around this level. (6) By 17:20, the high humidity current in the lower PBL has travelled to coordinate 210 km, where the first Hector is triggered. 30 minutes later, the upper level ice clouds merge with the rapidly developing storm and reduce dry air entrainment. The strong wind shear between the westerly in the PBL and the easterly in the lower free troposphere establishes strong slantwise rainfall. (7) As from 17:50, rather than feeding into the updraughts of the Hector, the mid-PBL flow builds up against the storm outflow, is dragged downward, folds, and flows back toward the west over the surface. An indirect PBL circulation is

established, with its own front facing westward. The feeding current is short-lived, since as the strong rainfall in the first Hector decays, the converging PBL flow is no longer blocked and can continue eastward. (8) The indirect circulation cell maintains itself and is not much wider than 10-15 km. Frontal ascent lifts high θ_e air masses to condensation level atop. (9) Between 18:30 and 18:40, the front steepens over the wetlands, and the second Hector is triggered. (10) At 18:50, the first strong precipitation downdraught splits the circulation cell in two and installs a strong vortex in the frontal part. The trailing part will collapse under the downdraught.

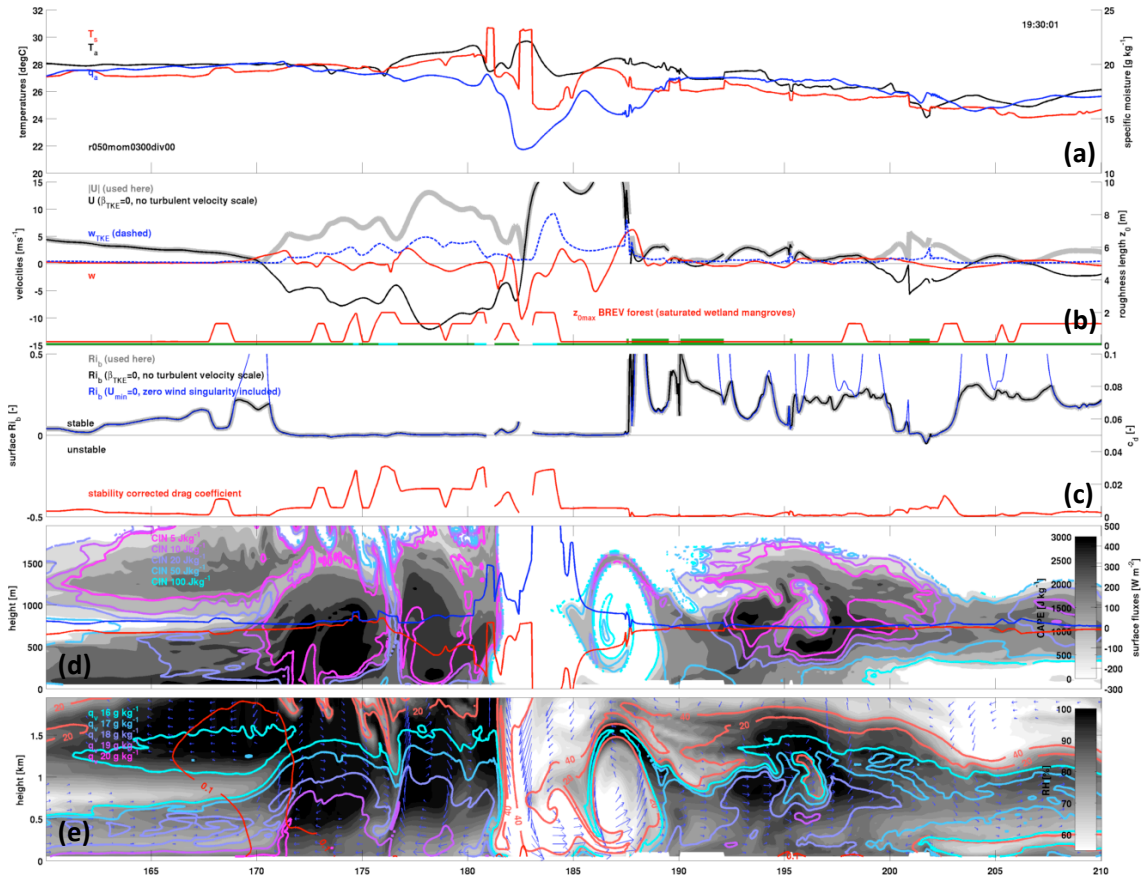


Fig 38 Same as Fig 37, but corresponding to Fig 35(d).

Turbulence and energetics

It is interesting to investigate to what extent the previously described complex dynamics can be synthesized in terms of turbulence power spectra. Besides, turbulence spectra within the PBL as a function of model grid-spacing are a good way to check if the basic assumptions related to the subgrid-scale turbulence closure scheme are met, and how the model behaves at different resolutions. In Fig 39 and Fig 40, we show time-averaged energy spectral densities of vertical velocity w (Fig 39) and of potential temperature fluctuations in space θ' (Fig 40), after Fourier decomposition of the original data extracted along a single line at a given height, within the PBL (at 500 m), the lower

free troposphere (at 4 km) and the lower stratosphere (at 19 km). Since the mean of w is close to zero at any given height, we used the raw field rather than spatial fluctuations; we are interested in the shape of the spectra, their relative differences and variations over time rather than in their absolute values. Our PBL r50 spectra closely follow those in Schröter, Bange, and Raasch (2000), estimated from a 3D 50 m homogeneous PBL LES, with a similarly narrow $k^{-5/3}$ power law wavenumber-range (compared to, e.g. the very wide Kolmogorov scaling in Sullivan and Patton (2011)). Our spectra are also qualitatively similar to those calculated by Bryan, Wyngaard, and Fritsch (2003) for a squall line simulated in 3D, taken at a height of 5 km over a similar range of resolutions. We do, however, not find a similarly pronounced energy peak corresponding to the largest eddies.

Independently of the question whether the model is capable of resolving it, we expect from Kolmogorov's theory a fully developed turbulence spectrum to characterize the unstable PBL, with eddies within an energy producing range, an inertial subrange (IS), where energy cascades without losses down the scales towards a dissipation range, where molecular viscosity becomes effective and energy is lost as heat through friction. The latter occurs at the Kolmogorov microscale, unresolved in geophysical fluid dynamics simulations ($\sim 0.1-1$ cm). The subgrid-scale turbulence closure model used in an LES model presupposes that the smallest of the resolved eddies, determined explicitly by the cut-off filter or implicitly by the model grid-spacing wavenumber, are set within the IS, if possible. The energy cascade in a log-log depiction of the IS for fully developed spatially homogeneous and isotropic 3D turbulence is usually assumed to be characterized by Kolmogorov's $-5/3$ slope, shown in the graph for reference. Our simulations are in 2D. Turbulence, especially during deep convection and near surface obstacles, is heterogeneous. Given the buoyant nature of convection, it is also necessarily anisotropic. The comparison to Kolmogorov's slope is useful nonetheless, as the eddies within the IS are supposedly much smaller in size than the anisotropic energy producing ones, and can often be assumed to be locally both homogeneous and statistically isotropic.

From the previous *a priori* assumptions and the analysis of shallow convection, we would expect to find a peak in turbulent energy production corresponding to PBL height-sized eddies matching the thermals' buoyant updraughts and their characteristic spacing, estimated at roughly 1-2 times z_i (here 0.8-1.5 km), i.e. at wavelengths/scales of 1-3 km (see also Fig 30) or angular wavenumbers of roughly $k_x=6-2$ km⁻¹. This peak can be found in the morning and early afternoon spectra of w (Fig 39(a), (d) and (g)), and to some extent in those of θ' (Fig 40(a), (d) and (g)). Note that the w spectra concentrate more energy within the individual buoyant convective updraughts, whilst in θ' spectra, the largest scales harbour most of the energy, presumably representing the average heating

over the islands. Also, the asymmetry of the signal used, with narrow updraught peaks separated by broader and less intense subsidence regions, may deviate the calculated spectra from their theoretical shape. If our representation is correct, the IS surprisingly starts around wavenumbers of similar order, and is well represented in our higher-resolution runs up to roughly $k_x=10 \text{ km}^{-1}$ (Fig 40), i.e. scales of the order of 500-600 m. Within a neutral boundary layer, the Kolmogorov IS is expected to have an upper bound at scales similar to z_i , or $k_x=8-4 \text{ km}^{-1}$, since larger eddies get sheared on the ground, producing TKE. In the convective PBL, buoyant plumes at scales smaller than z_i may decrease that upper bound to smaller values (Bou-Zeid, 2012, personal communication). Also, the 2D turbulence we simulate within our model setup does not necessarily have to cascade down an IS characterized by a slope of $-5/3$, constituting a reference established in 3D.

Energy decreases much faster at large wavenumbers in the case of the w spectra. The sharp drop towards higher k_x , both for w and θ' , does not represent a resolved dissipation range. It is likely due to a decrease in model performance as we approach the grid-scale. Grid-spacing, although often used interchangeably with resolution, does not represent the effective resolution of the model. Towards the grid-scale, the possible incompatibility of the eddy viscosity-type subgrid-scale model with the filter (implicit grid filtering in ATHAM), as well as numerical errors, increasingly affect the ‘resolved’ flow (see Moeng and Wyngaard (1988)). Eddies smaller than those at scales of roughly 500 m (in r50) are thus unlikely to be captured accurately. Furthermore, the extent to which energy cascading can be discussed, subgrid-scale TKE be trusted, and a 3D eddy viscosity subgrid-scale parameterization be used for simulating 2D dynamics, is uncertain (see Moeng et al. (2004) for a more in-depth discussion on the topic of 2D modelling of PBL convection). The levelling off of the spectra at the upper end of k_x is probably due to numerical noise or under-dissipation of the subgrid-scale model (Bou-Zeid, 2013, personal communication). It also remains obvious from a turbulence spectra point-of-view that simulations at 500 m grid-spacing do not capture the full range of energy-producing large eddies within the PBL during the shallow convection phase, and that the assumption of a model cut-off within the IS is violated. Indeed, cut-off is set at a wavenumber where turbulent energy production is maximum, i.e. at the scale of the convective thermals. At 500 m, these are erroneously simulated at a 2 grid-points scale ($2\Delta x$), i.e. around wavenumbers of 6 km^{-1} . We speculate that this possibly produces a more homogeneous inversion layer moistening and disturbance regime, and therefore, contributes to a delayed triggering of deep convection in those runs.

This mismatch improves later in time during the transition to deep convection, when energy is pivoting towards larger scales in the case of w , and when the shape of the

spectra gradually becomes more comparable for r50, r100 and BL_r. Spectral energy is now higher at largest scales, associated with deep convective circulations. The spectra at different times cannot be directly compared one to another and benchmarked against r50, since all runs follow different evolutions in time. We can assume that a grid-spacing of 500 m is more appropriate for dynamics associated with deep as opposed to shallow convection. Nevertheless, a persistent ‘overestimation’ of turbulent energy at the larger scales within the PBL may be indicative of a misrepresentation of cold pool dynamics.

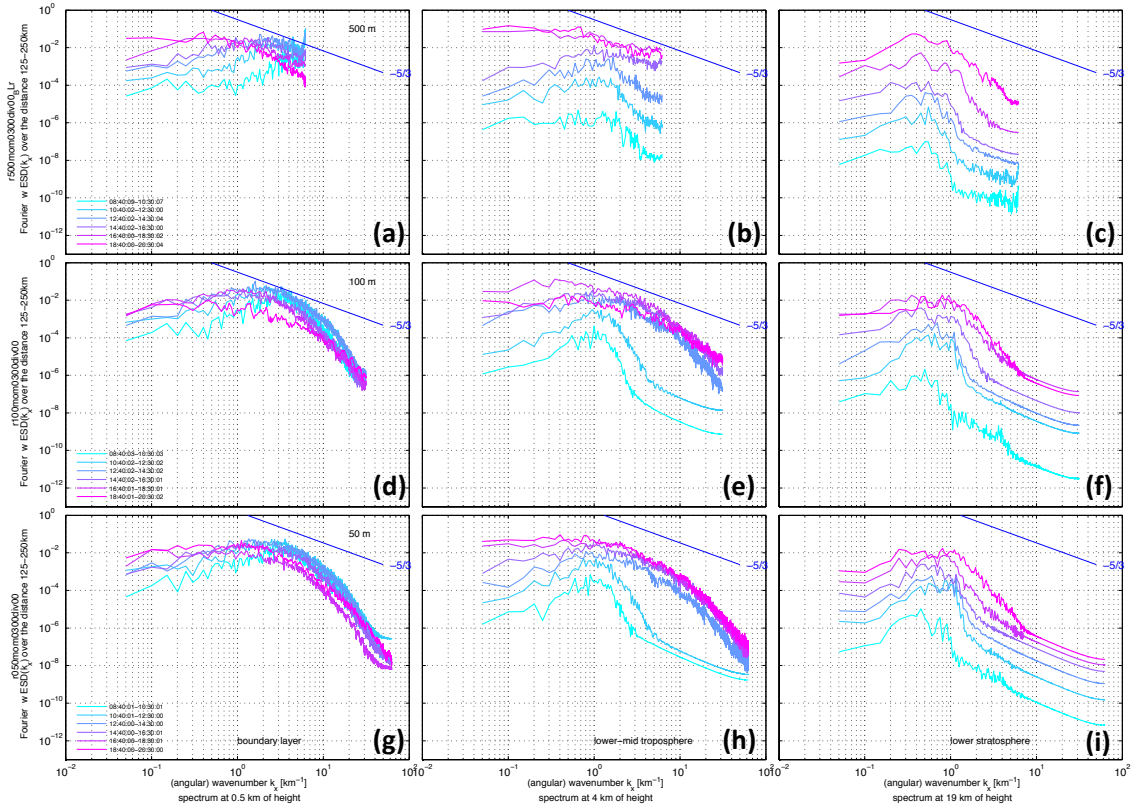


Fig 39 Energy spectral density as a function of wavenumber k_x calculated for simulations with horizontal grid-spacing of 500 m (first row), 100 m (second row) and 50 m (third row), extracted within the mid-PBL (first column), lower free troposphere (second column) and lower stratosphere (third column). The spectra are computed for single horizontal w -transects (i.e. lines) at the given height, and are limited to an area covering the islands (to remove the mean island convergence updraught and the stretched portions of the grid). The largest scale ($2\pi/k_x(1) = 125$ km) matches the size of the analysis window. The smallest scale is limited to twice the grid-spacing. 12 spectra are averaged to smooth 2-hourly ones (coloured). A $-5/3$ slope in log-log space is traced for reference, corresponding to a typical energy cascade in Kolmogorov’s inertial subrange for homogeneous isotropic 3D turbulence.

The spectra within the free troposphere and the lower stratosphere (second and third columns in Fig 39 and Fig 40) are interesting by themselves, even if fully turbulent regimes are not necessarily expected here. The $-5/3$ slope is displayed for reference only. The stratosphere is thermodynamically stable and so is the dry adiabatic troposphere, suppressing (buoyancy-generated) turbulence. It is therefore conceivable that the characteristic peaks in the spectra represent gravity waves excited by convective

development. Interesting also is the presumed transition towards a turbulent regime within the lower free troposphere, earlier for the higher-resolution runs than for BL_r, when the spectra adopt the typical shape for homogeneous isotropic 3D turbulence. We do expect the atmosphere in clouds to be turbulent. Whether the averaged spectrum over the full length of the island, situated slightly above the shallow clouds field, can indeed be characterized by fully developed turbulence, requires further study. Suffice to say that our spectra provide some support for that assumption, though the intersected deep clouds may dominate their shape.

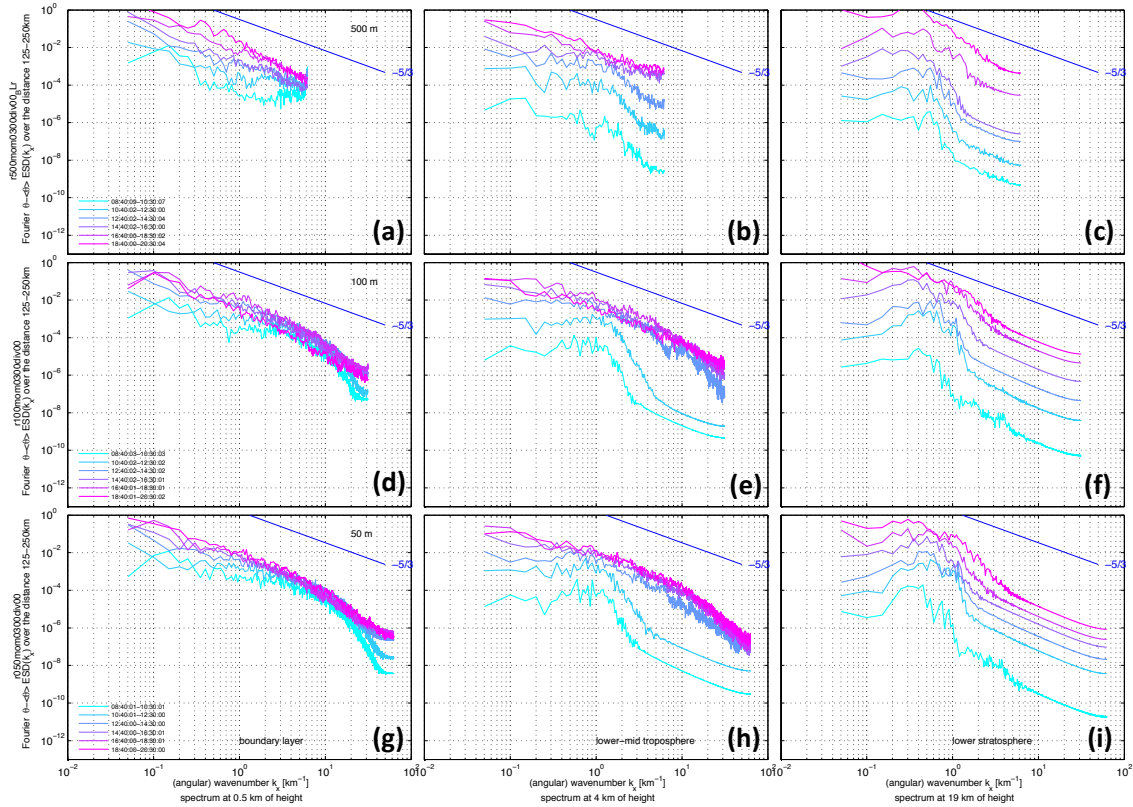


Fig 40 Same as Fig 39, but for spatial potential temperature fluctuations, $\theta(x, z = z_k, t = t_l) - \langle \theta(z = z_k, t = t_l) \rangle_x$

From a grid-convergence point-of-view, analysed through vertical profiles of the subdomain spatial average of u and θ and variance of w , time-averaged over the shallow convection phase between 10:00 LT (excluding spin-up) and 13:00 (onset of first deep convective cells, Fig 41), we verify that r100 converges toward r50. The r100 and r50 mean profiles are nearly confounded. In terms of θ , BL_r develops a less pronounced surface layer when averaged between 10:00 and 13:00, even if in Fig 41(b), this is predominantly the result of partial cancellation between opposite surface layer profiles over land and over sea. The $\langle \bar{\theta} \rangle$ profile is at most <0.2 K higher for BL_r within the PBL, compared to r100 and r50, and the PBL slightly deeper (50-100 m) with a more abrupt

inversion layer. The $\langle \bar{u} \rangle$ peak in the upper half of the PBL is at most $<0.4 \text{ ms}^{-1}$ lower for BL_r , and the surface layer $\langle \bar{u} \rangle$ higher by a similar amount, possibly because of an under-representation of PBL-scale eddies and their effect on the mean flow. Resolution obviously has a strong influence on how well the surface layer can be simulated. The peak in the time-averaged σ_w^2 profile is at a similar height for r100 and r50 as it is in the $\langle \bar{u} \rangle$ profile; it is lower in BL_r (situated around 500 m). Its magnitude is 6% lower for r100 compared to r50, and 39% lower for BL_r . Relative differences between r100 and r50 are largest within the inversion layer and above (up to -39%), but these are less relevant as the absolute values decrease. These larger differences in the inversion layer and above also reflect differences in timing regarding the penetration of buoyant plumes into the layer. Overall, a grid-spacing of 100 m may be sufficient to accurately represent shallow and deep convective processes, even if the trajectories start diverging significantly after the triggering of deep convection.

In general, the previous profiles are similar for runs performed at the same resolution, even if momentum diffusion does have a non-negligible influence. With smaller diffusion time scales $\tau_{\text{diff},\text{mom}}$ (blue solid and yellow dashed lines), absolute values of u decrease, as expected. The variance of w is also reduced. Lower (or no) momentum diffusion (yellow and black solid lines, respectively) enhances u extrema throughout the atmospheric column (only shown up to 4 km in Fig 41(a)), increasing vertical wind shear between the layers. It is possible that increased vertical wind shear, in simulations where deep convection is essentially represented by single columns or updraughts of a few grid-points' width, may have contributed to less intensive convective development compared to simulations with lower shear.

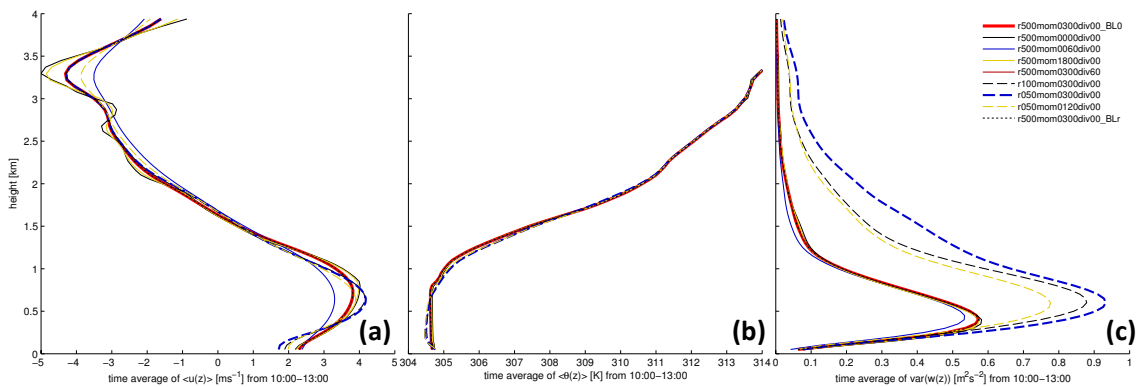


Fig 41 Grid-convergence and influence of model dynamics parameters on lower tropospheric profiles of (a) subdomain-averaged horizontal wind, (b) subdomain-averaged potential temperature, and (c) the subdomain variance of vertical velocity, for land and sea surface areas, and averaged in time between 10:00 and 13:00 LT

We close our investigation into the influence of model grid-spacing and parameters and into the development of convection with a short discussion on latent heat availability, release and consumption throughout the atmospheric column, to provide a link to large-scale model convective parameterizations. The availability of water vapour within the PBL is a major factor influencing the results of a CAPE sounding. CAPE soundings calculated for every model grid-column as a function of time, then averaged over land and sea surfaces separately, are shown in Fig 42(a) and (b), respectively. In spite of the considerable spatial variation in estimated CAPE values, as we found in our previous PBL-surface interactions analysis, the averaged values remain largely monotonous over time, until exposed to deep convective overturning. The light increase over the course of the day mostly reflects the PBL development and the gain in equivalent potential temperature (θ_e) of the lowest 500 m of air parcels that are lifted to estimate CAPE. Over land, the gain in θ_e within the lower half of the PBL is driven by the large increase in θ , as q_v is actually decreasing over time due to PBL growth (see following section for further details). The opposite is true for the inversion layer, where θ_e uniquely increases due to moistening. Over the sea, if anything, the PBL stabilizes slightly and the highest increase of θ occurs at the base of the inversion layer. However, q_v rises dramatically within the surface layer, explaining the average rise of CAPE over time. CIN, calculated for the same rising parcels (not shown), slightly decreases by a few Jkg^{-1} from an initial value around 20 Jkg^{-1} over sea, presumably because of a fast moistening of the surface layer, which lowers the lifting condensation level. It then rises constantly over time by $10\text{-}20 \text{ Jkg}^{-1}$ during the shallow convection phase, as the inversion layer intensifies. Average CIN over land (not shown) quickly falls by almost 20 Jkg^{-1} in BL_r and then remains low during the shallow convection phase, as the gain in θ overcompensates for the dilution of q_v . We do not know to what extent, if at all, longwave radiative cooling of the tropospheric column contributes to the rise of CAPE over the course of the day. The significant differences between runs at different resolutions in Fig 42(a) however suggests that changes in the thermodynamic properties of the rising parcels, and maybe of the inversion layer, are more relevant, since model horizontal grid-spacing should hardly influence free tropospheric radiation during the unperturbed shallow convection phase.

Except for r100, the sharp drops in CAPE arise just after the onset of the phase of most intensive rainfall (Fig 26(a)) and can most likely be associated with the spreading dry cold pool density currents, reducing θ_e within the lowest 500 m dramatically, and stabilizing the boundary layer. CAPE will therefore not give any information on the adjustment of the free tropospheric profiles. As the currents sweep over the ocean, they reduce CAPE equally. More interesting are the outliers in CAPE trajectories. None of *r500mom0000div00* (black solid), *r050mom0120div00* (yellow dashed) and to a lesser

extent r100 (black dashed) produce significant cold pools (Fig 27), which mostly explains their partially maintained levels of CAPE. In spite of *r500mom0000div00*'s and *r050mom0120div00*'s boundary layer θ drops, for example, q_v (and hence θ_e) have small positive anomalies with respect to initial conditions, keeping CAPE up.

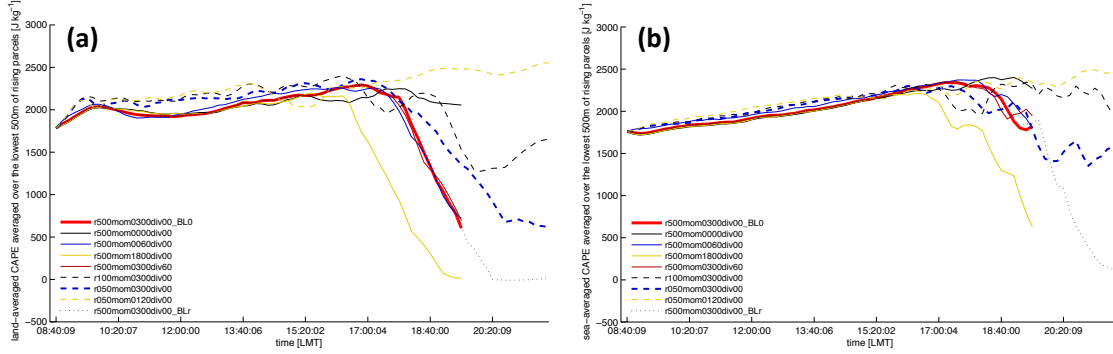


Fig 42 CAPE averaged over the lowest 500 m of rising parcels, and averaged (a) over all land surface grid-points, and (b) over all sea surface grid-points within the analysis subdomain

These outliers are characterized by overall mostly negative subdomain-averaged θ anomaly profiles within the mid-troposphere, roughly between 5 and 13 km (not shown). These are in turn consistent with much-reduced net latent heat release profiles, integrated during model runtime over the entire domain (Fig 43(a)). Integrating all latent heat conversion processes over time, such profiles highlight the dominant effects of sub-cloud evaporation (negative latent heat release in the lowest 1 km) and shallow convection (positive latent heat release peak within the inversion layer). From individual phase transition plots (not shown), we confirm that liquid-gas conversion processes dominate in the model's lowest 5.2 km, i.e. up to roughly above the freezing isotherm. Above, solid-gas conversions dominate. Between 4.7 km (the freezing isotherm) and about 9 km, both coexist. There is hardly any freezing of liquid to solid water and only little melting of solid to liquid, between 3 and 5.5 km, corresponding to falling graupel melting into rain drops. Note that evaporation of liquid to gas reaches much higher up (9 km) than condensation (virtually absent above 6 km); this liquid must have existed either in super-cooled form or in warmer updraught cores.

The net latent heat release in Fig 43(a) is the rather small residual from much larger opposite phase changes in space and in time. The profile is best understood through the analysis of the net effect plotted over time (e.g. Fig 43(c)) and through similar plots for the individual phase changes (not shown). The net latent heat release peak just above 1.5 km is mostly due to the shallow convective phase. Condensational heating is mostly limited to the thin region between cloud base and the neutral buoyancy height. Evaporational cooling peaks around the neutral buoyancy height but has a wider vertical distribution, resulting in negative net latent heat release between the neutral buoyancy

height and the maximum cloud top height as well as below cloud base. The strong sub-cloud cooling is predominantly established during the peak rainfall intensity, but precipitation from shallow convection, whether it reaches the ground or not, also contributes.

During the shallow to deep transition, condensation and evaporation of the developing cumulus congestus and early cumulonimbus clouds nearly balance within the lower free-troposphere. During early mature deep convection, condensation dominates here, whilst the re-evaporation of rained-out cloud elements dominates later. On average, condensational heating decreases with height, albeit less quickly than evaporational cooling does in the lower free-troposphere, roughly between 2.5 and 4.5 km. This results in the second local maximum in the net latent heat release profile, which is thus not due to stronger condensation aloft than below. At 5 km, i.e. just above the freezing level, there is a sharp drop in condensational and a sharp rise in depositional (or ice nucleation) heating. Since latent heat of deposition is slightly higher than that of condensation, given the (small) peak in graupel melting at the same height, decreasing evaporation and increasing sublimation with height, we get a second local minimum followed by a third local maximum in the net latent heat release profile. It is possible that the model crudely captures a Bergeron-Findeisen mechanism between 6 and 8 km.

Because the ice crystals do not precipitate, a large stratiform anvil remains suspended in the upper atmosphere at the end of the simulation. If we transfer this back into the vapour phase without further vertical redistribution, we modify the latent heat release profiles to Fig 43(b), exhibiting a large cooling within the upper troposphere. We have already discussed the potential effect of this cooling and interactions with radiation previously. The vertically integrated energies released (values given in Fig 43(b)) closely match (i.e. are slightly less than) the total amount of deposited rainfall multiplied by the latent heat of deposition/sublimation. This corresponds to only a small proportion of the total amount of energy that has been released as latent heat during the convective overturning; most of it has been consumed again during evaporation and sublimation and consequently led to the vertical redistribution of water vapour. The latent heat release in time for BL_r, r100 and r50 (Fig 43(c)-(d)) merely provide another perspective on the evolution of deep convection as a function of grid-spacing already extensively discussed before.

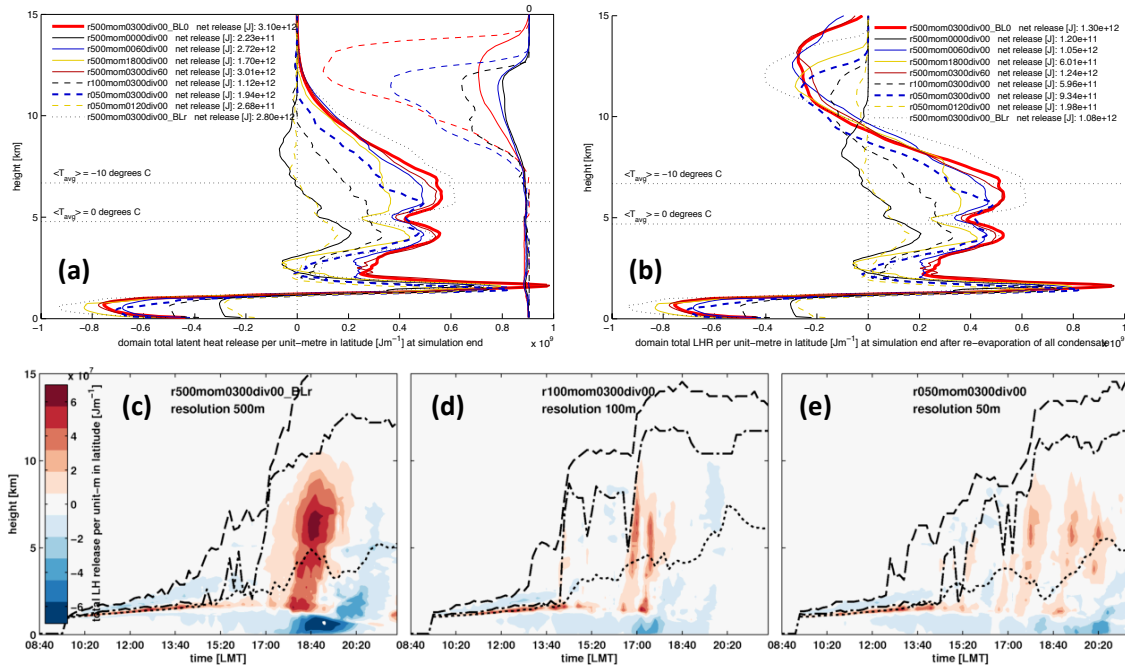


Fig 43 Total energy released over the full model domain per unit-metre in depth, due to all thermodynamic phase changes of water, integrated over the full simulation period. The curves on the right-hand side of (a) further display subdomain-averaged suspended condensate content at the end of the simulations (dashed lines) and total condensate content averaged over time (solid lines) in arbitrary units, for BL_r (red), r100 (black) and r50 (blue). The integrated net release over the profile is given in the legend. The time- and space-averaged 0°C and -10°C isotherms are also indicated; (b) same as (a), but where all the suspended condensate remaining in the model domain at simulation end has been re-evaporated into the vapour phase at the appropriate heights; (c)-(e) total latent heat release as a function of time for the 3 different model grid-spacings. Also given are the maximum cloud top height (dashed line), the neutral buoyancy height, and the subdomain-mean cloud base height as defined in Fig 26.

To what extent is it possible to draw general conclusions regarding the influence of model grid-spacing and momentum diffusion on the development of deep convection from these simulations? In their more rigorous analysis of 3D model convergence with resolution, Bryan, Wyngaard, and Fritsch (2003) remarked upon the lack of convergence down to grid-spacings of 125 m, and the unpredictability of specific trends in analysed diagnostics (precipitation amount and distribution, flow patterns, stability structure, amongst others) as the resolution was systematically increased. They did, however, by far not come across such dramatic differences as we presented here. In line with our findings, their maximum cloud top heights were mostly somewhat higher for coarser grids as well.

Considering the problem of convection initiation from the angle of boundary layer inversion erosion, Sullivan and Patton (2011) remarked from high-resolution LES studies of the convective PBL that the inversion layer entrainment (i.e. erosion) rate increases with increasing grid-spacing due to an inadequate resolution of the mean temperature gradient. We would assume this to lead to an earlier triggering of deep convection at higher grid-spacing, but the key here is the vertical resolution, which remains invariant across all our runs. At higher horizontal resolution alone, we can envisage this turbulent

entrainment rate to actually be faster. We could also argue that the averaged thermodynamic properties within a coarse-grid parcel should make it more diluted and convey it less extreme behaviour than better-resolved parcels or plumes. Likewise, since narrow updraughts need to displace less ambient air, we'd expect them to produce larger vertical accelerations or velocities, as reported for grid-spacings varying between 1600 and 400 m in Khairoutdinov et al. (2009). The opposite seems to be true: subdomain maximum and core mean updraught velocities are less for the higher than for the lower-resolution runs, although there is hardly any difference between r100 and r50. We tentatively attribute this to the nature of entrainment and the width of the cores we discussed previously, in line with the interpretations in KR06. The subgrid-scale turbulence scheme has to handle mixing with environmental air through cloud lateral diffusive entrainment for the coarsely resolved plumes, which might not be very efficient. Yet, we have found the actual turbulent entrainment at higher resolutions to operate mostly through vortex circulations in the wake of the rising bubbles. The latter may be more efficient and occurring on faster timescales. The rising bubbles may also have less straightforward trajectories as the purely vertical motion of grid-column updraughts and eventually succumb to more dilution due to resolved turbulence. Less dilution at coarser grid-spacing has also been found in pure shallow convection studies (B. Stevens and Seifert (2008)), leading to increased precipitation. During the shallow convection phase in our simulations, though, stronger narrower updraughts and an earlier onset of drizzle seem to prevail at high resolution. Moreover, peak downdraughts, less susceptible to changing properties due to dilution, are generally stronger for the higher-resolution runs, apart for the two isolated events in *r500mom0060div00* and *r500mom0300div60*. Mean core downdraughts are of similar magnitude during deep convection across all the runs.

We can also look for explanations in terms of total energy content, and argue that at lower resolution, the available energy gets concentrated into bigger structures, resulting in larger storms, and incidentally, stronger and better-defined cold pools, maintaining and propagating these storms. In essence, grid-spacing acts as a filter on scales. This seems to be consistent with our 500 m grid-spacing diagnostics trajectories (accumulated precipitation, cloud top height, core mean updraughts), subjected to varying degrees of momentum diffusion. From no diffusion (black solid lines) to highest diffusion at the shortest $\tau_{diff,mom}$ timescales (60s, blue solid lines), the intensity of convection steadily increases. In analogy therefore to the resolution argument, higher momentum diffusion concentrates more energy in the larger structures, smoothens the fields, and decreases random convective events (including artefacts) in favour of a more intense and better organized Hector. Interestingly, it does this without accessing more latent heat energy: the core updraughts and maximum cloud top height are higher for *r500mom0060div00*

than for BL_0 (thick solid red lines), although accumulated rainfall and total latent heat release at simulation end are slightly lower. If our argument is correct, the concentrated energy is thus kinetic, as expected for momentum. Deep convection under larger diffusion also takes longer to trigger, presumably because the more organized structures are slower to build up and early risers are suppressed. It is also possible that triggering thus delayed made it possible for more PBL energy to accumulate, fuelling stronger convection. Another argument which is perhaps more physically intuitive is that on average, higher momentum diffusion decreases vertical wind shear in the mean profile, increasing the opportunity for grid-column updraughts to remain intact.

Additional divergence damping at the model top (thin red lines) raises maximum cloud top height and neutral buoyancy height in accordance with strongly enhanced peak updraughts during maximum development (i.e. when updraughts reach highest), narrowing the precipitation distribution.

The startling outcome is that at highest resolution, the impact of momentum diffusion is seemingly reversed. At a diffusion acting roughly twice as fast (yellow dashed lines), convective precipitation is dramatically reduced, even if the maximum cloud top height remains indeed higher. The transition to deep convection is now earlier, rather than later. We could tentatively attribute this to similar arguments as above. With reduced vertical wind shear, narrow but strong early updraught plumes may be more likely to overcome the inversion barrier and reach great heights. Simultaneously, in a better resolved and more turbulent flow, excessive momentum diffusion may impede the growth and evolution of coherent and organized structures.

These arguments are of course rather speculative and are not grounded in solid or statistically-relevant evidence. Also, for shallow convection, the behaviour under increased momentum diffusion seems to remain consistent, in as much as the onset of early precipitation formation (DRZ) is delayed. Here, we may reason that less diffusion increases the likelihood of random shallow updraughts to go high enough for sufficient cooling to produce precipitation. Another avenue left unexplored leads to possible interactions between momentum diffusion and surface roughness z_0 , with potential changes of surface flow convergence and convection anchoring in regions with strong roughness gradients. These, if present, are not obvious in our simulations.

To recapitulate, we find model resolution and momentum diffusion to have an important influence on the overall evolution of deep convection simulated in 2D. Given median convective updraught cores that frequently do not exceed 1000 m in diameter, turbulent entrainment in the wake vortices of rising air parcels is possibly largely underestimated, when unresolved at coarsest grid-spacing. This may then yield more

intensive storms. Lower resolution also possibly acts as a low-pass filter, concentrating the available kinetic energy in the larger, more organized structures. Stronger momentum diffusion conceivably contributes to this energy concentration at coarse grid-spacing, whilst we found it to have the opposite effect when resolution is improved, in which case it may diffuse energy away from coherent structures before they can build up.

The transition to initial deep convection is much earlier for *r050mom0120div00* than for the other simulations, and the sharp rise in cloud cover after 14:00 produces an equally sharp drop in incoming shortwave radiation, reflected as a decrease of the land-averaged surface heat fluxes. It is possible that higher diffusion and reduced structural coherence did not determine a trajectory towards reduced deep convection, but that less available θ_e in the PBL did. In other words, how do the timing and location of deep convection triggering matter? Is our previous interpretation in reality flawed by fortuitous outcomes in a stochastic world? This seems to contradict the findings by J. W. Wilson et al. (2001) who discuss some skill in forecasting, at least roughly, the triggering and evolution of Hector storms, although our simulations might turn out to be more robust in 3D as they are in 2D. It is clear that our quest for finding key elements governing the transition from shallow to deep convection has not come to an end.

An important aim not further stated in the introduction to this study was to verify whether our parameter choices for the much more computationally expensive 3D simulations are justified. We claim that they are, at least within the realm of feasibility, requiring a grid-spacing of 500 m for the Tiwi Islands study. There is some degree of convergence for the simulations with the lower values of $\tau_{diff,mom}$; since the momentum diffusion is artificial by nature, we stick to the upper bound of the analysed values. Clearly, the storm features are not as detailed as when simulated at 50 m, resulting in one big as opposed to two separate Hectors. A 3D 50 m simulation of the event might produce a more accurate depiction of the observed storms, in particular in terms of reduced total deposited rainfall. That said, cloud top height and neutral buoyancy height (a proxy for anvil height) were not high enough in any of our 2D simulations compared to observations, and generally even lower at higher resolution.

5.5 Deep convection triggering in 2D: influence of surface properties

Objectives, setup and simulations performed

From the detailed analysis of snapshots in section 5.4, deep convection triggering, development, and interactions between individual convective cells and storms seem to be

interlinked at multiple levels. These include, but may not be limited to, the erosion and moistening of the inversion layer through shallow convection, the transport of water into the upper atmosphere in successive stages, the role of the sea breeze, of density currents and of indirectly induced circulations, all influencing the boundary layer flow and moisture convergence and forced ascent, and finally the interactions with the surface itself through the exchange of momentum, heat energy and water. Since there is a consistent line of deep convection emanating over the mangrove wetlands, it is intriguing to ask why this is so, and to what extent the surface configuration influences convection, in particular through factors with a possible influence on (moisture) convergence.

To test whether flux anomalies over wetlands, surface roughness, or topography, are likely to contribute to preferred deep convection triggering, we have repeated the BL_r simulation with several idealizations: first, with all topography removed (**flat island**), second, with island-wide averaged roughness lengths (z_0) and displacement heights (d_0) and with the wetlands' soil field capacity and humidity adjustments removed (**smooth z_0/d_0 + no wetlands**), third, with averaged z_0 and d_0 only (**smooth z_0/d_0**), and fourth, with the wetland soil anomalies removed only (**no wetlands**). We revert to the coarser 500 m grid-spacing simulations because of their more straightforward dynamics and lesser computational expense.

Integrated diagnostics

Again, differences in the rainfall diagnostics (Fig 44) are striking. All sensitivity runs produce less rainfall than BL_r. Most surprising is the non-linear and non-additive response of 'mangroves removal'. Removing their impact on sensible and latent heat fluxes (no wetlands) reduces convective rainfall. Removing their impact on energy and surface momentum fluxes through roughness modifications (smooth z_0/d_0) almost completely eliminates precipitating deep convection³⁴. Removing their impact through the combined action (smooth z_0/d_0 + no wetlands) results in an intermediate response³⁵. Fig 44(b) hints at a potential reason for the different rainfall amounts. With the exception of the case where no deep convection occurred, the 4 rainfall spatial distributions taken after the decay phase have similar skewed characteristics. They have an initial peak in the east, where surface accumulated rainfall is greatest, which then drops less rapidly towards the west, often with a reasonably long tail of lower values of rainfall. This is easily misinterpreted as an eastward-moving squall line with trailing stratiform precipitation.

³⁴ Note, however, that z_0 is not only reduced where it is highest (i.e. over forested areas), but increased elsewhere to compensate. This presumably also affects fluxes everywhere else.

³⁵ On a side note, this serves as a stark reminder that *a priori* predictions based on presumed effects are likely to fail in such strongly interconnected non-linear systems.

The motion is, on the contrary, westward, consistent with the BL_r case described previously. Short-lived but intensive Hector storms develop and propagate through forced ascent on their upstream-moving gust fronts. The squall lines possibly decay because the gust fronts are too fast with respect to the westward advection of their parent storms in the steering-level flow. Our simulations produce little deposited rainfall from the trailing stratiform cloud, a consequence of the non-precipitating ice crystals. Total deposited water decreases strongly with a westward shift of the location of the mature phase of the storm. A possible explanation is that a westward-propagating squall line has more space to develop and to intensify by drawing in high- θ_e air originating over land areas within the lower PBL, and resupplied with moisture from the sea via the downstream sea breeze, when triggered further east on the island. Indeed, J. W. Wilson et al. (2001) state that a Hector's dissipation can be anticipated as it moves westward from land to ocean, and occasionally, over land masses cooled by previous storms.

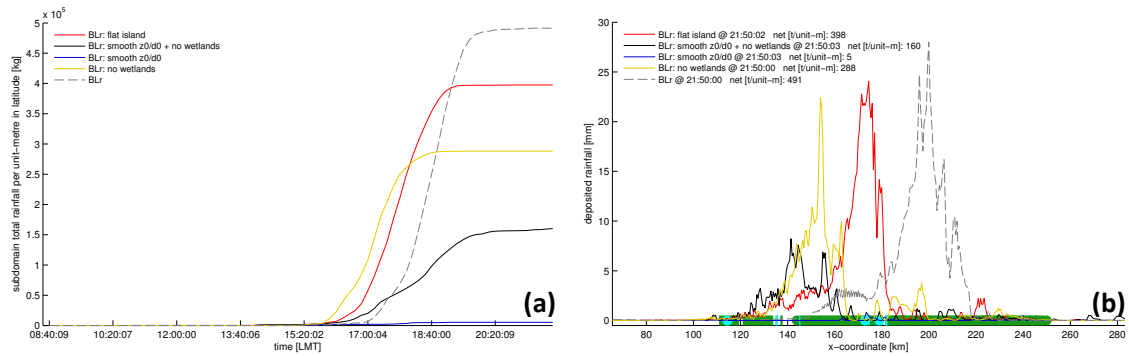


Fig 44 Same as Fig 26(a) and (b), but for the surface sensitivity analysis runs

The Hovmöller diagrams in Fig 45 (and Fig 29) are to some extent compatible with this interpretation. In this line of thought, the location where Hector is triggered might thus influence the intensity of the developing storm. It also seems like 3 (or 4) reasonably clear lines of deep convection emanate from or close to the main regions of strong roughness heterogeneity over Melville Island and that they are triggered more or less simultaneously around the time identified as the ‘drizzle’ (DRZ) onset (Fig 45(a) and (d), Fig 29(a), (c) and to a lesser extent, (d), z_0 not shown). The spacing between high condensed water path columns is roughly equidistant, (which might be indicative of a dynamics effect), but so is that between the z_0 heterogeneities. Without the latter, there is neither such ‘simultaneous’ onset of deep convection, nor is there as clear a spatial pattern (Fig 45(b) and (c)). In the two runs without wetlands, Hectors develop in the westernmost region of Melville, i.e. over the dry mangroves in the run where z_0 remains heterogeneous (Fig 45(b) and (d)). Note also that deep convection was not completely

'blocked' in Fig 45(c). Even if the neutral buoyancy height did not exceed 5 km, several updraughts reached up to 8 km, with vertical velocities up to 6 ms^{-1} .

Otherwise, the shallow convection and boundary layer development is nearly identical across all the sensitivity runs. This can be qualitatively perceived from the individual cloud elements and their condensed water path, as well as in a more aggregate form from the average cloud cover in Fig 45. From a series of figures identical to those in section 5.4, we found that the statistics of the PBL thermals during shallow convection, i.e. up- and downdraught core number, properties, mean and maximum velocities, as well as their qualitative aspects, remain very similar up to 15:20 LT. Only the number of convective cores is delayed in time by about 25 minutes over the flat island up to 10:10, and then remains slightly lower than in the other runs until after 12:00. The area-averaged f_h and f_e hardly differ across the runs in time, and neither does the total shortwave radiative input R_s (Fig 45). If this is surprising at first glance given the extent of the anvil cast over the domain, considerable differences in cloud cover only arise after 17:00, when the solar input starts to decrease rapidly.

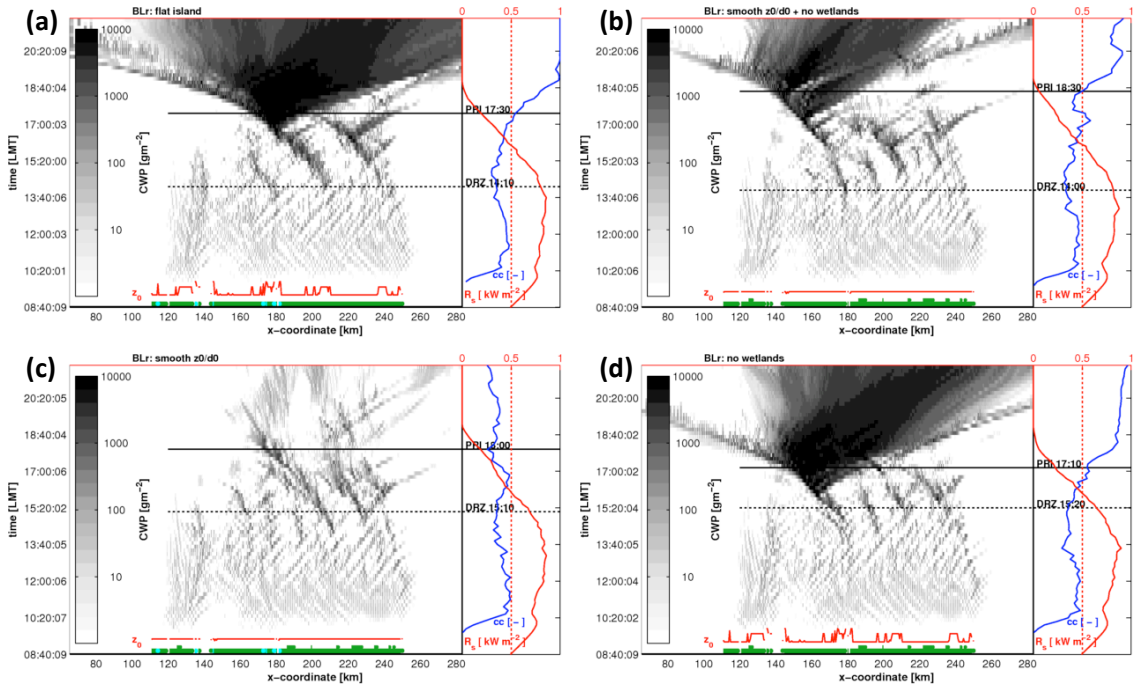


Fig 45 Same as Fig 29, but for the surface sensitivity analysis runs. The surface z_0 used in the respective simulation is qualitatively depicted as the red line.

By 15:20, the average PBL development over land (and ocean) areas hardly differs across the runs in terms of θ and q_v profiles (Fig 46); for example, the largest relative difference in q_v between the simulation with highest humidity in the PBL (flat island, red lines) and that with the lowest (smooth z_0/d_0 + no wetlands, black lines) remains less than 1% all throughout the PBL and reaches a lower free-troposphere maximum value of just above -5% around 2.6 km in height.

We therefore assume that differences in average boundary layer development are unlikely to have contributed much to changes in storm development, even if local effects cannot be excluded.

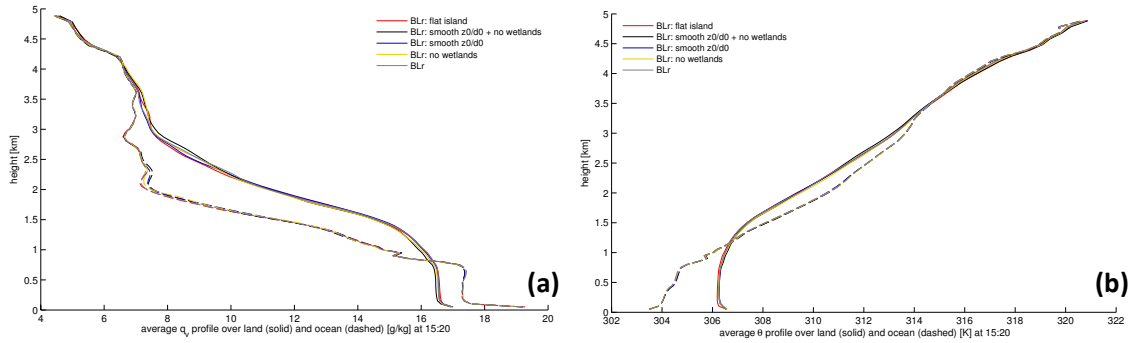


Fig 46 Lower tropospheric (a) specific humidity and (b) potential temperature profiles at 15:20 LT, spatially averaged over land (solid lines) and sea (dashed lines) surfaces.

Surface fluxes, surface layer, atmospheric boundary layer and triggering

Sensible and latent heat fluxes display a very erratic behaviour in time and in space, which mostly reflects varying shading due to elusive shallow cumulus clouds above. Still, we cannot exclude that changes in deep convective development under various surface configurations are directly linked to local changes in fluxes. In order to qualitatively assess the variations in surface heat fluxes across the runs, we have plotted Hovmöller diagrams of f_h and f_e , two examples of which we show in Fig 47 for illustrative purposes; the visible differences for the other simulations are of similar magnitude. The impact of the density current's gust front on heat fluxes is intense but short-lived. The large differences during deep convection set aside, there are few obvious variations in the preceding features during the shallow phase that we can readily link to the different triggering locations in the previous cloud plots. The influence of the wetlands on both heat fluxes (decreased f_h , increased f_e) is easily discernible, but much less so that of z_0 heterogeneity, even if it slightly increases flux variations as well.

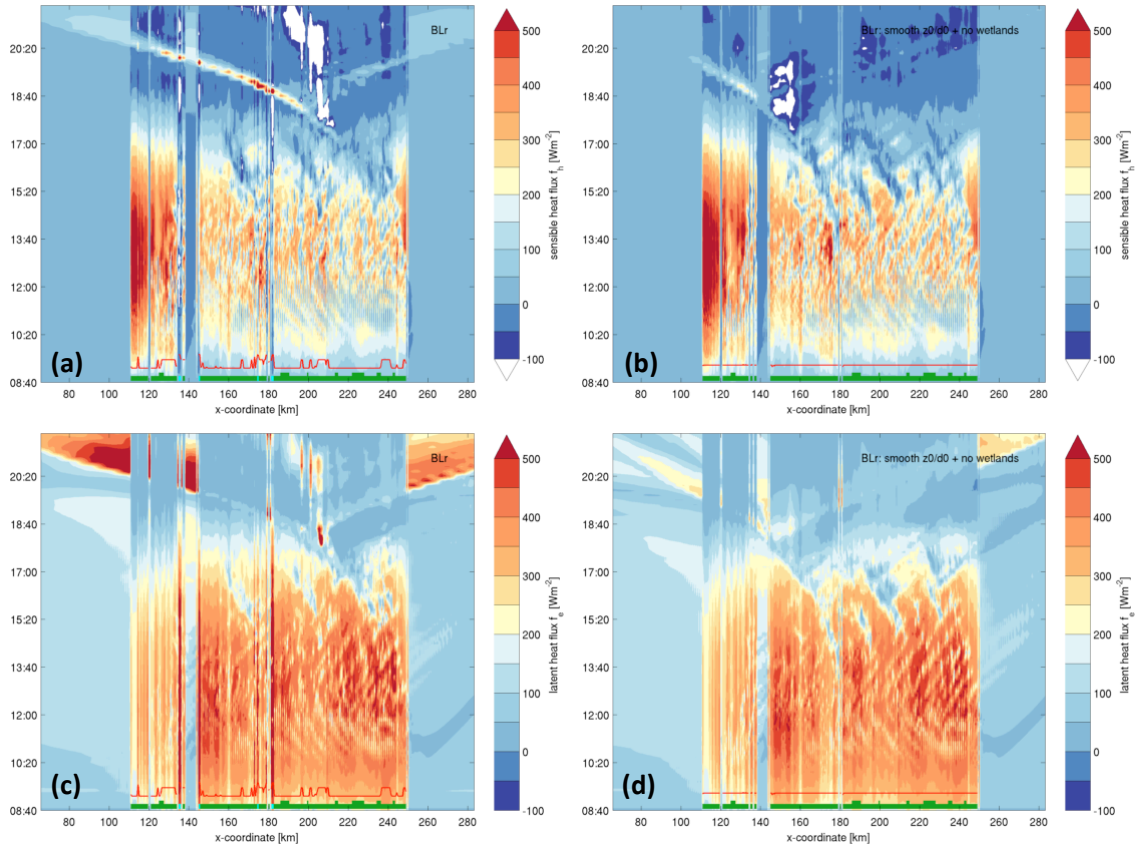


Fig 47 Hovmöller diagrams of the 10 min-averaged sensible (first row) and latent (second row) heat fluxes with surface configuration depicted as in Fig 45.

Spatial similarities and differences in the PBL development across the various runs and over time, as well as interactions with the surface and the free troposphere, are shown in Fig 48-Fig 50, and put the aggregate profiles in Fig 46 into perspective. The erosion of the inversion layer with the associated turbulent entrainment of dry and warm air masses into the PBL is well visible during shallow convection (Fig 48). It is clear that entrainment drying (compare e.g. to observations by Bennett et al. (2010)) and PBL expansion contribute faster to a decrease in q_v over the island than the large f_e over land can compensate for, or than the sea breeze and mean flow advection can replenish.

The turbulent motions set up by the convective updraughts, even if only coarsely resolved, produce a statistically similar but otherwise very heterogeneous entrainment pattern at the top of the PBL. Spatial differences get amplified over time. Random thermal updraughts may be sufficient for the triggering of some initial deep convective cells. By 16:40, circulations and overturning are widely different in the PBLs of the various runs (Fig 49). Hectors have started to form in the flat island simulation (likely triggered on an existing cold pool density current) and in the simulations without wetlands (with associated cold pool currents). The strong drying and cooling of the PBL at different stages of a Hector storm with an associated cold pool is shown in Fig 50.

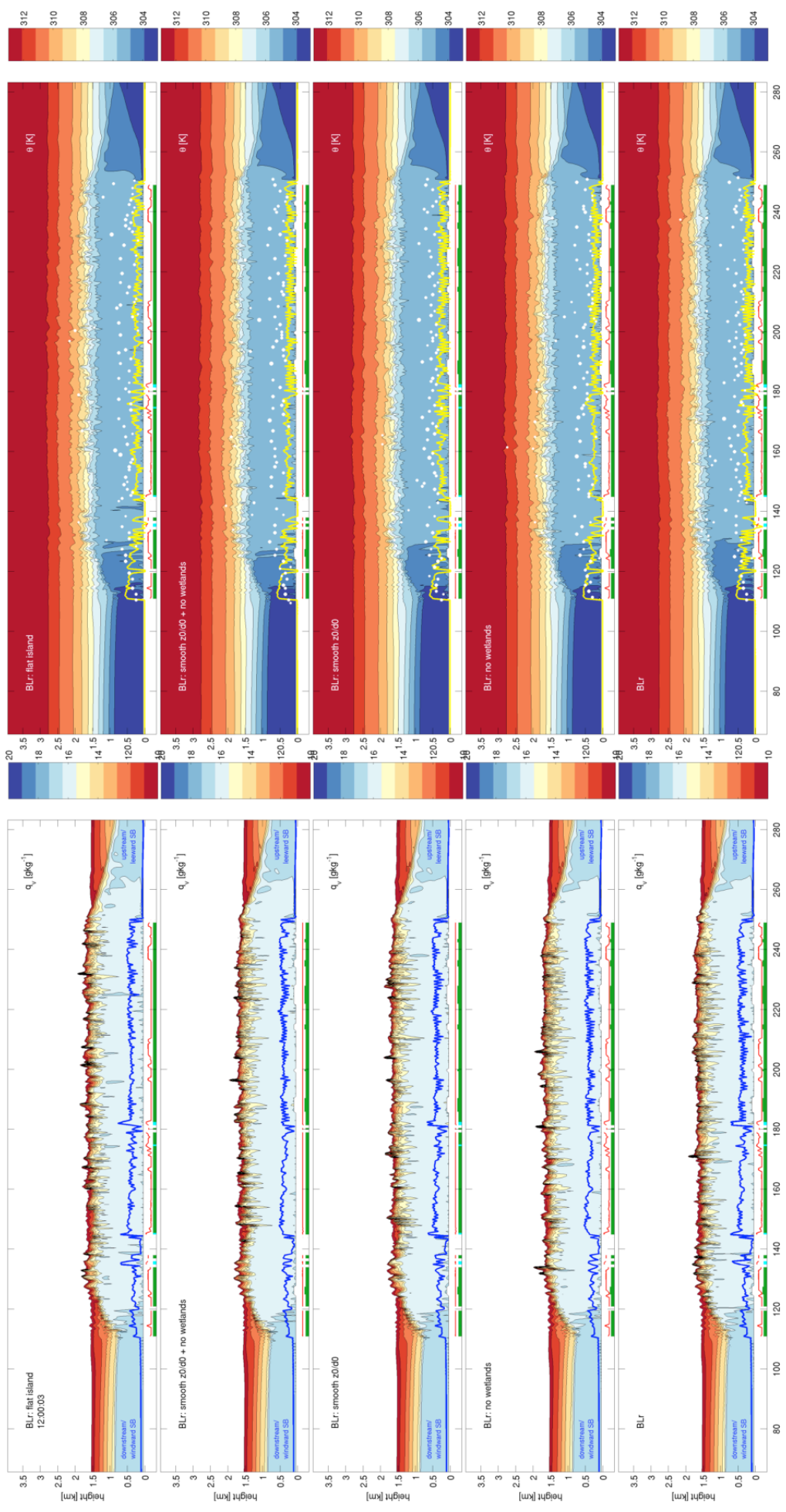


Fig 48 Specific humidity (first column) and potential temperature (second column) as filled contours within the lower troposphere and the PBL for the various sensitivity experiments (rows) at 12:00 LT. Superimposed are the surface latent heat flux (blue line, first column) and sensible heat flux (yellow line, second column). The white dots in the second column are updraught core centroids with size representing their average vertical velocity.

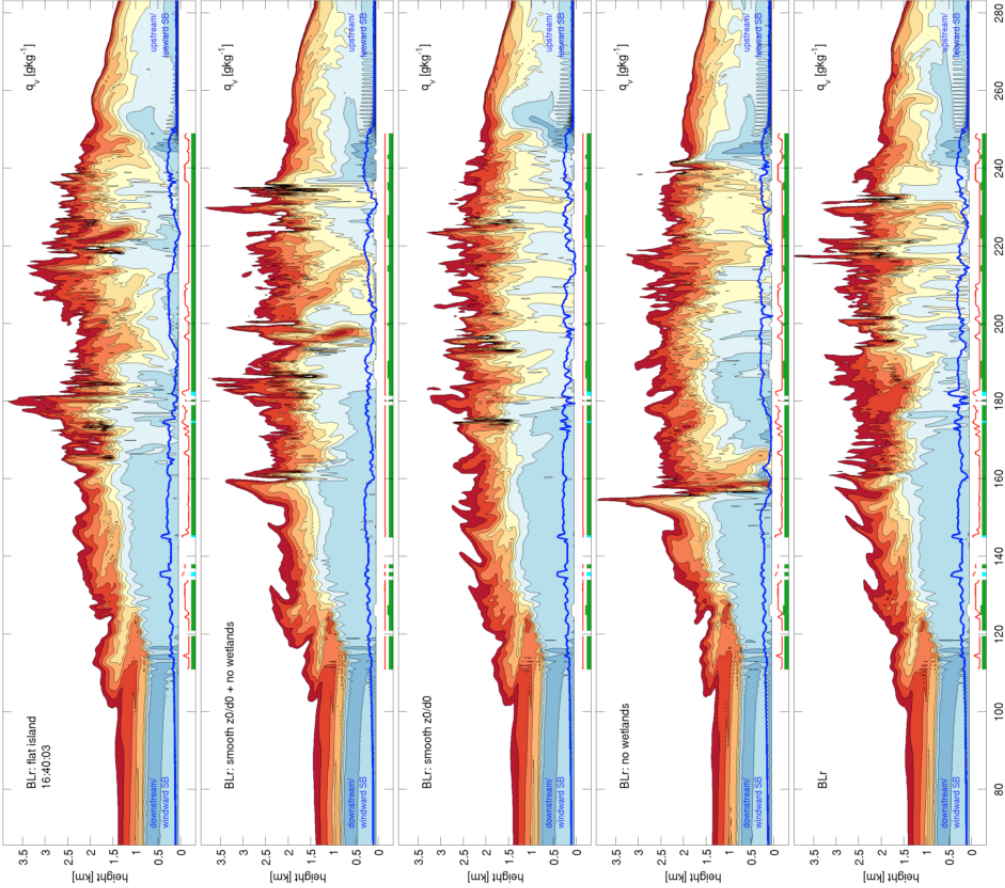
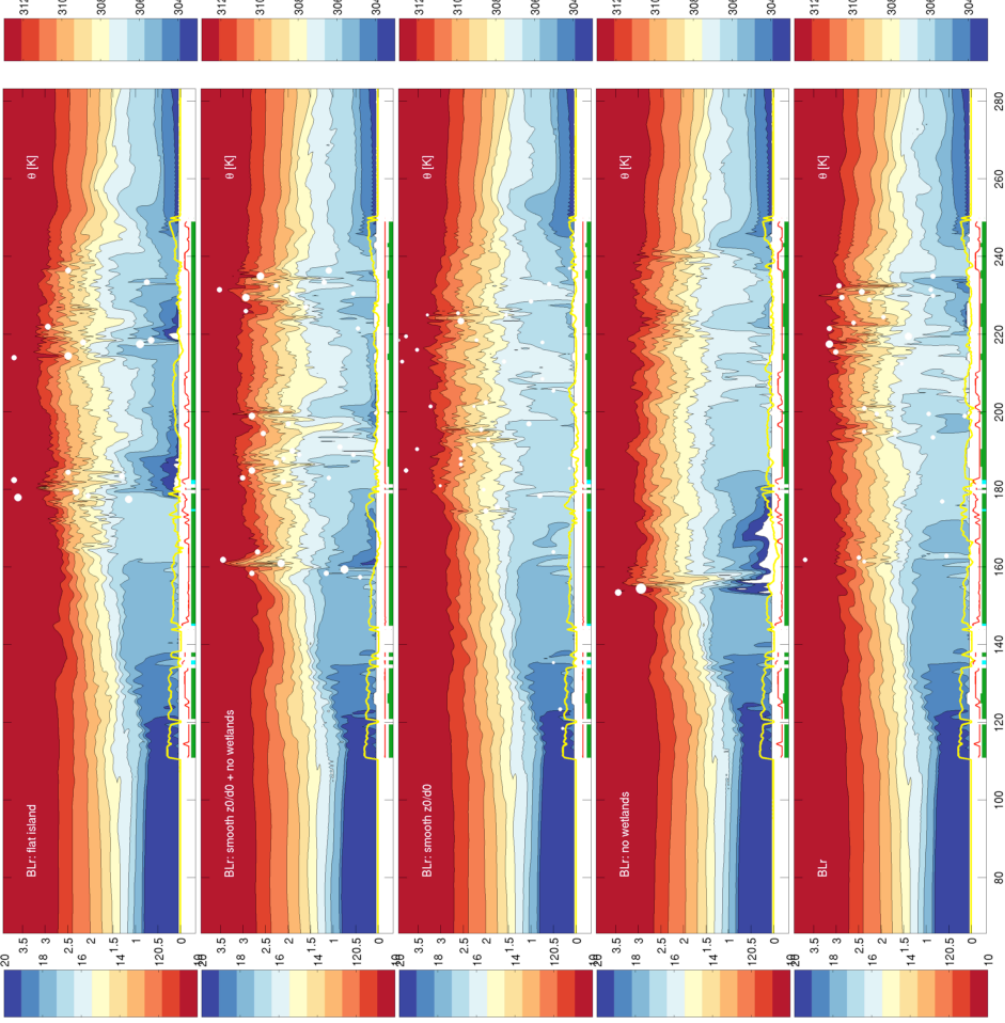


Fig 49 Same as Fig 48, but taken at 16:40 LT



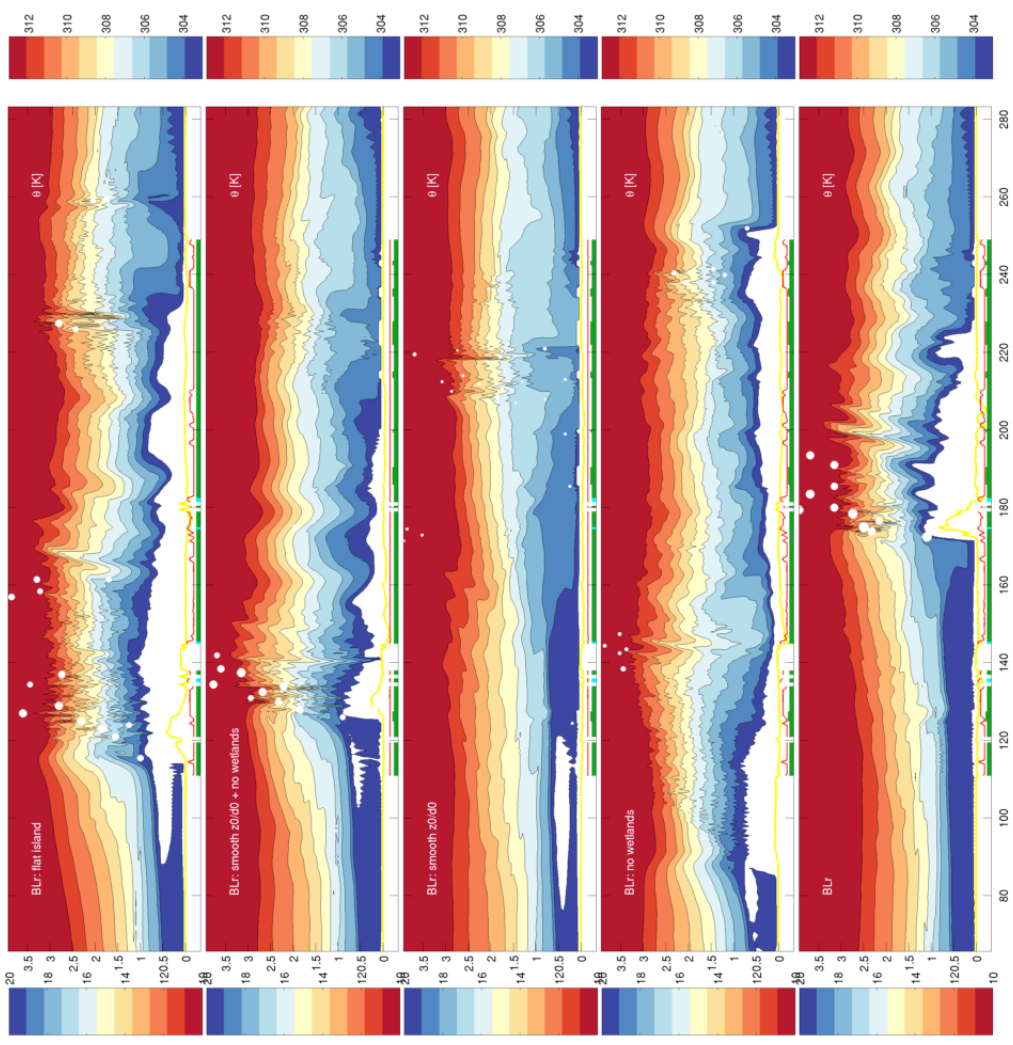
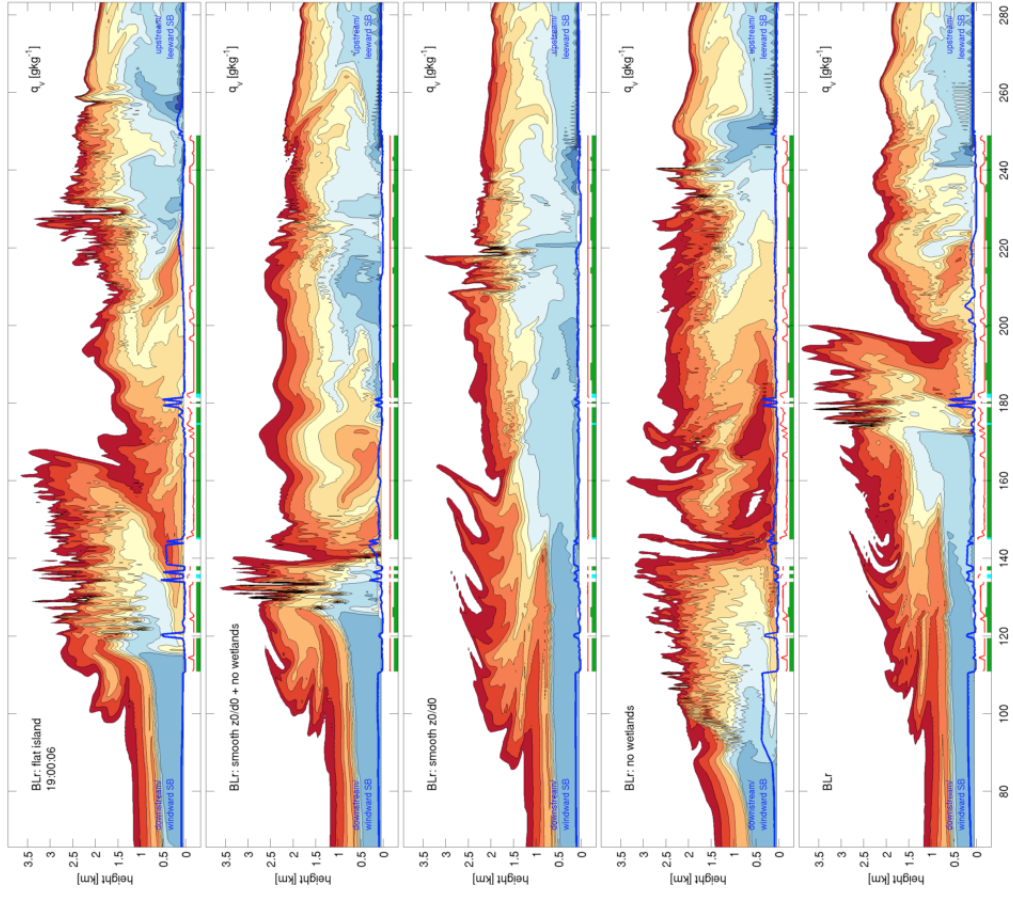


Fig 50 Same as Fig 48, but taken at 19:00 LT

Overall, a clear feedback linking deep convection triggering to surface fluxes is difficult to discern from the previous figures. Since the parameterized fluxes are proportional to the relative differences (gradients) in temperature and moisture between the surface and the overlying air, they are coupled through a regulating negative feedback to atmospheric conditions, in the absence of continuous free or forced convection or advection maintaining that gradient. On the other hand, if we exclude the fortuitous ‘free convection’ sensible heat flux described in section 4.1 for the limit where U tends to zero, heat and moisture transfer from ground to atmosphere increases with increasing winds and thus with advection, given a fixed gradient and z_0 . In the presence of lateral advection, though, the fluxes are not reflected in the actual temperature or moisture changes in the columns directly above and may convey a false perception of the spatial distribution of surface and boundary layer properties. As a matter of fact, when the surface wind U is large enough to significantly enhance the fluxes, so is advection, such that modifications in surface layer heat and tracer concentrations travel downwind considerably. Downwind advection is a possible interpretation of Fig 51(a) and (b), where we depict surface layer, (defined here as the lowermost 150 m to incorporate some vertical mixing), averaged θ and q_v , further averaged in time over the 3 hours preceding deep convection. The period between 12:00 and 15:00 LT captures the highest diurnal fluxes, and time averaging removes the strong fluctuations in the signal due to shallow cloud shading and translates into an integrated effect. We furthermore applied a moving average in space to improve the visual discrimination between the various surface configurations.

It is clear that surface layer θ is largest in the eastern half of Melville (Fig 51(a)), and given that f_h in Fig 47(a) and (b) is largest over Bathurst, this could be readily attributed to downwind heat advection from the westernmost landmasses. The large f_h over Bathurst, in particular towards its western shoreline, is a combined effect of highest U due to the sea breeze (Fig 51(e)), the strong temperature gradient induced by cold ocean air mass advection over the surface (Fig 51(a)), and the unabated solar input due to the absence of clouds (Fig 45)³⁶. Rather than being due to advection, though, an animated sequence of PBL θ (for which a series of snapshots is depicted in Fig 48-Fig 50) suggests that PBL warming predominantly occurs due a combination of surface warming and in particular strong inversion layer air entrainment, which is reduced or blocked towards the west because of the downwind cool sea breeze penetration. The sea breeze and the mean PBL flow thus slowly advect cooler and moister air masses eastward towards areas undergoing strong heating and drying due to PBL deepening.

³⁶ Even if cold ocean air over a warm surface enhances the sensible heat flux, the advected surface layer air would still presumably be cooler.

The surface layer q_v (Fig 51(b)) can be explained by similar arguments, and it initially comes somewhat as a surprise, given that f_e is consistently larger over land than over sea (Fig 47(c) and (d)) and that we initialized the whole domain with a single profile. Over land, entrainment drying exceeds evaporative moistening. Much reduced boundary layer development over the sea provides a concentrated lower-level moisture input from the west with the mean PBL flow and the downwind sea breeze penetration. In essence, the available moisture over sea gets mixed through a shallower PBL, less dry air from the free troposphere gets mixed downwards in an overall more strongly stratified inversion layer (Fig 46(b)), which does not act as a moisture sink through cloud formation and re-evaporation. Furthermore, the temperature drops rather than increases in the atmospheric surface layer over the sea (Fig 46(b)), which stabilizes it. As a consequence, whereas within the PBL at 15:20, q_v is less than 1 gkg^{-1} larger over the ocean than over land, this difference increases to over 2 gkg^{-1} within the lowermost surface layer (Fig 46(a)). Whilst an increased level of moisture gets advected into the drying land PBL with the downwind sea breeze, this moisture is not directly available to deep convection as the sea breeze itself constitutes a negatively buoyant density current that suppresses convection. It will be available later if forced ascent upon collision with a cold pool density current is strong enough to lift it to the level of free convection, but lower temperatures will offset the gain in θ_e due to humidity. Of course, mean flow advection also transports moisture from the sea inland.

The surface layer zonal wind u , here identical to the mean wind U , corresponds to the average value of roughly 2.5 ms^{-1} reached after spin-up of the model, modified by the developing sea breezes (Fig 51(e)). The leeward sea breeze shifts the wind direction in the surface and lower boundary layer, setting up a maximum speed at the shoreline. The windward sea breeze accelerates the flow over Bathurst; after which u steadily decreases towards the gust front of the leeward sea breeze, only several km inland from the eastern shore. This creates the typical average convergence zone in the leeward central part of the island also described by Saito et al. (2001). There is a reduction in speed of the mean flow over the Apsley Strait, which is likely due to another set of sea breeze cells. The other wind speed ‘troughs’ only start appearing after 12:00, and their relationship to heterogeneities in the surface configuration, if present at all, is difficult to determine. It is just as well possible that they can be attributed to local circulations set up by convective cells. This makes causality between lower-level wind convergence and triggering of deep convection equally difficult to ascertain, except in those regions where it is straightforward. In our case, only two such regions exist: at the leeward sea breeze front, and at the eastern shoreline of Bathurst bordering the Apsley Strait. Convergence over the latter (negative $\partial u / \partial x$ in Fig 51(g)) did not trigger deep cells in any simulation.

Convergence over the former triggered deep convection in all our simulations (Fig 29 and Fig 45), but only the cell in BL_r (Fig 29(a)) grew into a Hector storm.

Another region of consistent convergence is located on the western bank of the river crossing 180 km; the river and mangroves on the eastern bank harbouring a region of divergence, at least in Fig 51(g). One could tentatively argue that convergence and a local flow minimum is due to surface roughness, or that surface-level divergence is the consequence of subsidence over the mangroves where f_h and buoyancy are locally reduced. Yet, it is precisely the consistency between the runs that casts doubt upon the relevance of the mangroves, since the only feature present in all simulations is the narrow river itself. In other words, if either the wetland or the roughness characterizing the small patch of mangroves were relevant for local flow divergence or convergence, respectively, we would expect wind field divergence to be different in all the runs where their effects have been removed. This is not the case. We think that it is rather a consequence of the reduced u due to a local convective circulation cell not necessarily linked to the particular surface characteristics. Removing the wetlands changes the Bowen ratio and does have an influence on surface-layer air by locally increasing θ and decreasing q_v , but it does not completely remove the ‘trough’ in θ . The effects remain perceptible downstream of the wetlands up to the eastern sea breeze gust front, probably due to advection. These differences are reflected and amplified in the PBL (lowermost 500 m) CAPE values (Fig 51(d)), which mainly mirror the aggregate θ and q_v values (i.e. θ_e) of the parcels rising from within the PBL. CAPE is largest within the downstream sea breeze and just ahead of the upstream sea breeze gust front. Both boundary layer CAPE and CIN (Fig 51(f)) are highly variable in space and in time, reflecting changes in PBL properties; neither seems to be an obvious well-adapted predictor where, when and how intensively deep convection will occur over the island. That said, when averaged between 14:00 and 16:00 LT, both CAPE is higher and CIN lower over the western half of Tiwi Islands (not shown). This is where most convective rainfall is deposited in all the runs but BL_r (Fig 44(b)), but may be due to initial cold pool spreading in the eastern half. Largest values of CAPE occur within the simulation with flat topography and are due to slightly increased q_v . Increased specific humidity can be a consequence of higher u and thus higher f_e or advection. The sharp rise of CIN towards the coastlines will block storm progression over the sea in the absence of very strong lifting due to, say, intense enough a cold pool density current.

Buoyancy, computed from the model’s density field (Fig 51(c)), incorporates temperature, pressure and specific humidity perturbations, as well as the condensed water mass loading; its variability is almost fully captured by variability in θ alone, and thus provides no further insight into preferential areas of convective updraughts. Surface layer subgrid-scale TKE (Fig 51(h)) predominantly reflects z_0 and topography, modified by

the magnitude of and changes in wind speed. Simulations with averaged z_0 (black and blue lines) generally have higher subgrid-scale TKE over previously smooth areas and lower values over rough areas compared to the other runs with heterogeneous z_0 . Subgrid-scale TKE is overall lowest over a flat island (red line), but with a consistent peak over the mangrove region.

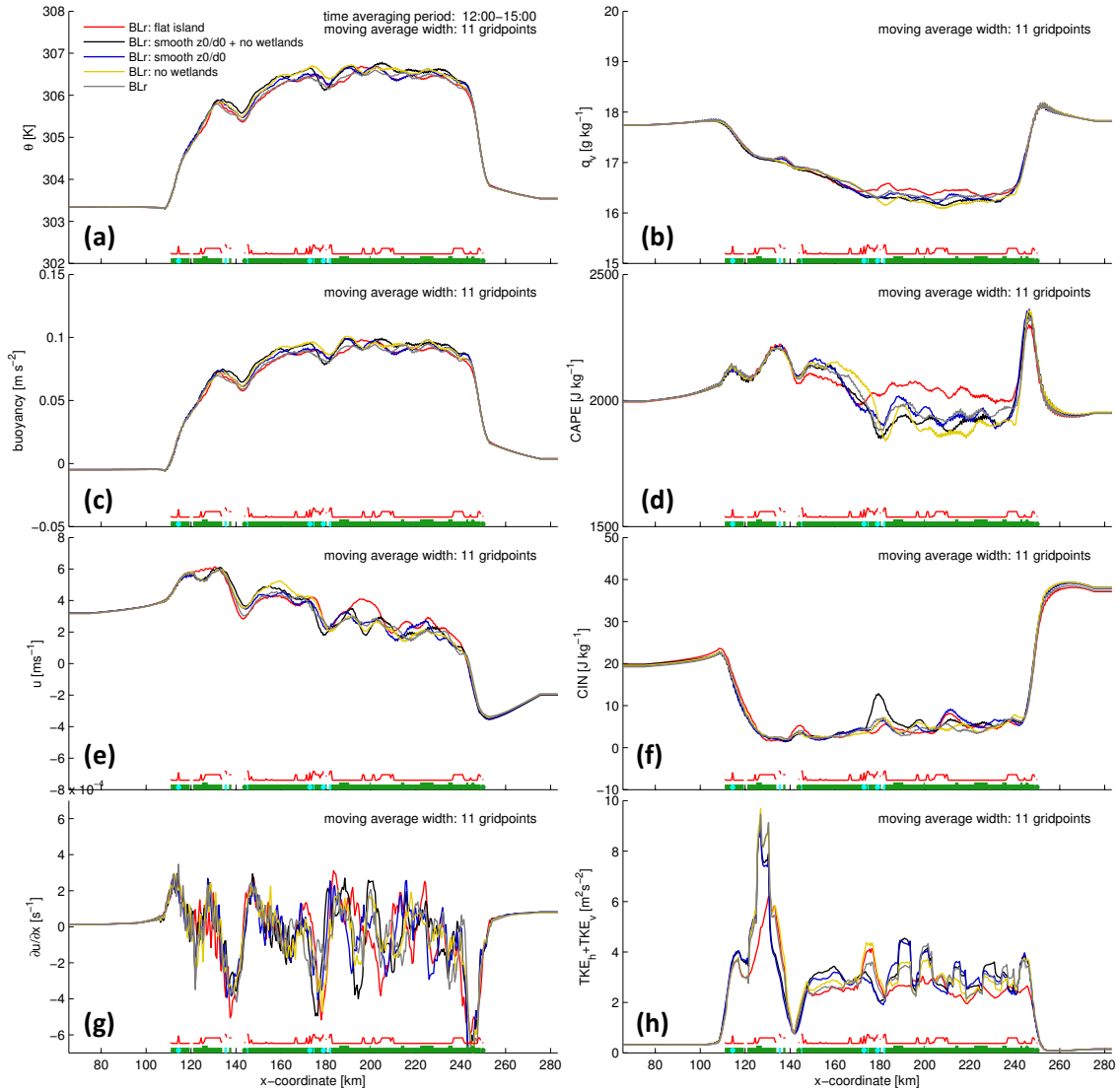


Fig 51 Response of several surface layer diagnostics to changes in the surface configuration. All curves correspond to 3h time-averages between 12:00 and 15:00 LT, the period with strongest fluxes and preceding initial deep convective development; a moving average with a width of 11 grid-points (5 km over land and adjacent ocean areas) has also been applied to smoothen highly heterogeneous signals due to shallow cumulus cover. The surface configuration is depicted as in Fig 45. All diagnostics except for CAPE and CIN have been calculated as vertical averages over the lowermost 3 grid-points (150 m); CAPE and CIN correspond to the same lowermost 500 m averages as used before. Buoyancy B has been estimated from the density field ρ as $B = -g \cdot ((\rho - \rho_0)/\rho_0)$, where ρ_0 is the initial field in hydrostatic balance. The gradient $\partial u/\partial x$ is the only nonzero term of the horizontal wind divergence $\vec{\nabla} \cdot \vec{U}$ in a 2D setup.

A clear link between small-scale surface heterogeneity and deep convection triggering and development did not emerge from the previous qualitative inspections, in spite of the large differences in deep convective rainfall across the set of simulations. To test whether convective updraught cells, starting in the convective PBL, can be associated in a statistically more meaningful way with the surface configuration, we applied the same convective core identification and selection procedure as described in section 5.4 (Fig 52(a)). There is a clear gap of inversion layer-top weak updraughts downwind of the Apsley Strait. Convective activity occurs almost exclusively over the islands. The strongest updraughts seem to agglomerate slightly in 3 clusters: these correspond to the 3 Hector storms also visible in the rainfall distributions in Fig 44(b). By means of core centroid location, we selected only those within the PBL and plotted histograms of their spatial (longitudinal) distribution. We repeated the same exercise for free tropospheric cores, which resulted in a distribution similar to the deposited rainfall (Fig 44(b)). Fig 52(b) shows the distribution of all the thermals limited to the shallow convection and transition phase, and Fig 52(c) the distribution of those preselected on the basis of their mean updraught velocity, prescribed to exceed the average thermal updraught velocity at a given time by 1σ . Since at a grid-spacing of 500 m, the model predominantly produces grid-column updraughts alternating with grid-column downdraughts, (especially during the first few hours), which are advected downwind, it is not surprising that the distribution is relatively flat. Few easily interpretable differences exist across the various runs. For comparison, the spatial distribution of r50 thermals is also plotted, as it resolves PBL processes in a more realistic way. The peak over Bathurst taken aside, even this distribution is relatively flat, indicating that thermals tend to be located everywhere in similar proportions. More revealing should be the distribution of the stronger (significant) thermals, as these may hint at preferential locations for deep convection triggering, if concentrated in space. Significant thermals occur much less over Bathurst, and are more frequent within inner Melville than around its shores, consistent with Fig 47. But clear preferential areas of updraught formation linked to surface properties are also missing here. The strongest peak in the vicinity of the mangroves corresponds to the run where their effects had been removed.

We tentatively conclude that these results do little to support our initial hypothesis that small-scale natural surface variability and an interactive surface response have a palpable influence on the development and evolution of convection. Shallow convection statistics and their effects on PBL development remain robust and unaltered across the various sensitivity studies. The heterogeneous surface fluxes are likely a response to the atmospheric and radiative forcings, governed by internal circulations and cloud formation, but are not necessarily exerting a strong feedback onto these circulations. Since the

transition to deep convection completely differs across the runs, we ascribe this tentatively to unresolved, fortuitous, and hence stochastic and unpredictable, differences of ascent into a conditionally unstable atmosphere. Limitations to the predictability of deep convection over homogeneous land in CRMs have been emphasized through significant variations in convective rainfall (e.g. by a factor 10 in accumulated rainfall) in 2D ensemble runs at 250 m grid-spacing, which differed only in the lowest 200 m white-noise temperature perturbations, especially when the number of deep cells was small (Petch (2004)). The study also suggested that the location and separation of these deep cells was stochastic, hence unpredictable, with fixed surface forcing, whilst little spread over the ensembles was observed during the shallow phase, i.e. before the onset of precipitation, as in Kirshbaum (2011). Petch speculated on the influence of deep cell separation on precipitation efficiency, through hypothetical competition for PBL moisture, organization or radiative feedbacks. He reduced the ensemble spread by strengthening the surface flux forcing. The seemingly stochastic nature of deep convection may indeed warrant the adoption of an ensemble approach, as implemented in various 2D CRM studies (see e.g. Clark et al. (2003) for the simulation of the influence of PBL moisture on squall lines, Kirshbaum (2011), amongst others). In our runs, the lower atmosphere and inversion layer are preconditioned in the same way, the same large triggering mechanisms such as sea breeze convergence are present, and yet a Hector may develop, or not, and attain different intensities. One possible explanation for the successful growth of certain deep events may be a pre-moistened free troposphere in the wake of a previous event. This is, however, difficult to test.

From our 2D sensitivity studies with differences in realistic heterogeneity of various surface properties (soil moisture, surface roughness due to vegetation, shallow topography), we find little evidence for a clear deterministic influence of these properties on the transition between shallow and deep convection in 2D simulations, and tentatively ascribe triggering to stochastic features in the flow. This does not, however, lessen the relevance of convergence lines produced by mesoscale density currents, such as the sea breeze and cold pool storm outflows. Single 2D simulations are unlikely to be suitable for deterministic predictions.

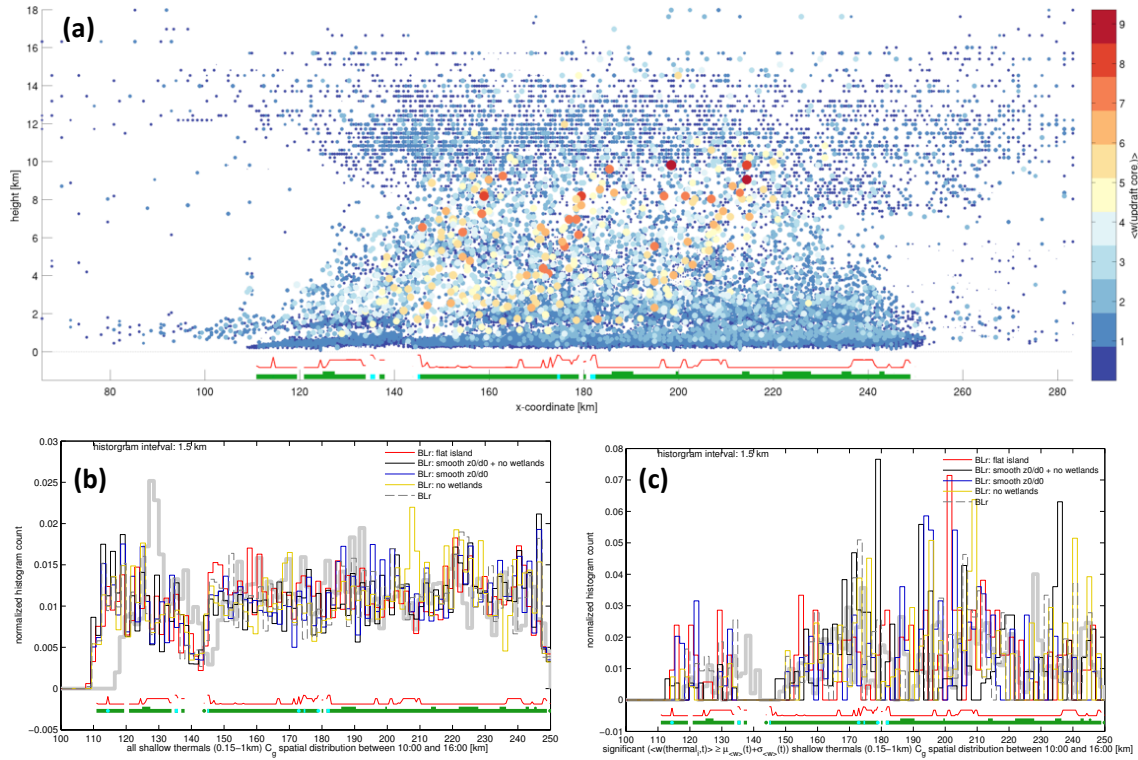


Fig 52 (a) longitude-height distribution of all updraught convective core centroids for every run over the full simulation period. Size and colour of centroids correspond to their average vertical velocity; (b) and (c) spatial distribution histograms of shallow updraught core (thermal) centroids during the shallow convection period, excluding spin-up time. Surface layer centroids (below 150m) have not been selected to exclude small updraughts locked to topographic elements. The successive histograms are each shifted in space by an incremental 100 m to facilitate their discrimination. The thick grey histogram corresponds to the 50 m version of BL_r (r50), shown for comparison; the histogram interval is 1.5 km. (b) all thermals; (c) significant thermals, i.e. only those for which the respective average vertical velocity at a given time exceeds the mean plus one standard deviation calculated across the thermal population at the same time.

5.6 The diurnal cycle in 3D: structure in a convective cloud field and the competing roles of surface interactions and self-organizing circulations

Surface fluxes and comparison to measurements and other models

Before wrapping up this study with a brief analysis of the organization and evolution of shallow convection, the Hector storm and associated statistics under various surface configurations in 3D, it is worthwhile to assess how the simulated interactive surface response compares to that in other models and to verify that it remains consistent with observations. To this aim, we have plotted the diurnal evolution of surface sensible and latent heat fluxes, their distributions, as well as the Bowen ratio, $\beta = f_h/f_e$, estimated as a function of surface cover type, corresponding to the baseline simulation introduced in section 4.4 and compared to remote sensing observations in sections 5.1-5.3 (Fig 53).

Surface heat fluxes over the ocean (simulated with COARE) compare reasonably well to those simulated by Chemel et al. (2009) with the UK Met Office's Unified Model (UM) for the same Hector on 30th November 2005 (Fig 53(b)). The very low f_h evolves nearly identically in both models, and the slow increase over time of f_e is captured by both models. The latter is consistently higher in the UM than in ATHAM-COARE, which may be partly due to a fixed SST in the UM (303.83 K) that is slightly higher than it is in ATHAM-COARE ($303.73 \pm 0.06(1\sigma)$), though more likely reflects a difference in the parameterization and/or the prevailing atmospheric surface layer conditions and winds. Our simulated spatial variability in f_e is comparatively low during the shallow convection phase, presumably because of the very limited extent of the ATHAM domain and the use of homogeneous SST and of periodic boundaries. The sharp increase in both fluxes' mean and spatial variability after the onset of deep convection is due to the extensive cold pool and gust front that develops in the ATHAM simulation, sweeping over the coastal waters.

The picture is significantly different for fluxes over land areas (simulated with HYBRID in ATHAM, Fig 53(a)). If f_h displays a similar magnitude of spatial variability and evolution over time, (governed mostly by the Sun's zenith angle, shallow cloud cover and significant Hector anvil shading), the spatially averaged f_h remains consistently higher in the UM than in ATHAM-HYBRID. Note that Chemel et al. (2009) simulated sensible heat fluxes with the Advanced Research Weather and Research Forecasting model (ARW) and the UM that differed by up to 20-30%, with higher fluxes in the UM. More striking is the difference in latent heat between ATHAM-HYBRID and the UM, in magnitude, time evolution and relationship to f_h . Even though both models exhibit a plateau during peak daylight hours, this is much more extended in the UM, which does not produce a similar stark response to deep convection as does f_h or f_e in HYBRID. In the UM, f_e spatial variability is equally much less during most of the day, not just during the Hector decay phase.

Differences between the two models are best appreciated in space- and time-agglomerated histograms (Fig 53(c) and (d)). Here, the differences in f_e are most obvious. Over sea surfaces (Fig 53(d)), the mode is displaced by roughly -50 Wm^{-2} for ATHAM-COARE compared to the UM. The tails in both surface fluxes are due to the passing gust front. ATHAM-HYBRID's f_e (and f_h) distribution is bimodal (large fluxes during the morning and early afternoon, low fluxes after the onset of Hector), whilst the UM produces a very prominent peak just in between these two modes. Latent heat in the UM is thus presumably much less susceptible to atmospheric surface layer conditions and variations in insolation. The f_h distributions are similar, ATHAM-HYBRID produces larger extreme values in both directions and for both fluxes.

Differences in latent heat can have many origins, both in model initialization as in parameterization, as well as in the state of the simulated atmosphere. Some obvious candidates are soil moisture content and soil physics, as well as vegetation type, abundance and modelled physiology (provided transpiration is not much lower than evaporation). Since the partitioning between sensible and latent heat fluxes, often measured through β , is important for convection and atmospheric processes, and is strikingly different between ATHAM-HYBRID and the UM over land areas, we estimated β for dominant ecosystems in our simulation. These have been determined as a function of percentages of Generalized Plant Types (GPTs) in each grid-box, to reflect the expectedly different physiology and transpiration of the various dominant vegetation types (Fig 53(e)). Also, these β -values can then be more easily compared to point observations at specific sites (as in Beringer and Tapper (2002)) than the fluxes themselves, which will be highly dependent on the local meteorology and conditions. We emphasize that there is not necessarily a direct correspondence (in vegetation type, height or density) between the ecosystems with which our model has been initialized and those found in the field.

During the October-December 1995 Monsoon transition MCTEX experiment, observed ensemble-averaged net radiation peaked at around 600 Wm^{-2} during local noon (Beringer and Tapper (2002)), midday f_e over forests and savannahs lay between 200 and 300 Wm^{-2} . On any typical day at the savannah site, net radiation could peak at 700 Wm^{-2} , fluctuating in the range 300 - 600 Wm^{-2} due to cloud cover (Keenan et al. (2000)). Simultaneously, f_e was easily between 300 and over 400 Wm^{-2} , fluctuating by over 100 Wm^{-2} , which agrees reasonably well with our simulation in terms of both mean values and variability (Fig 53(a), σ roughly between 70 and 110 Wm^{-2} up to $15:00$ LT, not shown), even if our mean value may still be overestimated.

Based on ITEX data, Simpson et al. (1993) had already previously commented upon remarkably high levels of evapotranspiration, dominating over other fluxes, and Bowen ratios similar to those over the ocean (a value of 0.15 is cited). They mentioned average f_e estimates at Pickertaramoor of 450 Wm^{-2} (and correspondingly low f_h), deemed conservative, but consistent with budget estimations of the convective subcloud layer. Along a similar line, surface fluxes should produce enough moisture within the sub-cloud layer to lower the cloud base sufficiently for convection to be triggered and to maintain the observed precipitation with a convective rain production efficiency of between 30 and 50% . Rough calculations, based on coarse estimates of island-wide sea breeze moisture fluxes and vertical ventilation, thus led Simpson et al. (1993) to an attribution of approximately 15% of the moisture source for rainfall to evapotranspiration, compared to 45% attributed to the direct supply of moist oceanic air by the sea breeze convergence and another 40% to downdraught-related exchange processes after precipitation onset.

From the Penman-Monteith method applied to the combined fluxes residual in the energy balance, Skinner and Tapper (1994) derived slightly higher Bowen ratios over Pickertaramoor, on average around 0.29 (pre-Monsoon only, 0.24 for whole period). From point observations, they also estimated a peak value of island convergence due to onshore sea breeze flow of $0.6 \cdot 10^{-4} \text{ s}^{-1}$ around 13:30 LT (their Fig 4). When we average our horizontal wind field³⁷ divergence over all island grid-points, we obtain a similar time evolution for the onshore flow (convergence), but a much more dramatic reversal to offshore flow (divergence) due to our strong density current (not shown). Our convergence, however, peaks around 14:00 LT at values of roughly $1.8 \cdot 10^{-4} \text{ s}^{-1}$. Even if these values are not necessarily directly comparable, our higher convergence hints at a potentially stronger moisture influx from the sea (or, at least, within our model).

Indeed, Keenan et al. (2000) later suggested that the Bowen ratio should be higher still than the previous estimates by Skinner and Tapper (1994), further emphasizing a bigger role of advective moisture transport through sea breeze convergence. In comparison to the more recent gradient-based β -estimates from MCTEX by Beringer and Tapper (2002), our simulated ratios for the dominant ecosystems, dry forests ($\beta_{\text{HYBRID}} = 0.65$ vs. $\beta_{\text{BT02}} = 0.65$) and savannahs ($\beta_{\text{HYBRID}} = 0.46$ vs. $\beta_{\text{BT02}} = 0.50$), match extremely well, even if they are characterized by broad distributions (Fig 53(f)), strongly reflecting the diurnal variation and surface-meteorological dependence of β (not shown). The obvious outlier is grassland ($\beta_{\text{HYBRID}} = 0.53$ vs. $\beta_{\text{BT02}} = 1.08$), but given the fact that our simulation has very few such grid-points and that these still encompass a significant fraction of trees, we prefer to discard these estimates of ours. Also, the measured grassland β was actually recorded during a much drier period (low soil moisture) preceding the other measurements. We simulated very low Bowen ratios only under saturated soil conditions, i.e. in the forest wetlands (previously referred to as mangroves), which yield ratios ($\beta_{\text{HYBRID}} = 0.16$) similar to those referenced by Simpson et al. (1993) and a high likelihood of negative values, arising particularly during the storm outflow. Note also the secondary modes of all Bowen ratios in the negative section of Fig 53(f). These are the result of a positive f_e and more or less strongly negative f_h (see Fig 53(c)), modelled when warm air passes over a cooler surface at a wind speed large enough for stability to tend towards neutral.

It is not possible to tell without further investigation whether the bulk of f_e in HYBRID results from soil evaporation or plant transpiration. Also, Skinner and Tapper (1994) mention measuring a negative substrate flux, i.e. a net heat flux out of the soil, contributing energy to the net radiative input, and Tapper (1988) suggested that advective

³⁷ Averaged vertically over the lowest 500 m

sensible heat flux can supply energy for evapotranspiration. The measured mean surface albedo over the savannah (0.19, Beringer and Tapper (2002)) was higher as the corresponding value we retrieved from satellite data (~ 0.13), affecting the net radiation term. Given certain issues identified previously, simulated fluxes could indeed be too high or off in either direction. These issues include the use of grid-point temperature instead of potential temperature to estimate air temperature in the surface layer, the incorporation of a TKE-based gustiness term and minimum winds to remediate singularities in low-wind conditions and possibly excessive surface layer wind speeds given the treatment of the lower boundary in ATHAM. Further, they include the lack of a canopy temperature and the use of the Ri-number approach for stability in HYBRID, and the possibly inadequate specification of surface aerodynamic roughness length and of the derivation of roughness lengths for tracers.

Nevertheless, we are tempted to claim that ATHAM-HYBRID does a reasonably good job of flux partitioning, even if we cannot ascertain that this happens for the right reasons or that the bulk magnitude of fluxes is adequate. Whilst awaiting more thorough flux validation of the coupled models, we remain confident that the interactive surface responses of both HYBRID and COARE are suited for the purpose of simulating convective processes.

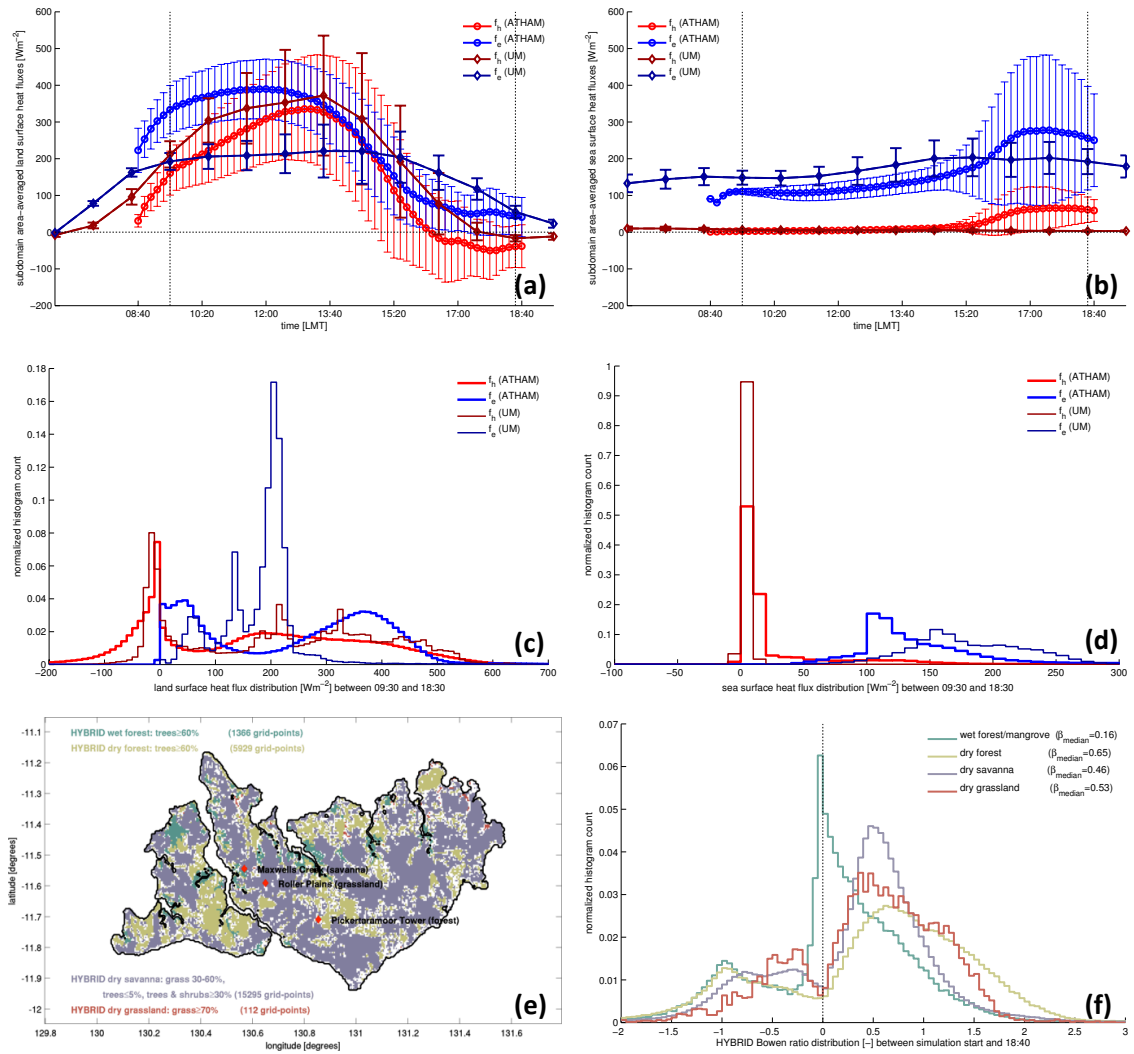


Fig 53 Interactive surface heat fluxes from the 3D Hector baseline simulation (CONTROL). The time evolution of the area-averaged sensible (f_h) and latent (f_e) heat fluxes, bounded by 1σ (standard deviation) in grid-point space, is given separately over (a) land and (b) sea surfaces. Fluxes used are the time-averaged values over each 10 min integration cycle between successive model outputs. The densely-spaced curves correspond to our ATHAM simulation, coupled to HYBRID (a) and COARE (b) for surface interactions; the 1h curves correspond to the UM-simulated data in Chemel et al. (2009), drawn for comparison. The matching histograms for a time period limited between 09:30 and 18:30 LT (vertical dotted lines) are plotted in (c) and in (d), respectively. Major ecosystem types over Tiwi Islands, with which we have initialized HYBRID, are plotted in (e), with their Generalized Plant Type (GPT) composition criteria and total number of grid-points in the legend. The location of 3 of the flux-measurement stations in Beringer and Tapper (2002) is given by the red diamonds. The conditionally-averaged Bowen ratios (f_h/f_e) by ecosystem type are plotted as histograms in (f).

Objectives, setup and simulations performed

In order to investigate to what extent this interactive, highly heterogeneous and transient surface response actually influences convection, we have performed 3 further 3D sensitivity studies with respect to the initial baseline run (CONTROL). The first introduces as the sole difference a small change in the initial upper-layer soil temperature of 0.5 K, raising $\langle T_1 \rangle$ (see Fig 10e) from 30.10°C to 30.60°C (SOILDIFF). This essentially

represents a difference that falls easily within the uncertainty range of observations and one amongst many potential initialization ‘errors’. Note that given the quadratic extrapolation of surface skin temperature, the initial difference of skin temperature is actually somewhat larger. We confronted this small change with a radical simplification of the initial configuration (**ELLIPTIC**). Here, we replaced the realistic heterogeneous initialization with an elliptic, homogeneous and flat island. Surface properties, such as land cover, roughness, albedo and LAI were set to averaged values, and we added a random 0.1 K perturbation to $\langle T_1 \rangle$, to provide seeds for initial shallow convection. The semi-major and semi-minor axes were set to 75 and 35 km, respectively, to produce an island area roughly equivalent to the realistic one ($\sim 8320 \text{ km}^2$), avoiding a significant change of bulk surface energetics³⁸. An ellipse also changes the predominantly concave Tiwi coastlines to convex, even if the realistic SE coastline, giving rise to the strongest upstream sea breeze, was originally also of slightly convex curvature. Last, we repeated the baseline in uncoupled/prescribed mode, releasing over the prescribed surface, set at grid-point-averaged skin temperature, the grid-point-averaged land and sea surface fluxes from the baseline (**SURFPRESC**). The 4 simulations have a very similar land-area-averaged flux evolution (not shown). Only the elliptic case has a slightly lower f_e and slightly higher f_h up to the flux peak in the early afternoon, and thereafter slightly lower values for both fluxes, as well as the expected much-reduced initial spatial variability. Total fluxes and their partitioning thus remain virtually unaltered across all runs.

Integrated diagnostics and statistics

The time evolution of the total accumulated surface rainfall (Fig 54(a)), the most fundamental integrated indicator for the evolution of the convective storm system, already hints at both a much higher robustness of a 3D simulation compared to a 2D simulation, and a fairly low sensitivity of convection to even significant modifications of the surface configuration. Even if initial deviations from the baseline trajectory are larger for the experiments with bigger changes (**ELLIPTIC** and **SURFPRESC**), final amounts remain within a maximum difference of roughly 10% to the baseline, and indeed this difference is amongst the largest for the experiment with a small initialization difference only (**SOILDIFF**). This suggests that our 2D simulations may be excessively sensitive and potentially unreliable.

³⁸ Note that we realized only during post-processing that our original island was actually 10% smaller, covering an area of $\sim 7410 \text{ km}^2$ only; the integrated heat release in the elliptic case is therefore actually somewhat larger.

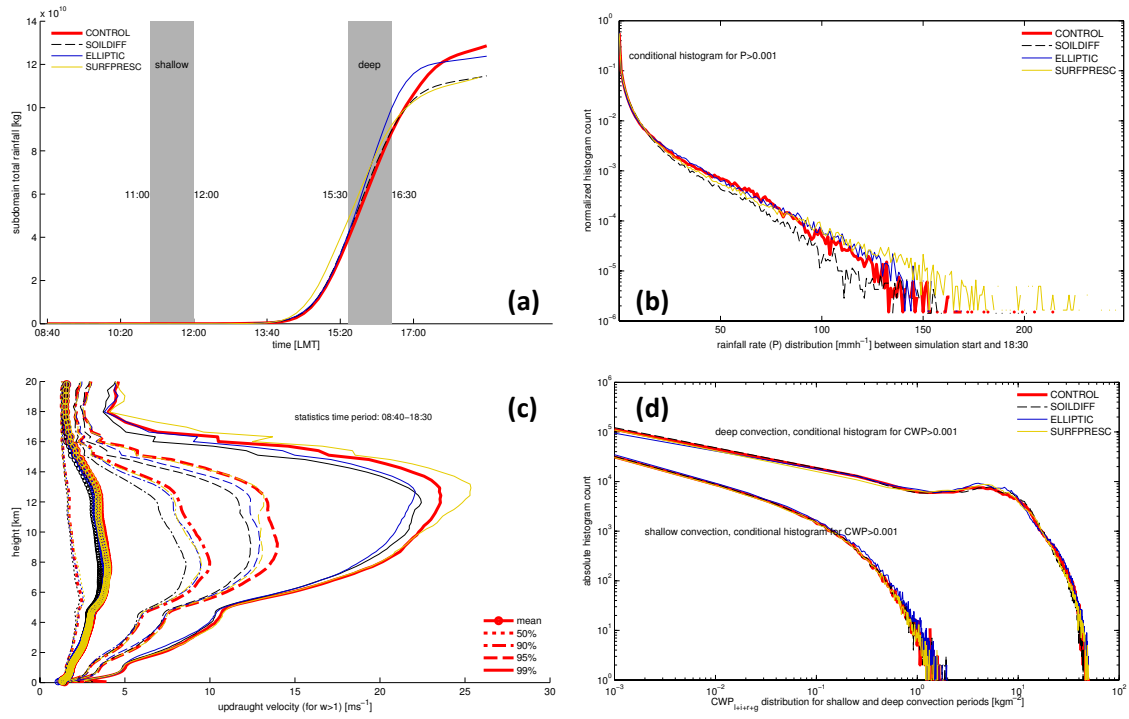


Fig 54 (a) Area-integrated total deposited rainfall over the analysis subdomain, for the CONTROL and 3 sensitivity runs. The two 1h periods highlight time spans used for averaging diagnostics over an arbitrarily-defined shallow and deep convection phase (Fig 55), the latter identified by the maximum rainfall rate (or precipitation intensity), P ; (b) histograms of P , for a range of 10^{-3} - 250 mmh^{-1} ; (c) mean values and percentiles of convective updraught velocities (1 ms^{-1} w threshold applied, no cloud condensate threshold applied); (d) histograms of the condensed water paths, including all condensates, separately computed for the shallow and deep phases (1 gm^{-2} condensed water path threshold applied). Statistics have been computed over all grid-points of the subdomain in space (irrespective of their size) and over all snapshots in time within the specified period, unless otherwise indicated.

The statistical distribution of the rain rate P (Fig 54(b)) does not reveal a largely different picture. If anything, rain rate extremes may be slightly more common in the prescribed-surface simulation, possibly because of a missing coupling between storm outflow characteristics or anvil shading and surface fluxes. The extreme values are, however, very uncommon (log-scale), and the 4 distributions are essentially confounded.

With respect to updraught dynamics (Fig 54(c)), the slightly higher peak in w for SURFPRESC seems consistent with the preceding statement; though mean and median profiles are again hard to dissociate. As before, the impact of major configuration changes on the statistics is small, and less than that for a run within the range of potential initialization uncertainties. In absolute terms, the profiles compare very well in shape to those simulated with WRF by J. Wu et al. (2009) (their Fig 3(c), in pressure coordinates), although our mean and median profiles are significantly lower and our upper percentile peaks at roughly 10 ms^{-1} less than theirs. Some of these disparities are not surprising, as J. Wu et al. (2009) perform an additional in-cloud conditional sampling, (though apparently affecting the results by $<1 \text{ ms}^{-1}$), and the size of their space and time domains for statistics is unknown, and thus necessarily different from ours. We include (existing) updraughts in

the stretched domain over the sea, though these enter as grid-point averages, rather than being area-weighted. Their simulation was run at a 1.3 km grid-spacing (and with 30 vertical levels only), and given our previous findings, a coarser grid might result in stronger updraughts. A sensitivity run of theirs at higher resolution did not significantly decrease their mean updraught speed profiles, though. Discrepancies can also be simply due to the fact that they modelled Hector on a different date (Monsoon break period in February 2006). Note here that early 1D numerical studies were already consistent with observed updraughts exceeding 30 ms^{-1} , confined to regions above the freezing levels (Simpson et al. (1993)). Our simulated maxima are within the range $48\text{-}62 \text{ ms}^{-1}$.

The statistics of clouds, reduced to the total condensed water path (Fig 54(d)) distribution, also do not reveal any obvious variations amongst the runs. During deep convection, a slightly higher cover of thick clouds around the mode centred on 5 kgm^{-2} , (i.e. a slightly larger anvil and stratiform region extent), might exist in the ELLIPTIC case at the expense of the optically very thin columns, but the signal is so low that it does not warrant interpretation.

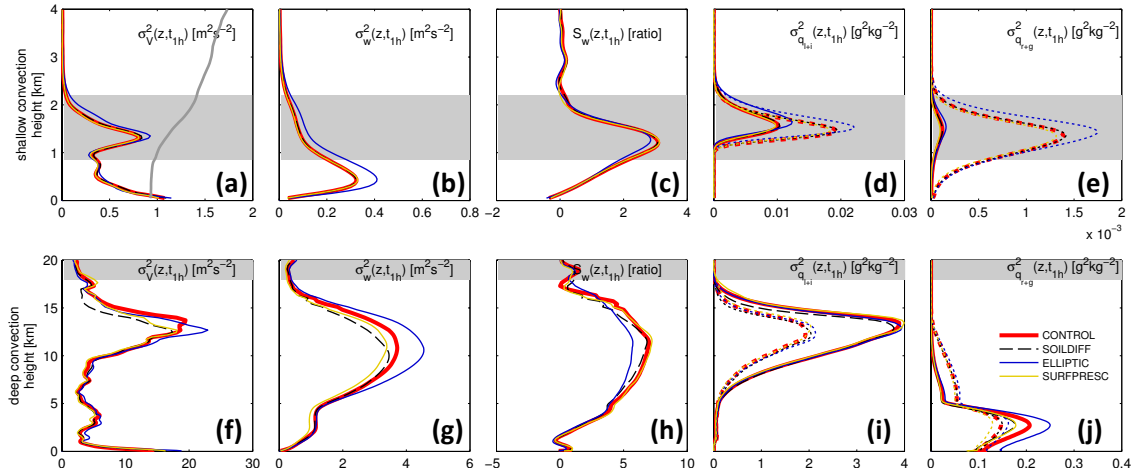


Fig 55 Profiles of horizontal (grid-point) statistics from instantaneous snapshots over the whole subdomain, averaged over 1h periods during the shallow (top row) and the deep (bottom row) convection phases (see Fig 54). The principle stable θ -inversions (PBL inversion layer for shallow convection, tropopause layer for deep convection) are shown as grey shading; they are both diagnosed from the 1h-averaged CONTROL mean θ -profile around 11:00 LT. Layer bottom heights are roughly identified as inflection points (lowermost significant extrema in gradient) in the profile (given for reference as the grey line in (a)), the inversion layer top height is identified here as the very prominent peak in the 1h-averaged θ -kurtosis-profile (and is slightly higher as may be found through other indicators). Shown are ((a), (f)) the variance of the horizontal wind speed V ; ((b), (g)) the variance and ((c), (h)) the skewness of the vertical velocity; ((d), (i)) the variance of cloud condensate (droplets and ice crystals) specific concentrations, and ((e), (j)) of precipitating condensate (rain drops and graupel) specific concentrations. The dotted lines in the last 2 columns show mean values.

Further (higher-order) statistics are presented in Fig 55, time-averaged separately over a pre-defined shallow and a deep phase. Their general features are similar to those

presented in many other LES studies (see e.g. B. Stevens et al. (2001) for shallow convection interpretations). Profiles during deep convection roughly suggest a scaled-up version of the convective PBL shallow plumes. Less detailed structure compared to typical LES studies is expected due to our coarse horizontal grid-spacing. During the analysed shallow convection phase, it is obvious that the thermals penetrate into the inversion layer and rise above the lifting condensation level in the lower third of the layer (Fig 55(d)), which provides additional buoyancy, and reduces the gradient of the w -variance slope aloft in this stable layer (Fig 55(b)). At this moment in time, energy is mostly insufficient for shallow cumuli to break through the inversion and to grow into deep convection; cloud top entrainment is likely to quickly dissipate any plumes that succeed in penetrating into the free troposphere. Peak horizontal top detrainment (Fig 55(a)) is on average just above cloud base. Increasing w -skewness with height (Fig 55(c)) may represent the concentration of upward motion in narrowing (increasingly compact) plumes but S remains a concept challenging to interpret; surprisingly, there is no kink at the bottom of the inversion layer, which suggests that most thermals penetrate to some depth into the inversion. Average precipitation (Fig 55(e)) is very low, with a comparatively high spatial variability. Deep convection mostly detrains at a level lower than the tropopause (Fig 55(f)). Convective cores are most intense, i.e. produce highest w -variance (Fig 55(g)) in the upper parts of the troposphere (compare to Fig 54(c)), variance clearly increases strongly above the freezing level that is just below 5 km. The cloud condensate variance is larger than its mean (Fig 55(i)), but the standard deviation is of similar magnitude, characterizing a relatively uniform cloud deck (the anvil). As for precipitation, the fact that variance is lower than the mean for shallow convection (Fig 55(d)) is misleading, given the fractional numbers. Standard deviation is indeed much larger than the mean, and of similar magnitude as the individual clouds (0.1 g kg^{-1}), as is expected for a highly scattered (popcorn) cloud field. Some precipitation from deep convection re-evaporates before reaching the ground (Fig 55(j)). The kink above freezing level is surprising and is likely due to discontinuities in the parameterized microphysics between the liquid and solid water phases.

Again, the main message however is the virtually identical structure of the profiles for the various sensitivity experiments, with some deviations of the elliptic island profiles.

Structural evolution and storm propagation

Even if the statistics across the various experiments remain similar, one may question whether the detailed evolution of structure in the convective cloud field does not vary greatly if submitted to different surface configurations and interactive versus prescribed fluxes. To address this issue, we have plotted a horizontal cross-section

through the lower-mid-PBL w -field at various characteristic instants in time (Fig 56), except for the SOILDIFF run assumed too similar to CONTROL. Apart for some differences in the details and in location, the structures (size of pattern units, depth of sea breeze penetration, extent of cold pools, approximate location of major downdraughts, direction of system propagation) remain remarkably similar. This further implies the dominant role of internal (self-) organization over the influence of small-scale patchiness in surface forcing and feedbacks between atmospheric circulations and the surface response. In particular, we can identify the familiar pattern of hexagonal open cells with updraughts concentrated around the vertices and outer walls, as well as some horizontal convective rolls near the upwind coastlines, even if our default grid-spacing does not resolve clear features. They have, however, also been emphasized in many previous Hector studies; and Chemel et al. (2009) recently also simulated horizontal convective rolls perpendicular to the sea breeze front within their highest-resolution (250 m grid-spacing) run, characterized by wavelengths of the order of 3-4 km. In a preliminary simulation with a wind field reversed by 180°, we simulated very clear horizontal convective rolls over the entire island in the morning hours, before these decayed into open cells due to the wind slowing down following sea breeze convergence and the heat over the island building up (not shown). This suggests that the relatively straight (slightly convex) SE coastline might be more conducive to roll generation, maybe because it is less likely to moderate the flow and retains the dynamic-thermodynamic balance in favour of dynamic instability for longer. Since other parameters have also changed in the current suite of simulations, this finding would require further simulations and study. Likewise, repeating our runs at higher resolution would be required to investigate whether there is indeed a very faint difference in linear versus cellular organization between CONTROL and SURFPRESC.

Be this as it may, we have also re-plotted Fig 56 with the virtual potential temperature field, a proxy for flux-generated buoyancy (not shown). Here too, the similarities are striking, especially for the fine details in the shallow convective structure. Some larger-scale magnitude differences are fleetingly apparent, presumably because of the averaged effect of a patchy ecosystem distribution in CONTROL. This adds substance to the hypothesis that this structure results from organized turbulent eddies, even if the latter are ultimately driven by (some averaged amount of) thermal instability due to surface fluxes.

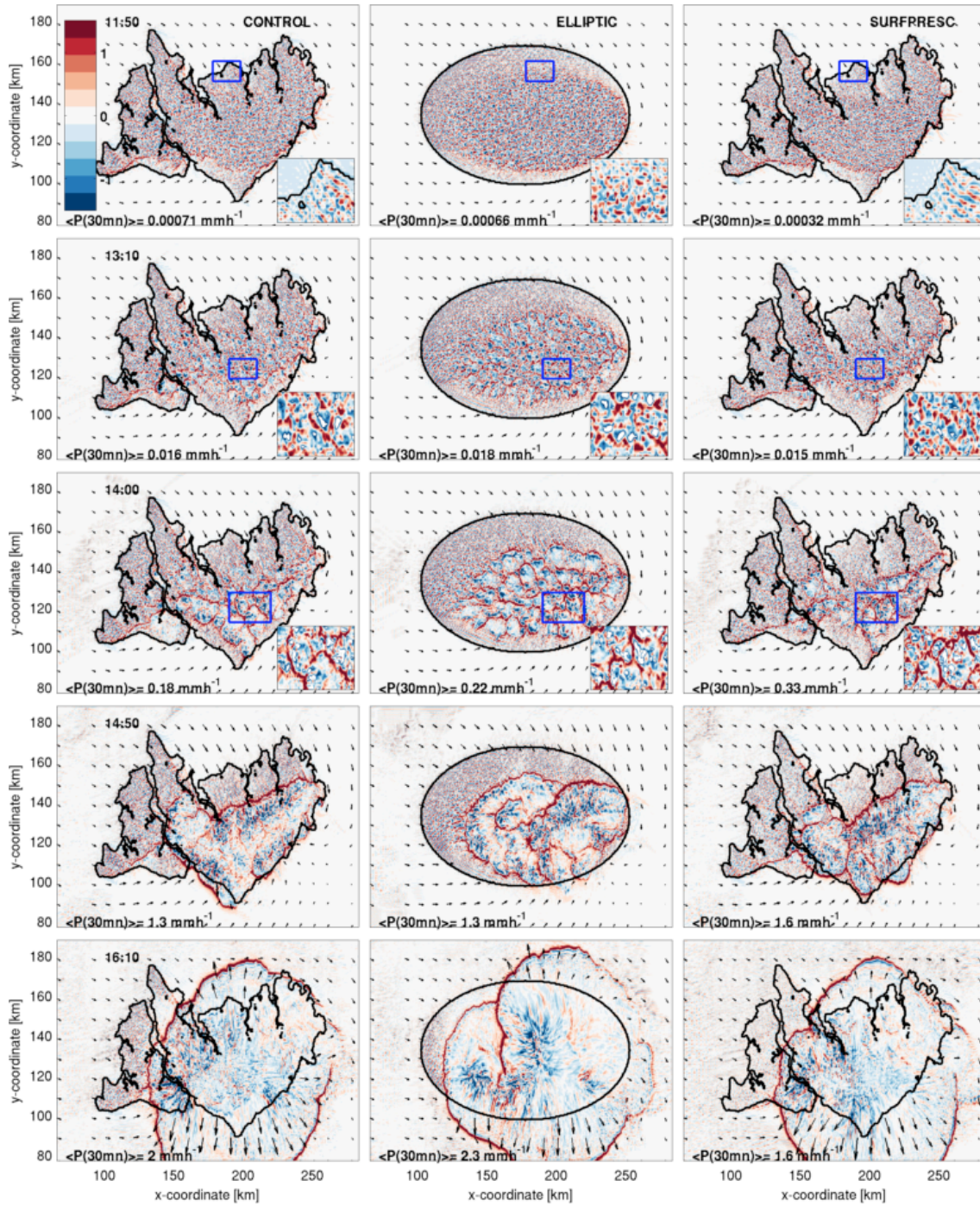


Fig 56 Vertical velocity (w) field snapshots at a height of 300 m, for 3 experiments (columns) and at 5 characteristic times (rows), with magnified areas (blue box) shown in the insets. The superimposed horizontal wind vectors (displayed over the sea only) correspond to the PBL flow averaged over the depth of the lowest 500 m. The 30 min subdomain-area-averaged rainfall rate P is added in the legend.

These results find support in more idealized studies of the convective PBL alone performed at much higher resolution. In their coupled LES-land surface simulation of a convective PBL, van Heerwaarden, Vilà-Guerau de Arellano, and Bou-Zeid (2011) found a cellular pattern in the surface temperature estimated using a surface skin, and a significantly different streaky pattern aligned with the wind, when using a finite soil surface layer with a given heat capacity instead. The latter essentially acted as a low-pass

filter. Remarkably, in spite of these differences, they found similar cross-sections of vertical and horizontal wind speed at the first atmospheric model level, and equally similar averaged PBL profiles. They argued that the cellular pattern in the surface skin temperature represented an imprint of the thermals organizing themselves into the characteristic cellular convection at higher levels. Given their findings illustrated in their Fig 8, this consolidates our belief that surface temperature might be as much a response to convective eddies as their direct driver. In other words, since the same convective updraught patterns seem to occur both in their surface skin experiment, where they are located over areas of high surface skin temperature, and in their finite surface experiment, where they are not, it is difficult to claim that high local surface temperatures alone produce high local sensible heat fluxes which directly drive overlying thermals. In this view, an organized cellular convection pattern arises as much from homogeneous as from heterogeneous surface fluxes, as already found in the very early dish experiments by Bénard (1900). This pattern produces PBL-scale eddies with horizontal wind speeds that are lowest in the areas of convergence under the rising branches, possibly superimposed on an existing regional flow. Minima in wind speed result in reduced fluxes, and the energy balance closure responds via rising temperature, particularly in case of a fast-responding skin. This increases the temperature gradient, and hence, balances the flux again. In the words of the authors of the study, “turbulence can therefore be seen as the mechanism that drives the structure in surface temperature, but apparently, there is no significant feedback from the pattern in surface temperature back to the flow. (...) In a convective boundary layer, the self-organization of the turbulence is so strong that a field of surface fluxes containing small scale spatial variability leads to the same turbulence statistics as a field having spatially homogeneous surface fluxes as long as both have the same area-averaged heat fluxes”. This is in stark contrast to studies using one-way-coupled (surface flux driven) LES models with heterogeneity. In the latter, updraughts are (obviously) predominantly located, or stronger, above patches with higher sensible heat fluxes; and everything else being equal (!), sensible heat would be higher over patches with lower albedo and therefore higher surface temperatures. In similar terms, the simulated flow pattern and the horizontally-averaged vertical profiles of scalar and momentum convective PBL characteristics were found to depend on surface heterogeneity scales as short as hundreds of meters to several kilometres (H. -Y. Huang and Margulis (2009)), provided that these heterogeneities are strong enough to set up micro- or mesoscale circulations. Even in other fully-coupled LES-land surface model simulations with strong initialization heterogeneities (e.g. in soil moisture) on scales of 1-15 km, such differences in flow patterns and the influence on local circulations are still obvious

(Courault et al. (2007), Patton, Sullivan, and Moeng (2005), H.-Y. Huang and Margulis (2012)).

In the case of a passive tracer (dimethyl sulphide, DMS) emitted in a wind speed-dependent way from an ocean, Devine et al. (2006) found that provided that the average flux emitted was the same, surface layer spatial variability of emission mattered little to the (deep) convective transport and vertical redistribution. Even if a passive tracer has by definition no influence on buoyancy and dynamics (as surface heat fluxes do), we conceptualize that heat (as other) fluxes get drawn into a hypothetical surface layer reservoir. The latter gets depleted by convective updraughts that certainly feed on the buoyant instability within the reservoir, but organize themselves spatially into a pattern mainly determined by the dynamics of the fluid.

Ultimately, besides the total accumulated rainfall evolution over time, we should also check its distribution in space, which potentially matters for practical purposes and is a good indicator of the propagation path followed by the deep convective system. This distribution is roughly similar for the 4 runs, especially those with the realistic island shape (Fig 57), and dissimilarities are at least as great between the runs with only a minor initialization difference as between those with and without an interactively coupled surface. The main feature occurring in all simulations is the region of largest accumulated rainfall over SE Bathurst (or an equivalent location for the elliptic island). Allowing for some degree of stochasticity in deep convection triggering, the development of the Hector system over time, visualized by the contours of main precipitation centres during the various phases, also reveals a recurrent pattern. First, initial isolated precipitation clusters form mostly along the southern coastlines, some presumably driven by upstream sea breeze frontal lifting. This continues over Melville, whilst some centres also appear to be preferentially located on the northern side of the EW-orientated hilly escarpment. A strong core then forms just north of the centre of Melville, whilst another one develops in the SE of Bathurst. The latter, possibly triggered on a gust front, then develops into the strongest Hector propagating in a squall line fashion. Further details have been given previously. The massive, (possibly excessive), cold pool density current is central to the evolution of the system, and the location of its outer gust front is akin in all the runs. Beringer and Tapper (2002) estimated that once in a mature state, the interactive exchange of energy was unlikely to have a large influence on a Hector storm's life cycle, even if the surface and fluxes themselves are dramatically altered by the storm dynamics. An interesting follow-up simulation could start from an identical configuration with either the initial soil or the initial atmospheric moisture fields replaced by that at the end of our simulation, to investigate the impact on a successive storm. In reality, at least the atmosphere is likely to be completely recycled over night due to prevailing winds. For

soils, the extent of the precipitation anomaly and the strongly modified Bowen ratio over wetlands might be large enough to actually induce a response.

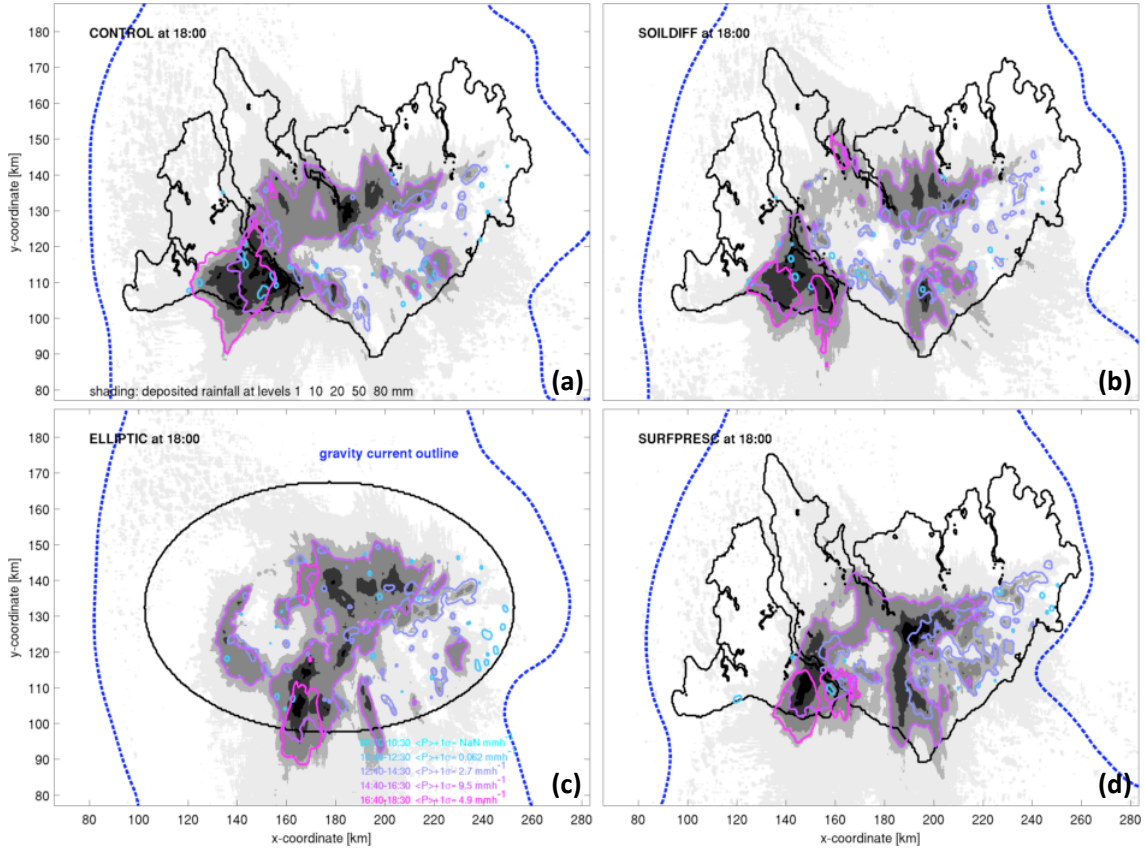


Fig 57 Total deposited rainfall distribution in space for the CONTROL and 3 sensitivity runs at 18:00 LT (shaded). The evolution in space and in time of the storm system is indicated through the coloured contours, delimiting the extent of the maximum rainfall rate, averaged over consecutive 2h periods and smoothed in space with a 3 grid-points moving average. The contours' values, taken as the mean plus 1σ of the 2h time-averaged rainfall rate spatial distribution in the CONTROL run, (and where values below a 10^{-3} mmh^{-1} threshold have been discarded), are shown in the legend. The dotted blue lines delimit the approximate extent of the cold pool density current (gust front) at 18:00. They highlight the edge of an indicator, $\left(\left(\rho_s - \langle \rho_s \rangle\right) / \langle \rho_s \rangle\right) \cdot \left(q_{v,s} - \min(q_{v,s})\right)$, calculated as a function of the density perturbation and water vapour specific concentration, vertically averaged over the surface layer (lowest 150 m, subscript s). Vapour anomalies are used to reduce the effect of dynamic pressure perturbations on the indicator, and all input fields and the indicator itself have been smoothed with a 5 km filter semi-width.

Contrary to our 2D simulations, the storm system evolution in 3D is robust, largely unaffected by differences in surface configuration and initialization, and likely to be predictable. The strong sensitivity of our 2D simulations to model initialization, parameters and resolution, discussed in the previous sections, casts some doubt on their reliability, and potentially on their usefulness as “superparameterizations” of deep convection. The prescribed surface experiment was run with a set of averaged fluxes over land and sea areas that matched those from a realistic and fully-interactive simulation. Further simulations would be required to test if convective development remained the same if the prescribed

fluxes were introduced from a priori assumptions, typically distributed symmetrically around local noon, and thus, if a coupled model is required at all. We can conclude that as long as the bulk magnitude of the surface energy fluxes, and their partitioning into sensible and latent heat (Bowen ratio), remain unaltered, as has been achieved in this case with a coupled model using averaged surface properties and a simplified initialization, the detailed heterogeneous spatial distribution of these fluxes might matter less to convective development, structure and organization. We need to stress, however, that our findings may not hold in an area less strongly forced diurnally as is the case for island convection, or when more pronounced differences exist in land surface properties, predominantly if characterized by patchiness scales of mesoscale extensions.

Chapter 6

Concluding remarks and outlook

In this dissertation, we have described the development needed for coupling an advanced physiology-based vegetation (and soil) model (HYBRID) and a state-of-the-art sea surface flux algorithm (COARE) to the Active Tracer High-resolution Atmospheric Model (ATHAM). Through the exchange of fluxes of sensible and latent heat, this interactive response links the surface to the atmosphere above, and provides the energy and moisture driving atmospheric convection. Using high-resolution detailed numeric simulations of the Tiwi Islands Hector deep convective storm as a test-bed, we studied the full diurnal cycle of the storm from initial shallow and dry convection to storm decay, with particular emphasis on the atmospheric boundary layer, structure and organization in convective cloud fields and the triggering of deep convection. Since these are likely to be driven as much by internal dynamics as by surface fluxes, processes strongly influencing buoyancy and convection-scale dynamics, in particular radiation, cloud microphysics and turbulence, and second-order effects due to model formulation, were investigated with separate idealized simulations. Of direct relevance to the life cycle of clouds is entrainment and mixing, the effects of which we have further investigated through simulations with different diffusion settings and grid-spacing. The influence of a realistic land surface cover with small-scale patchiness and heterogeneity has been explored both with 2D and 3D sensitivity studies. We have also extended the model with a remote sensing observations emulator (COSP). Comparison to satellite and radar observations reveals good agreement, especially in terms of storm timing and propagation, though it is possible that the extent of the Hector is overestimated at the baseline grid-spacing of 500 m. As we simulated median convective cores to be roughly 1000 m wide, we join a long list of references in the literature recommending a model horizontal grid-spacing of about 100 m at most for simulations of deep convection. Simulated fluxes and measured data documented in the literature and collected during separate field campaigns are consistent.

We therefore have confidence in the model to reproduce qualitative and quantitative features of a Mesoscale Convective System, even if there are some differences to the observed case we tried to simulate. In comparison to volumetric, actively- and passively-sensed cloud top and *in situ* properties, simulated convection may have been

slightly too extensive in area, whilst producing too low and too broad of an anvil. The timing and the temporal evolution of the system, including the development of squall line-type convection after initial triggering on the sea breeze front have been extremely well captured and also match with qualitative descriptions from field reports and the statistical description of Hector storms.

Beljaars and Holtslag (1991) concluded that it was unclear to what degree details in land surface physics needed to be captured in weather and climate prediction models. Our 3D simulations do not support a strong influence of small-scale realistic surface patchiness and of an interactive surface boundary on the convective field structure and storm dynamics or life cycle. These seem to be driven predominantly by organized turbulence and internal dynamics, provided that the mean energy fluxes are captured correctly, that they produce a thermodynamic profile with sufficient convective available potential energy, and capture the larger thermally induced mesoscale circulations, such as the sea breeze. An interesting extension would be a simulation over a hypothetical archipelago of islands with the same total area as the Tiwis. Since Tiwi Islands constitute a very particular environment, with finite winds, a strong sea breeze convergence forcing and large moisture availability from the Tropical Warm Pool surrounding ocean areas, we are wary to make statements regarding the extent to which these conclusions or other results presented herein can be generalized. Many studies support a stronger role of surface flux heterogeneity, but often rely on idealized, larger-scale and forced-flux patchiness. In any case, we doubt that further modifications, such as taking account of the Sun's zenith angle in computing sub-cloud surface insolation, will have strong effects on convection.

In hindsight, we also doubt that the application of gustiness velocities, and of the subgrid-scale TKE formulation given in equation (4.2) in particular, is appropriate in a CRM or LES framework, and we recommend setting the β_{TKE} parameter to 0 in future simulations. Aside potential double-counting of turbulence and hence violation of similarity theory, subgrid-scale TKE and mean wind are correlated in the surface layer through shear production of turbulence, such that the gustiness term is likely to strongly increase fluxes in high winds over rough terrain, whilst it is unlikely to contribute much to avoiding singularities in the flux parameterizations at low winds. It is therefore possible that the gustiness term actually contributed to the strong spatial and temporal variability of fluxes and to the occasional extreme values. Furthermore, with grid-spacings ($O100$ m) permitting the direct simulation of larger clouds but not resolving individual boundary layer convective updraughts, and with time steps on the order of seconds to minutes, there is little reason to believe that continuous or average free convection in the limit of vanishing winds should exist, as implied by the use of equation (4.3). The model and

parameterized processes are set at scales at which they may lose significant theoretical backing. Field campaigns focusing particularly on scales captured by a CRM/LES would prove particularly useful to validate, improve and inter-compare with data from the coupled models described herein, in terms of mean values, spatial and temporal variability and statistics. Boundary layer measurements should include flux and micrometeorological measurements networks, averaged fluxes (such as from scintillometry), and the remote sensing of heterogeneity in surface skin temperature as well as of the boundary layer structure at high spatial resolution, to measure surface, fluxes and thermal circulations both over homogeneous and heterogeneous terrain.

Additional composite and statistical analysis of our simulated results, along the lines of e.g. Chaboureaud et al. (2004), Kuang and Bretherton (2006), Khairoutdinov and Randall (2006), combined with the methods presented in this dissertation, should provide a powerful extension to this work, especially in the context of comparison to mass-flux convection schemes with variable entrainment. Four large datasets, corresponding to the 3D sensitivity studies presented in the last chapter, are available and well-suited for further exploration.

Our novel coupled biosphere-hydrosphere-atmosphere modelling suite provides an ideal tool to perform investigations into small-scale and short-term interactions between processes changing the composition of the surface layer and atmospheric convection, after some modifications to include material fluxes and cycles.

Over land areas, we expect it to generate new insights into feedbacks between the atmosphere and the biosphere, necessitating a mechanistic treatment of plant physiology, such as the suppression/modification of boundary layer clouds by plants in a CO₂-rich atmosphere and warmer climate that was suggested by Vilà-Guerau de Arellano, van Heerwaarden, and Lelieveld (2012). Since they did not explicitly simulate atmospheric processes or clouds, they were not able to capture truly interactive and potentially relevant feedbacks, or an equilibrium between the vegetation and photosynthesis, clouds and radiation. Herein lies the definite advantage of coupling an LES model to the biosphere, and the simplified boundary layer profile initialization described in section 3.4 would provide an ideal framework for such a study. Given observed mid-latitude grassland diurnal surface layer CO₂ mixing ratio variations on the order of 30-50 ppm (Casso-Torralba et al. (2008)), particularly due to the rapid changes in the early morning hours with the onset of photosynthesis, the erosion of the stable nocturnal layer and the mixing with residual boundary layer air during the transition to an unstable mixed layer, introducing CO₂ as a prognostic passive tracer into the model seems warranted.

Last but not least, we tentatively argue that a mechanistic treatment of plant physiology could be used simultaneously to parameterize the emission of Volatile Organic

Carbons (VOCs), such as isoprene (Kesselmeier and Staudt (1999)); even if stomatal conductance might only have a limited control over actual isoprene emission rates, at least for slow aperture change rates (Fall and Monson (1992)). Taking airborne measurements over heterogeneous (sub)tropical vegetation cover giving rise to thermally induced mesoscale circulations, Garcia-Carreras et al. (2010) retrieved strong peaks of isoprene concentrations in cumulus congestus clouds. This collocation was attributed to tracer accumulation and exclusive vertical transport in the small-scale convective updraughts or rising branches of the thermally induced mesoscale circulations. As isoprene is a precursor for secondary organic aerosol formation, it would be interesting to investigate to what extent natural VOCs in particulate form contribute to the observed cloud formation. Pöschl et al. (2010) pictured the Amazon as a “biogeochemical aerosol reactor” and hypothesized on potential feedbacks between atmospheric convection and secondary organic aerosol formation. Given the availability of a new two-moment cloud microphysics scheme for ATHAM, explicitly simulating the cloud droplet activation process (Griffiths et al. (2012)), our modelling suite shall be capable of including aerosol-cloud-precipitation interactions in the biosphere-atmospheric convection feedback. Including secondary organic aerosol from primary emissions would require a further chemistry package. Since cloud droplet nucleation and microphysics have obvious impacts on parcel thermodynamics and buoyancy, they could potentially alter internal flow dynamics. When emitted from the surface, this could possibly provide a stronger feedback mechanism between the surface and convection than heat fluxes alone, though their ingestion into the rising branches from our hypothesized surface reservoir is probably similar to that of the sensible and latent heat anomalies. Other future opportunities into this direction involve emission inventories for man-made components or parameterized dust uplift. Obviously, such analysis is not limited to the land biosphere. The coupled COARE sea surface model, with wave parameterizations (see Appendix A), provides an ideal framework for introducing further processes such as sea spray, bubble aerosol or other forms of tracer emission.

If further emphasis is put on simulating boundary layer and surface exchange processes, additional model development to improve the treatment of the interfacial sub-layer and of the surface layer in ATHAM might be warranted. Unfortunately, the development of HYBRID 6.5 seems discontinued, so future improvements or corrections are not necessarily quickly available. Future model versions have a different source code structure, which conflicts with our original intention to facilitate fast upgrades through subroutine intercomparison. For this reason, we cannot vouch for a continued use with the ATHAM framework. Many more physics features and parameterizations have been incorporated into the coupled models as have been actively used and exploited in this

study. Further testing and investigation is needed to evaluate their performance and effects.

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Acknowledgments

The hole-filled seamless SRTM V3 data has been provided by the International Centre for Tropical Agriculture (CIAT), and is available at srtm.csi.cgiar.org. Bathymetry has been derived from SCRIPPS DEM data and accessed as the Global 30 Arc-Second Elevation Data Set through the USGS Global GIS DB, available at webgis.wr.usgs.gov/globalgis/. Tiwi Islands soil properties have been defined based on data from the Australian Soil Resource Information System, online at www.asris.csiro.au/themes/Atlas.html. Soil Available Water Content data has been retrieved from the Harmonized World Soil Database, online at www.iiasa.ac.at/Research/LUC/External-World-soil-database/HTML/. The University of East Anglia Climate Research Unit's (CRU) climate data has been retrieved through the British Atmospheric Data Centre (BADC), available at badc.nerc.ac.uk/data/cru. The ESA Global Land Cover Product 2005-06 has been downloaded from due.esrin.esa.int/globcover/. MERIS broadband 16-day albedo has been retrieved from www.brockmann-consult.de/albedomap/. AVHRR AMSR OI SST data has been retrieved from ecco2.jpl.nasa.gov/data2/data/sst/Reynolds/. All NASA processed data products are best accessed through reverb.echo.nasa.gov. MTSAT-1R data was obtained through the Atmospheric Radiation Measurement (ARM) Program. The atmospheric profile has been initialized using a standard radiosounding launched from Darwin (WMO 94120, flight 440269442735). We thank Maria Russo for providing the surface fluxes simulated with the UK Met Office Unified Model for the Hector storm studied by Chemel et al. (2009).

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Appendix A: Note on wave parameterizations in COARE

Considerable debate remains on the topic of roughness' scaling with sea state and waves (e.g. Drennan, Taylor, and Yelland (2005)). In COARE, the roughness length can be made dependent on one out of 2 simple parameterizations of surface gravity waves, relevant for wind speeds above roughly 5 ms^{-1} and in situations where the prevailing wave climate is different from an average open ocean state as implied by equation (4.4). Roughness can therefore take on the following expressions, based on the empirical relationships proposed by P. K. Taylor and Yelland (2001)²⁰ (TY, dominant wave steepness (h_s/L_p)-based) and Oost et al. (2002) (Oe, wave age (C_p/u_*)-based):

$$\begin{aligned} z_{0,TY} &= 0.11 \frac{v}{u_*} + 1200 h_s \left(\frac{h_s}{L_p} \right)^{4.5} \\ z_{0,Oe} &= 0.11 \frac{v}{u_*} + \frac{50}{2\pi} L_p \left(\frac{u_*}{C_p} \right)^{4.5} \end{aligned} \quad (7.1)$$

for a significant wave height h_s , and a wavelength L_p associated with the dominant wave period T_p propagating with a phase speed C_p . The dominant wave corresponds to the peak in the frequency-size spectrum. Significant height corresponds to the mean height of the upper third of the height distribution. In equation (7.1), wave period, length and phase speed are linked using standard relationships for deep water gravity waves, i.e. $C_p = gT_p/2\pi$ and $L_p = gT_p^2/2\pi$. Wave period and significant height in Fairall et al. (2003) are adapted from P. K. Taylor and Yelland (2001) for a fully developed sea:

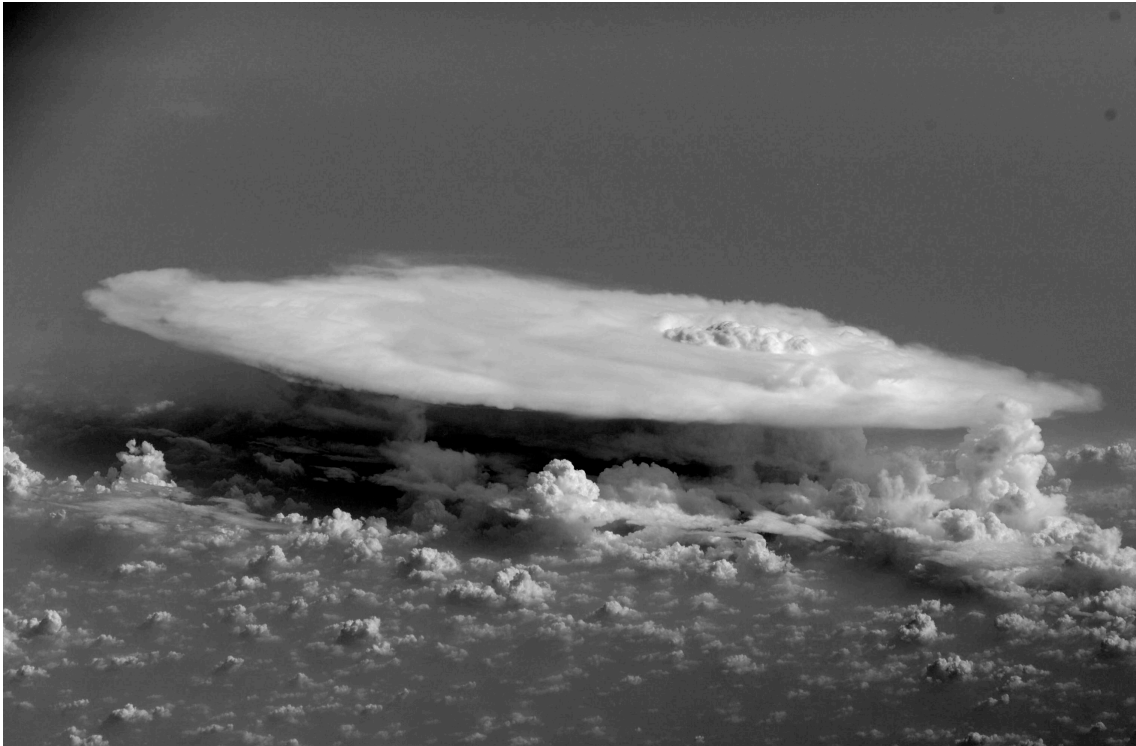
$$\begin{aligned} T_p &= 0.729U \\ h_s &= 0.018U^2 \cdot (1 + 0.015U) \end{aligned} \quad (7.2)$$

In the present implementation, either of these **wave parameterizations** can be switched on by changing a hardwired flag (jwave) in the interface's data module (surf_sea_IF_data). Neither is compatible with the shallow water adaptation outlined in section 4.1. They have not been tested within the COARE framework and **have not been used in this study**. Other forms can easily be added, we refer to the discussion on waves in shallow waters. Calculated wave parameters could potentially be used to estimate the transfer of liquid water and sea salt aerosol from sea spray into the atmosphere.

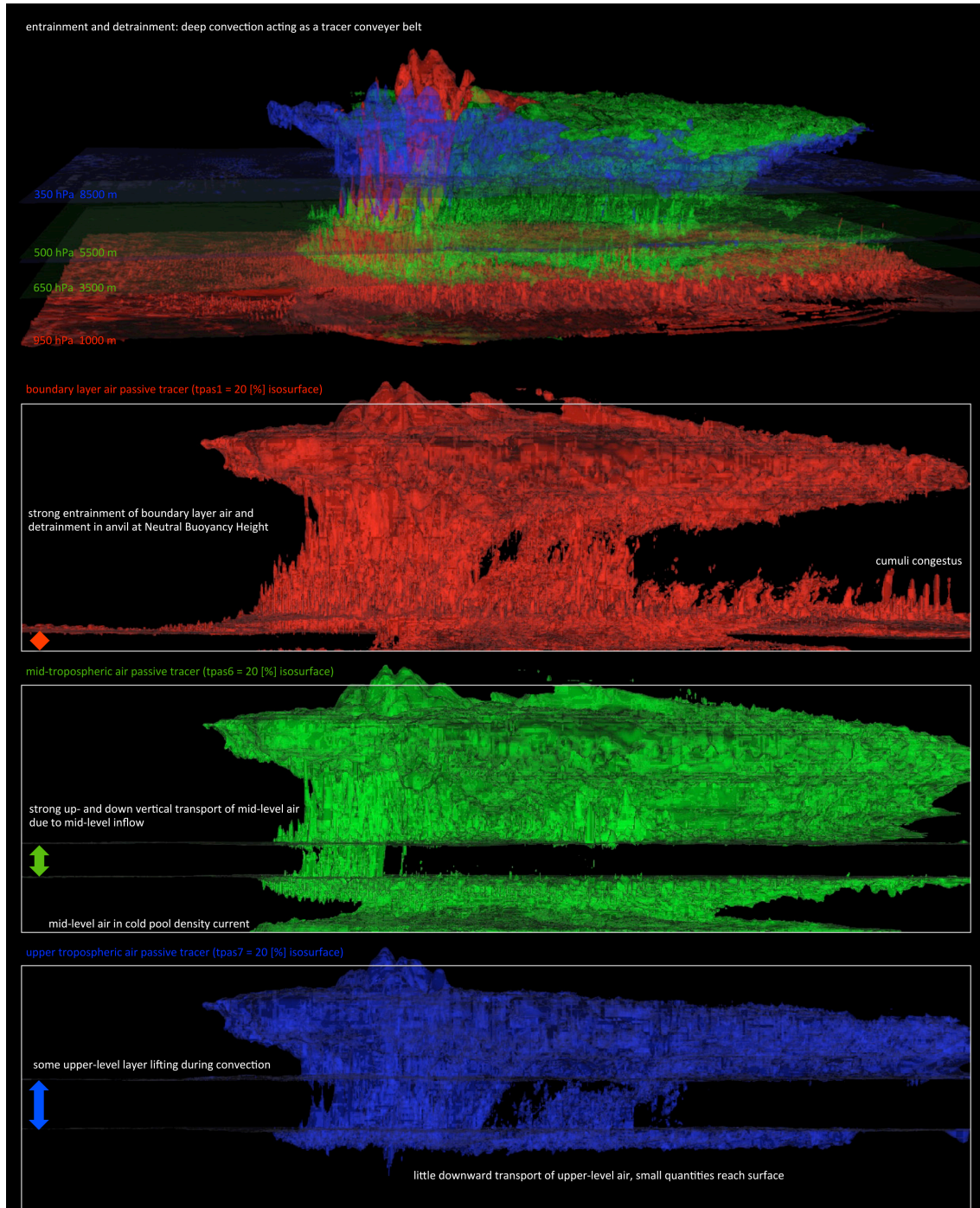
Appendix B: New serial/parallel output facilities and model versioning

We have fitted ATHAM with a new module to generate output data in the netCDF portable file format, the *de facto* atmospheric community standard. File metadata has been aligned with the Cooperative Ocean-Atmosphere Research Data Service (COARDS) and Climate and Forecast (CF) conventions, where possible. In order to safeguard model performance and to avoid a potential bottleneck from a serial file writing procedure when running ATHAM in a parallel environment, the parallel PnetCDF procedures (Li et al. (2003)), which support concurrent writing from each process into a single file, were implemented in an analogous fashion to serial netCDF. The new PnetCDF library used for this purpose builds on top of the MPI-IO parallel I/O interface specified in the MPI-2 standard. The surface model restart file reading and writing facilities have also been created within this framework.

In an attempt to make the code more accessible to a wider community, and to improve reproducibility and traceability (G. Wilson (2006)), we have set the coupled models source code and newly developed test cases, as well as the pre-processing platform and post-processing analysis and visualization tools into a server-based version control system (SVN) and a web-based collaborative management platform (Trac). Information on source code status and revision, as well as on system architecture, compiler and compilation flags, is now also routinely stored in dedicated log-files during a model build.



“A Cumulonimbus cloud over Africa is featured in this image photographed by an Expedition 16 crewmember on the International Space Station. [...] The image, photographed while the International Space Station was passing over western Africa near the Senegal-Mali border, shows a fully-formed anvil cloud with numerous smaller cumulonimbus towers rising near it. The high energetics of these storm systems typically make them hazardous due to associated heavy precipitation, lightning, high wind speeds and possible tornadoes.” © NASA, 5 Feb 2008, photo ID ISS016-E-027426



Hector storm from the baseline simulation in this dissertation, visualized in terms of its influence on the vertical redistribution of air masses originating at different vertical levels.