

Unification of thermodynamics

or

Unification steps via thermodynamics ?

in fact the presentation will oscillate between the two meanings ...

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(many thanks to P. Marquet, B. Catry, and M. Van Ginderachter)

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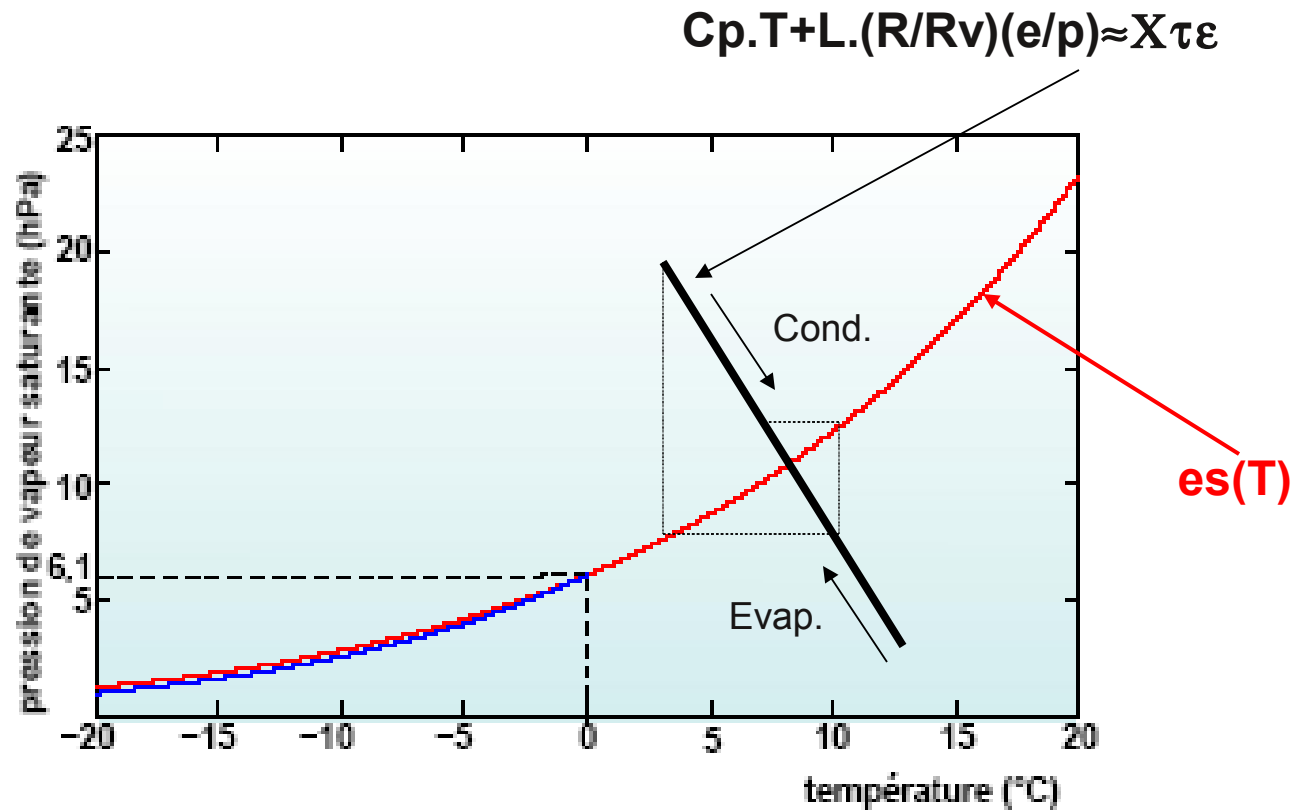
Introduction

- **Idea behind the talk: clean thermodynamics does not need to be too complicated ... and it has nice practical applications.**
- **But reaching this advantageous situation requires a good deal of consistency.**
- **This does not mean that there should be no simplifications with respect to the full complexity of the system ... but that they should be decided as a whole and ab-initio!**
- **But sometimes practical implementation decisions do have some level of arbitrariness => the transversal issues (critical if we want to work as a community), like for instance conservation properties, should in principle be treated through global constraints.**
- **But the devil is still sometimes in the details! Thus it matters to also think conceptually in all generality (barycentric view and exact specific weighting of dry air properties => consequences).**

Split of the presentation

- **Examples:**
 - A simplified ‘toy computation’
 - A curiosity concerning radiation and heat diffusion
 - The paradox of moist entropic considerations (Emanuel)
- **Rules:**
 - Additivity
 - Conservation of theoretical invariants
 - Practical consistency in discretisation
- **Conditions of application:**
 - Simplifying (and structuring) hypotheses
 - Algorithmic hurdles
- **A practical view of the three Laws of thermodynamics for the atmosphere**

Irreversible saturation adjustment calculation



The 'black line' is in fact not a straight line because C_p and R vary with q_v and L with $T \Rightarrow$ exact equation:

$$\left. \begin{aligned} C_p &= C_{p0} + (C_{p_v} - C_l) \cdot \delta q_v \\ L &= L_0 + (C_{p_v} - C_l) \cdot \delta T \\ C_p \cdot \delta T + L \cdot \delta q_v &= 0 \end{aligned} \right\} \Rightarrow \delta(C_p \cdot L) \equiv 0 \quad !!!$$

hyperbole branch

There is even an extension to the computation of the irreversible moist adiabat

Radiative-diffusive ambiguity: a curiosity

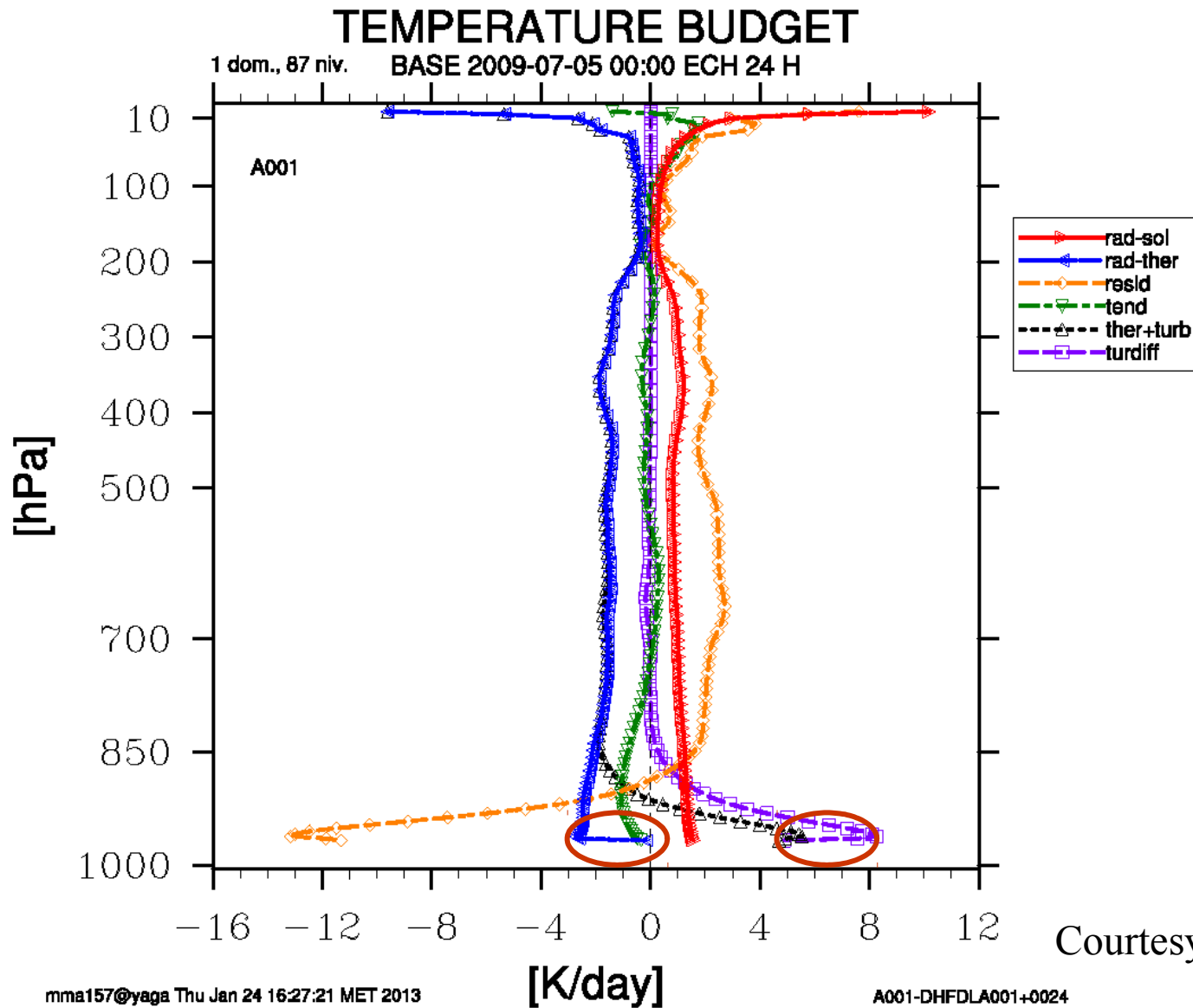
We shall come back to the equation below later (in more details).

$$\frac{\partial}{\partial t}(c_p T) = -g \frac{\partial}{\partial p} [(c_l - c_{pd})P_l T + (c_i - c_{pd})P_i T - (\hat{c} - c_{pd})(P_l + P_i)T + J_s + J_{rad}]$$
$$-L_l(T_0)(P_l' - P_l''') - L_i(T_0)(P_i' - P_i''')] = -g \frac{\partial J_{total}}{\partial p}$$

Here, what is important to notice is that the sum of the diffusive heat flux J_s and of the radiative flux J_{rad} makes them indistinguishable, from the point of view of what the dynamical part of the model will 'feel' from the parameterisation computations (all other terms have to do with independent water species' budgets, those not). Numerical compensations can therefore happen ...

And they indeed do !

Radiative-diffusive ambiguity: manifestation



K. Emanuel's example: dry convective turbulence

- A statistical approach to dry turbulence: system at radiative-(dry)convective equilibrium. The convection compensates the built-up of a temperature jump at the surface
- Entropy budget:

$$C_p \left(\frac{d \ln(T)}{dt} \right) - R \left(\frac{d \ln(p)}{dt} \right) = \frac{Q_{rad}}{T} + \dot{s}_{irr}$$

- Vertical integral:

$$\int \dot{s}_{irr} = F_{surf}^{net-rad} \left(\frac{1}{\bar{T}} - \frac{1}{T_{surf}} \right)$$

K. Emanuel's example: moist convective turbulence (the naive approach)

- Still statistical approach: dry convection with surface flux balance (radiation=heat) is a heat engine => what about moist convection?
- Simplify: $C_p=C_{ste}$, $R=C_{ste}$, $e \ll p$, etc...

$$C_p \left(\frac{d \ln(T)}{dt} \right) - R \left(\frac{d \ln(p)}{dt} \right) = - \frac{L_v}{T} \left(\frac{dq}{dt} \right) + \frac{Q_{rad}}{T} + \dot{s}_{irr}$$

- Vertical integral:

$$\int \dot{s}_{irr} = - \int \frac{Q_{cool}}{T} + \int \frac{L_v}{T} \left(\frac{dq}{dt} \right)_{cloud} = 0$$

- Zero (assuming solar heating is compensated by evaporation only at the [oceanic] surface)!

K. Emanuel's example: moist convective turbulence (the correct approach)

- Stop simplifying : $R/C_p=R(q)/C_p(q)$, $L_v=L_v(T)$, $e \neq 0$

$$C_p(q) \left(\frac{d \ln(T)}{dt} \right) - R_d \left(\frac{d \ln(p - e)}{dt} \right) - R_v \left(\frac{d \ln(e)}{dt} \right) = -\frac{1}{T} \left(\frac{d(L_v q)}{dt} \right) + \frac{Q_{rad}}{T} + \dot{s}_{irr}$$

- Vertical integral:

$$\int \dot{s}_{irr} = -\int \frac{Q_{rad}}{T} + \int R_v \ln \left(\frac{e}{e_{sat}} \right) \left(\frac{dq}{dt} \right)_{cloud} \neq 0$$

- The latent heat term disappeared and we have a new 'shape' for the heat engine expression!
- **Beware: even this is done with some simplifications (see later).**

Additivity rule

- When having a complete system of parameterisation algorithms, one must know how to combine the outputs of individual computations in terms of evolutions of the main-model's prognostic variables.
- In the case of water species (or any 'passive tracer' of course) things are simple thanks to the intrinsic linearity of the tendency equations.
- But for energy linked quantities ($cpT+\Phi$, $(u^2+v^2)/2$, ...), this is not anymore true.
- One must then realise that tendencies (which do have a lot of conditional aspects in their definition) **ARE NOT ADDITIVE**:
 $\delta(cpT) \neq cp \delta T + \sum T(\partial cp/\partial qx) \delta qx$ (in time discretisation)!
- Only fluxes (which have an intrinsic physical meaning) **ARE ADDITIVE**.

This gives a central role to the Green-Ostrogradsky theorem

Transversal conservation issue

Taking the 'heat part' of the 'specific moist enthalpy + geopotential' defines S'_{li} as the exact counterpart of $c_p T + \Phi$ for the fully dry case. It corresponds to the dry static energy in the unsaturated case got after evaporation (interpretation of Betts' system)

Moreover, in the general case, local conservation of S'_{li} is equivalent to conservation of the quantity $(c_p T + \Phi - L_v(0) q_l - L_s(0) q_i)$, with $L_v/s(0)$ the temperature-independent extrapolations of L_v/s at 0 K. The linearity of the last two terms allows to develop in function of the various transport fluxes of the water species (diffusion & precipitation) and to so obtain a Green-Ostrogradsky-type thermodynamic equation

$$\frac{\partial}{\partial t}(c_p T) = -g \frac{\partial}{\partial p} [(c_l - c_{pd}) P_l T + (c_i - c_{pd}) P_i T - (\hat{c} - c_{pd})(P_l + P_i) T + J_s + J_{rad}$$

$$-L_l(T_0)(P'_l - P'''_l) - L_i(T_0)(P'_i - P'''_i)] = -g \frac{\partial J_{total}}{\partial p}$$

Catry et al.,
2007, Tellus A

$$S'_{li} = (c_{pd} + (c_{pv} - c_{pd}) q_t) T + g z - L_v(T) q_l - L_s(T) q_i$$

$$\theta_{li} = \theta \cdot \exp\left(-\frac{L_{vap} q_l + L_{sub} q_i}{c_{pd} T}\right) \iff S'_{li}$$

$$q_t = q_v q_l + q_i$$

Basic assumptions for consistency

- **Two types of consistency ought to be sought when designing a parameterisation set:**
 - **Between the ‘dynamical’ and ‘physical’ parts of the model. Here the Green-Ostrogradsky approach is the easiest one (using the specific moist entropy as synthetic variable would be equivalent, but the way-back-computations are very complex; neither of the existing potential temperatures can help if one wants an exact solution). In the non-hydrostatic case, the issue about projecting the energy tendencies on the temperature and pressure prognostic variables also appear, but it exists in all solutions, albeit under differing shapes.**
 - **Between the individual parameterisation computations. There, if a policy for global conservation of the invariants exists (see just above), the issue is shifted to the one of having the same basic hypotheses on all sides. This requires a clear, compact and purposeful definition of so-called ‘simplifying hypotheses’ which become de-facto ‘structuring constraints’.**
- **All this appears simple and logical. Yet it is very hard to be enforced in models’ design. Nevertheless ...**

Impact of (no) enthalpy conservation (1/3)

- The following will have to do with the intra-time-step variations of C_p , C_v (and hence R), following the phase changes of a **barycentric** multi-phasic system (here *qv/l/i/r/s*)
- Using $C_p = C_v + R$ and the first Law of thermodynamics, one gets a Green-Ostrogradsky form for the evolution of enthalpy (with δm a tag for conservation or not of the total mass and with P' & P''' the mass-weighted vertical integrals of phase changes with respect to vapour):

$$\frac{\partial}{\partial t}(c_p T) = -g \frac{\partial}{\partial p} [(c_l - c_{pd})P_l T + (c_i - c_{pd})P_i T - (\hat{c} - c_{pd})(P_l + P_i)T + J_s + J_{rad} - L_l(T_0)(P'_l - P'''_l) - L_i(T_0)(P'_i - P'''_i)] = -g \frac{\partial J_{total}}{\partial p}$$

$$\hat{c} = \frac{c_{pd}q_a + c_{pv}q_v + c_l q_l + c_i q_i}{1 - q_r - q_s}$$

$\delta m = 1$

$$\hat{c} = c_{pd}$$

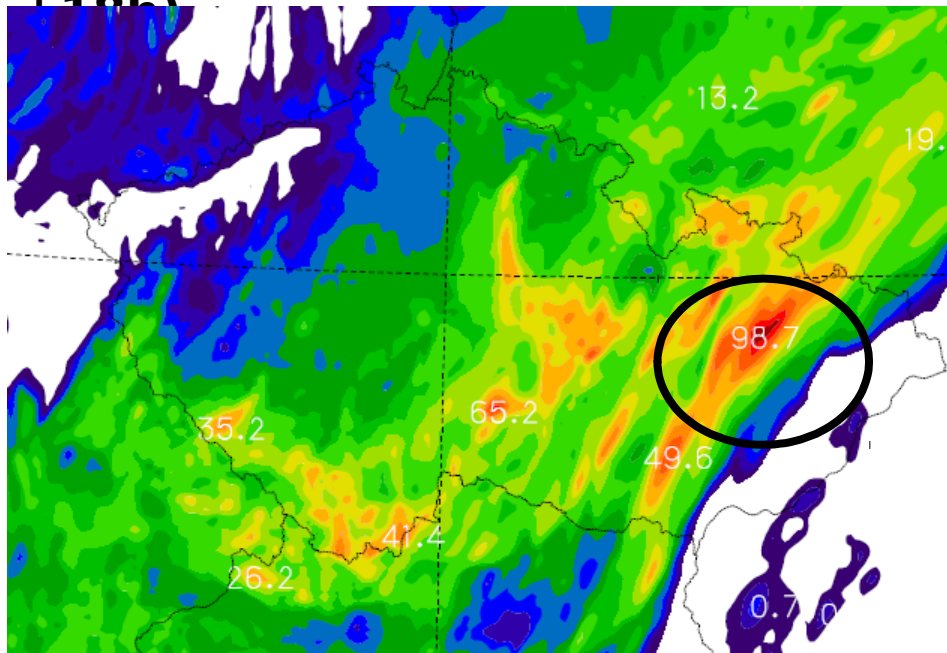
$\delta m = 0$

Impact of (no) enthalpy conservation (2/3)

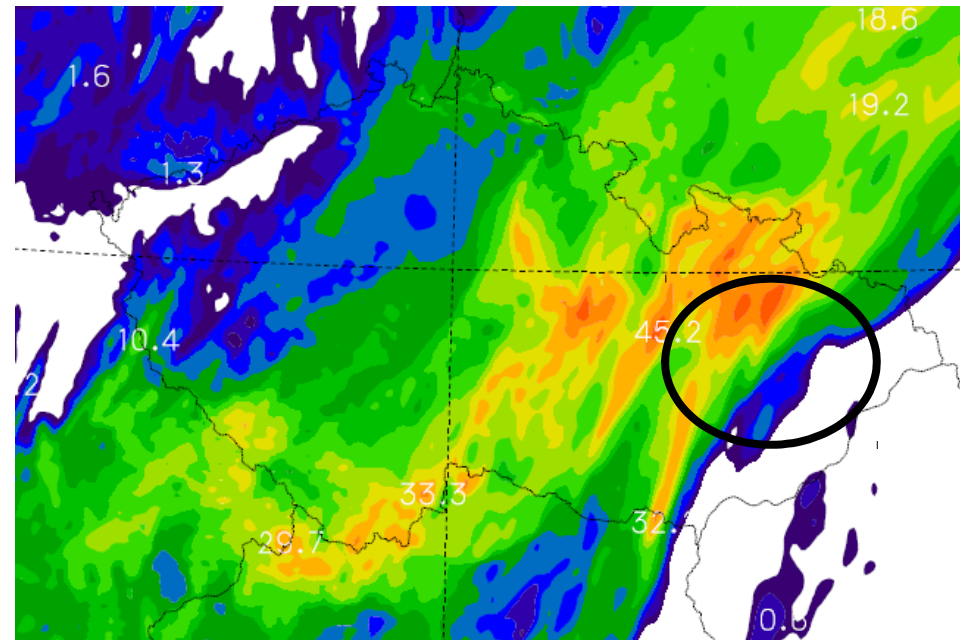
- It is sometimes customary to say that neglecting the time variation of C_p (or C_v , or R) during the ‘physical time-step’ (under the influence of phase changes) has little impact.
- We shall now see that this is not true at all at the ‘NH scales’.
- The trick, given the compact shape of the previous flux-conservative form of the enthalpy equation, is just to replace on the left-hand side ‘ $d(C_p.T)$ ’ by ‘ $C_p.dT$ ’ !

Impact of (no) enthalpy conservation (3/3)

ALARO test (with 3MT in order to make up for the difference between convection 'permitting' and convection 'resolving') on 2.3 km mesh (90s time step); 6h precipitation on 18/05/2008 (+12h to +18h)



without enthalpy conservation



with enthalpy conservation

Precipitation patterns are roughly the same, but the local intensity may be very different, nearly doubled at maximum

'Simplifying' assumptions and/or 'structuring' constraints

- **Barycentric system** (condensates are an integral part of the parcel)
- **Hydrostatism** (for the vertical gradient aspects in 'physics')
- **Zero assumed volume for condensates**
- **Gases obey Boyle-Mariotte's and Dalton's laws** (together with the previous one $\Rightarrow p/(\rho \cdot T) = R_d \cdot q_d + R_v \cdot q_v = R$)
- **Homogeneity of temperature across species** (**even for falling condensates**)
- **Constant values of specific heats across the atmospheric temperature range** (**a bit problematic for c_i**)
- **Linear variations of latent heats with temperature**
- **In presence of condensates, water vapour partial pressure around them depends only on temperature** (**no treble phase situation, though in practice many results may be robust to that ...**)
- **Clausius-Clapeyron relationship**

... and then nice analytical results (including the ones already presented) become possible!

A bit more detail about the 'barycentric' issue

- **Barycentric system** (condensates are an integral part of the parcel)
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The idea behind all this is the following:

- *The system of irreversible condensation/evaporation of drop/flakes is infinitely complex (should the surface pressure in a model know that a component aloft changed phase before or during its fall? rather not!).*
- *The best way of avoiding the problem is:*
 - *to make the simplification that the accelerations (positive or negative) are neglected \Rightarrow falling species are always at their equilibrium speed;*
 - *to consider that this equilibrium is reached because the existing differential of pressure between the 'below' and the 'above' of drops/flaxes is the way by which the information about the weight of condensates transfers to the averaged pressure of the atmospheric gas.*
- *This also automatically applies to non-falling cloud condensates, of course.*
- *The state equation $p = \rho \cdot R \cdot T$, preserved during phase changes, acts as a filter.*

Algorithmic hurdles (i.e. devils in the details) (1/2)

- **There are several types of them: linked to the (vertical) space discretisation, linked to the time discretisation (degree of implicitness), combination of both (fight against linear and non-linear instability), basic decisions about the considered process' behaviour.**
- **The latter are the most interesting ones from the purely thermodynamics point of view. The decisions are about:**
 - **Reversible or irreversible character (for instance condensation is reversible and precipitation irreversible; and yet microphysical packages sometimes mix them without caution).**
 - **Local adjustment or transport-type process (nature does not make such a distinction, but in models we need it most of the time, for the sake of simplicity).**
 - **How to deal with the treble phase problem (even if the final computations may be solved by linear combination tricks, this contradicts the way in which we obtained, in the case of two phases only, the simple formulae allowing this strategy).**

Algorithmic hurdles (i.e. practical consequences) (2/2)

- **Reversible or irreversible character:**
 - for irreversible saturation conditions (precipitation) we have

$$q_{sat}(T, p) = (R_d/R_v)[e_{sat}(T)/(p - e_{sat}(T)(1 - R_d/R_v))]$$

- for reversible saturation conditions (no precipitation) we have

$$r_{sat}(T, p) = (R_d/R_v)[e_{sat}(T)/(p - e_{sat}(T))]$$

- **Local adjustment or transport-type process. The issue is here:**
 - whether to use $(q/r)_{sat}$ as implicit target for a return to saturation (in the transport case where one cannot anticipate the change of [T,p] characteristics along the vertical displacements;
 - Or to use $(q/r)_w$ (wet-bulb value) as explicit target for a return to saturation (in order to implicitly couple the temperature and humidity evolutions in the local case)
- **The treble phase problem: there is no ideal solution; probably an additional prognostic quantity ought to be defined and added in order to keep both consistency and physical realism!**

Excursion towards turbulence: so-called 'moist conservative' transforms (1/2)

- **When trying to compute turbulent fluxes in a situation where cloudiness is different from 0 or 1, or simply when it changes along the vertical, one is facing two delicate issues:**
 - **(1) The calculation of the buoyancy flux $\langle w' \cdot \rho' \rangle$ becomes extremely non-linear and complex (we shall come back to this issue later);**
 - **(2) The interaction between phase changes and transport of heat, water vapour and condensate(s) during the 'physics time-step' is not tractable.**
- **Concerning the issue N°2, Betts (1973) proposed to use two so-called 'moist conservative' variables, namely the total water amount qt and the liquid water potential temperature θ_l (no consideration of the ice phase in those early years!).**
- **While the conservative character is only approximate and the advocated link with entropy wrong, what remains from Betts' idea is the 'transform' method: (i) evaporate (with temperature change), (ii) transport both variables and (iii) condense back.**
- **The last step needs additional hypotheses, linked to the issue N°1!**

Excursion towards turbulence: so-called 'moist conservative' transforms (2/2)

- **One very misleading idea is that Betts' method (despite its big practical advantages) makes transparent the transition from the 'dry only' case (θ) to the 'moist one' (θl), the latter starting only when condensation appears. This is thrice wrong.**
- **First of all the problems linked with the presence of water start even without latent heat release. Water vapour is lighter than dry air and this favours an increase in buoyancy with increasing qv .**
- **Second, and most importantly, θ plays a double role in the truly dry case (favorite to turbulence theoretical studies): tracer of density (buoyancy) and of entropy (conservation). In the moist case this is split: θv takes over the density role but is not conserved alike entropy (and neither is θl , see above and later).**
- **Third, there is a term in the buoyancy computation which does not scale with the presence of cloudiness and thus requires special attention (proportional only to the gradient of total water).**

Short reminder

- **First Law of thermodynamics**: Conservation of energy (heat Q + work W)
- **Second Law of thermodynamics**: For a closed system where the change of entropy S due to a heat source is the ratio of the latter to temperature T ($dQ=T.dS$):
 - Irreversibility (diabatism) implies increase of entropy;
 - Adibatism equals conservation of specific entropy.
- **Third Law of thermodynamics**: At 0 K, entropy vanishes.
- We shall now see what differences make the consideration of dry air also as an ‘interactive’ part of the air parcel (i.e. going for it from ‘conservative’ to ‘non-conserved’ ideas).

Computations of $s \rightarrow \theta_s$

A paradox, which constrains many aspects. Plus the need not to forget ‘dry air’, if wanting a comprehensive view.

Budget of entropy is difficult to $\rho T \frac{ds}{dt} = \rho (\dot{Q}_i + \dot{D}) - \rho \left[\mu_k \frac{d_i q_k}{dt} \right]$

Entropy = state function \rightarrow measurable at each point: $\mathbf{J}_k \cdot \nabla(h_k) - T s_k (\nabla \cdot \mathbf{J}_k)$

$s = q_d s_d + q_v s_v + q_l s_l + q_i s_i$

Paradox: it is the opposite for enthalpy (easy budget vs. uncertain absolute value)!

$$s_d = (s_d)_r + c_{pd} \ln(T/T_r) - R_d \ln[p/(p_d)_r]$$

$$s_v = (s_v)_r + c_{pv} \ln(T/T_r) - R_v \ln[e/e_r]$$

$$s_l = (s_l)_r + c_l \ln(T/T_r)$$

$$s_i = (s_i)_r + c_i \ln(T/T_r)$$

$s = s_{ref} + c_{pd} \ln(\theta_s)$

$s_{ref} = \text{Cste}$

$s \leftrightarrow \theta_s?$

$c_{pd} = 1004.7 \text{ J K}^{-1} \text{ kg}^{-1}$

The 2nd Law gives the specific moist entropy with exact consideration of the dry air part of the parcel ...

Computations of $s \rightarrow \theta_s (\rightarrow (\theta_s)_1)$

SPECIFIC MOIST ENTROPIC POTENTIAL TEMPERATURE

$$s = s_{ref} + c_{pd} \ln(\theta_s)$$

$$s_{ref} \approx 1138.56 \text{ J K}^{-1} \text{ kg}^{-1}$$

$$\theta_s \equiv \theta \exp(\Lambda q_t) \exp\left(-\frac{L_v q_l + L_s q_i}{c_{pd} T}\right)$$

$$(\theta_s)_1$$

$$\times \left(\frac{T}{T_r}\right)^{\lambda q_t} \left(\frac{p}{p_r}\right)^{-\kappa \delta q_t}$$

$$\times \left(\frac{r_r}{r_v}\right)^{\gamma q_t} \frac{(1 + \eta r_v)^{\kappa(1 + \delta q_t)}}{(1 + \eta r_r)^{\kappa \delta q_t}}$$

$$(\theta_s)_2 \approx 1$$

θ_s complicated ?

in fact "similar" to HH87, M93 ou E94, except...

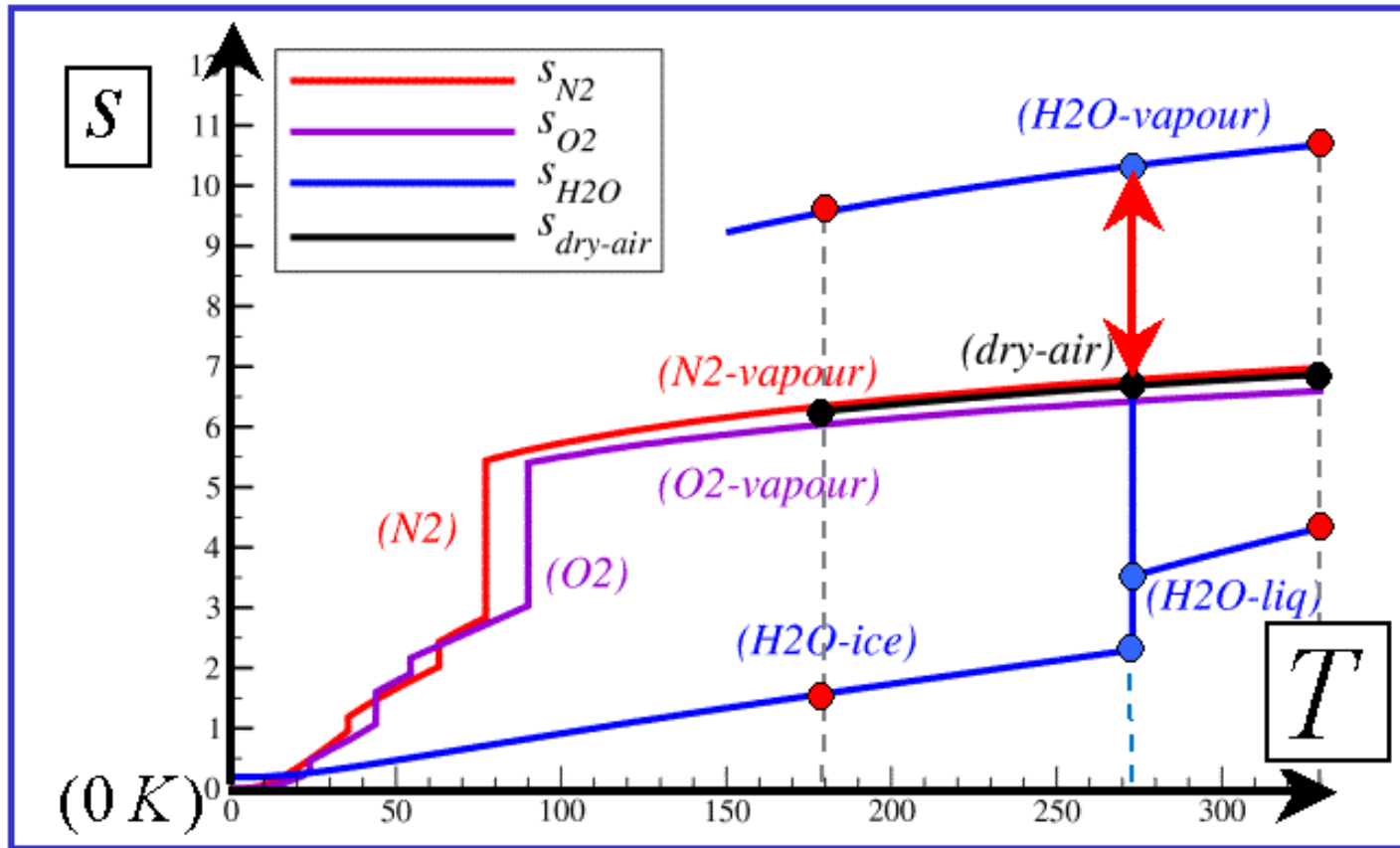
3-phase
Betts ?

$$q_t = q_v \oplus q_l + q_i$$

$$(\theta_s)_1 = \theta_l \oplus \exp(\Lambda q_t)$$

Marquet, 2011,
QJRMS

Practical application of the Third Law



Entropy diagram (in kJ/K/kg) for N₂, O₂, H₂O and for a 1000 hPa pressure

The vertical arrow is a symbol for the role of Λ (at T_0)

Computations of $s \rightarrow \theta_s (\rightarrow (\theta_s)_1)$: Additional remarks

SPECIFIC MOIST ENTROPIC POTENTIAL TEMPERATURE

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$$s_{ref} \approx 1138.56 \text{ J K}^{-1} \text{ kg}^{-1}$$

$$\theta_s \equiv \theta \exp(\Lambda q_t) \exp\left(-\frac{L_v q_l + L_s q_i}{c_{pd} T}\right)$$

$$\times \left(\frac{T}{T_r}\right)^{\lambda q_t} \left(\frac{p}{p_r}\right)^{-\kappa \delta q_t}$$

$$\times \left(\frac{r_r}{r_v}\right)^{\gamma q_t} \frac{(1 + \eta r_v)^{\kappa(1 + \delta q_t)}}{(1 + \eta r_r)^{\kappa \delta q_t}},$$

θ_s is independent of the choice of the reference values, but only if $rr=rr(esat(T_r), p_r)$, a situation which excludes the 3 phases case. This problem disappears with $(\theta_s)_1$ but it is displaced to the choice of Λ , which also depends on the reference values

θ_{li} is the obvious extension of Betts' θ_l , in the spirit of $(\theta_s)_1$

3-phase
Betts ?

$$q_t = q_v + q_l + q_i$$

$$(\theta_s)_1 = \theta_l \exp(\Lambda q_t)$$

Marquet, 2011,
QJRMS

Computations of $s \rightarrow \theta_s \leftrightarrow Th$

+ **absolute** values of partial entropies \rightarrow

$$\Lambda = [(s_v)_r - (s_d)_r] / c_{pd} \approx 5.87$$

The 3rd Law ...

+ **similar** computations for moist enthalpy \rightarrow

$$T_Y = [(h_v)_r - (h_d)_r - (c_{pv} - c_{pd})T_r] / c_{pd} = 2362 \text{ K}$$

$$h = h_{ref} + c_{pd} T_h$$

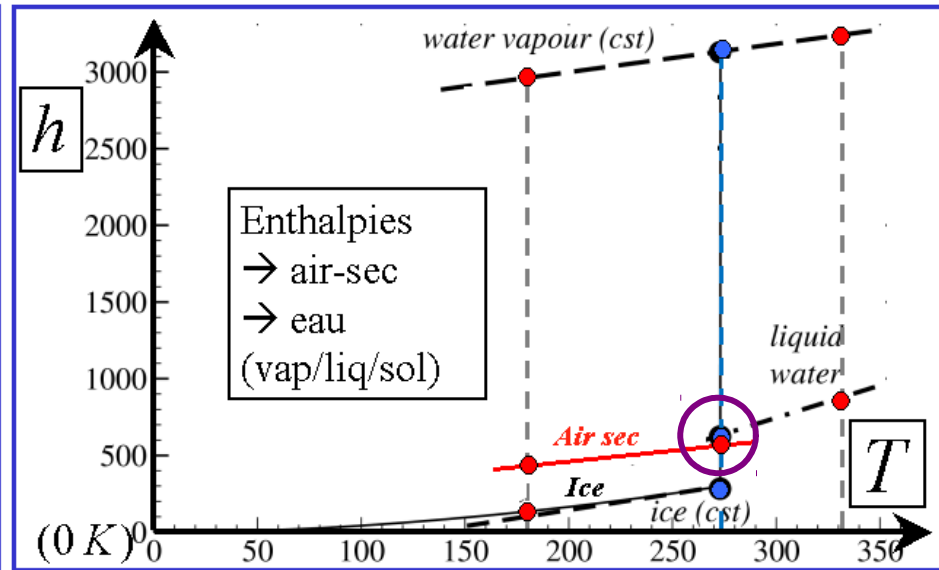
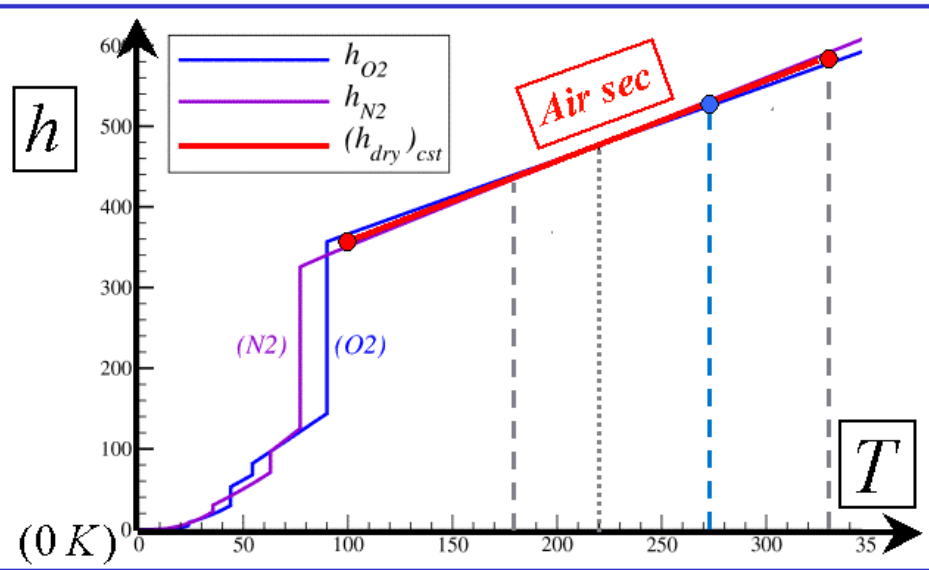
$$h_{ref} \approx 256 \text{ kJ kg}^{-1}$$

$$\begin{aligned} c_{pd} T_h &= [c_{pd} + (c_{pv} - c_{pd})q_t]T - L_{vap} q_l - L_{sub} q_i + c_{pd} T_Y q_t \\ &= S_{hm} - g z \end{aligned}$$

No need here for a leading term like $(\theta_s)_1$

It is easy to express a 'relative' specific moist enthalpy (\neq from the thermal part of 'Moist Static Energy' (MSE))

Practical application (bis)



Enthalpy diagrams (in kJ/kg) for N_2 , O_2 , H_2O and for a 1000 hPa pressure
 The circle indicates the ‘coincidence’ (see later for the consequences)

Computations of $s \rightarrow \theta s \leftrightarrow Th$: Additional remarks

There is no direct equivalent of the Third Law for the enthalpy 'h'. However a formal parallel integration from 0 K to atmospheric temperatures is possible. This is here the meaning of the dashed arrow.

$$\Lambda = [(s_v)_r - (s_d)_r] / c_{pd} \approx 5.87$$

The 3rd Law ...

$$T_Y = [(h_v)_r - (h_d)_r - (c_{pv} + c_{pd})T_r] / c_{pd} = 2362 \text{ K}$$

$$h = h_{ref} + c_{pd} T_h$$

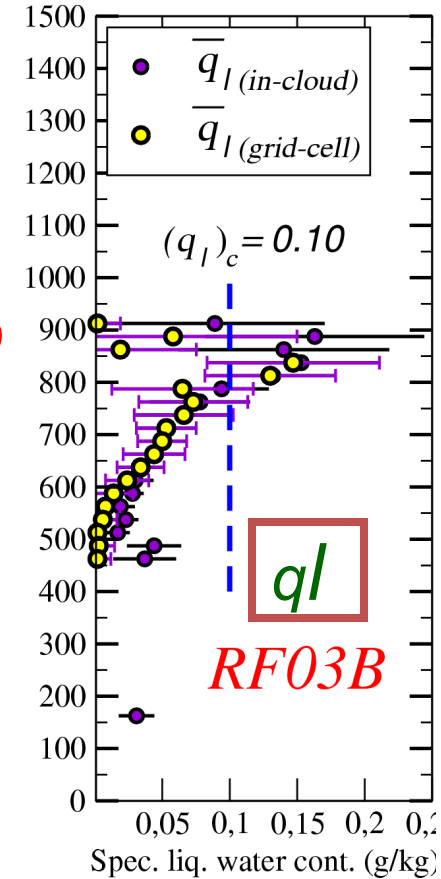
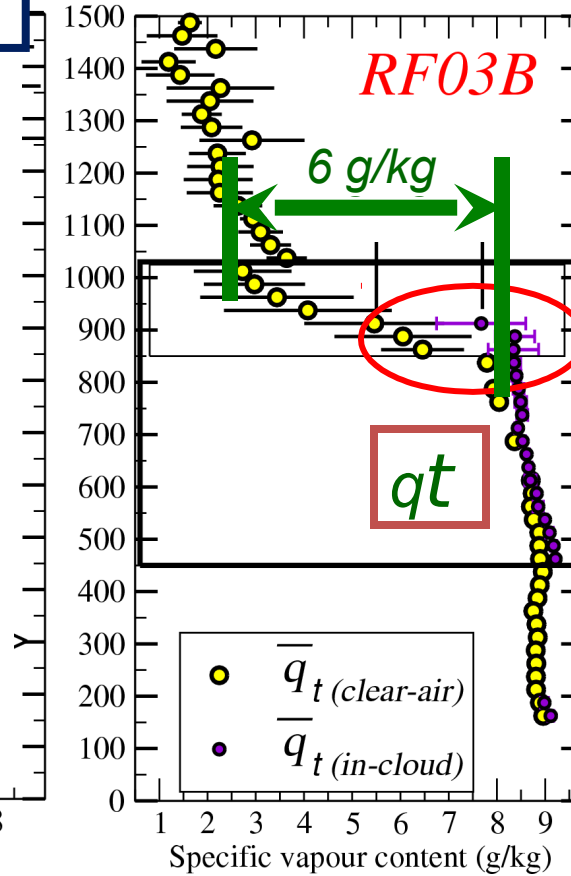
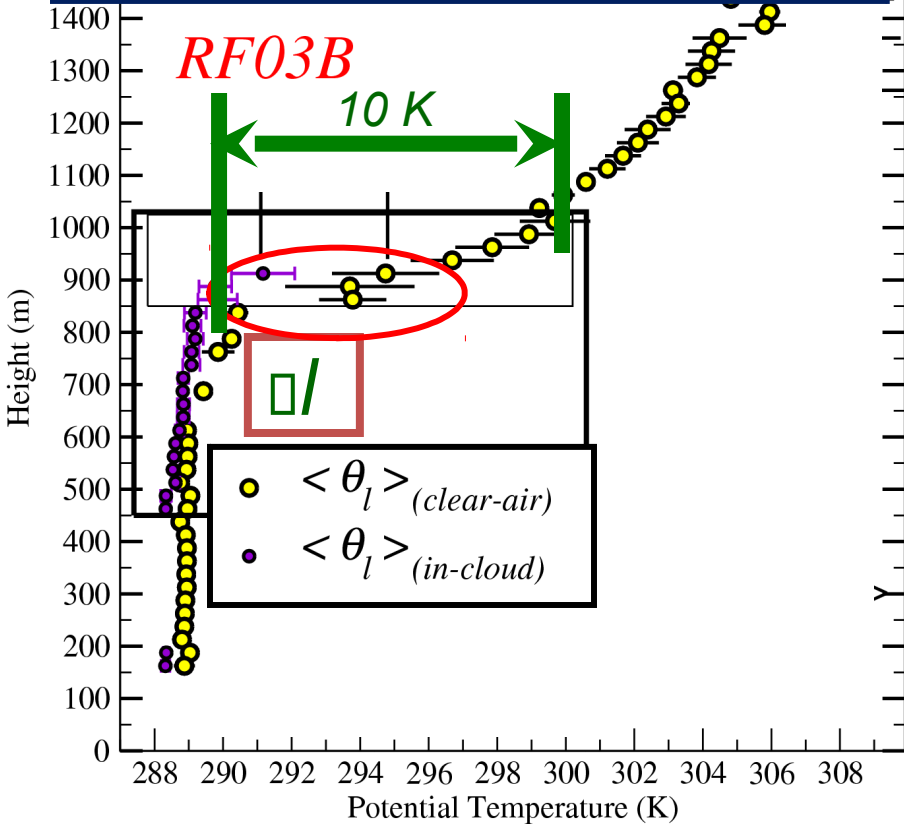
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Forgetting the (partly arbitrary) reference value and adding the geopotential, one obtains Shm as conservative quantity for vertical displacements and phase changes

Applications / FIRE-I : [θ_l ; q_t ; q_l] RF03B-hom.

Data flights NASA ← S. De Roode

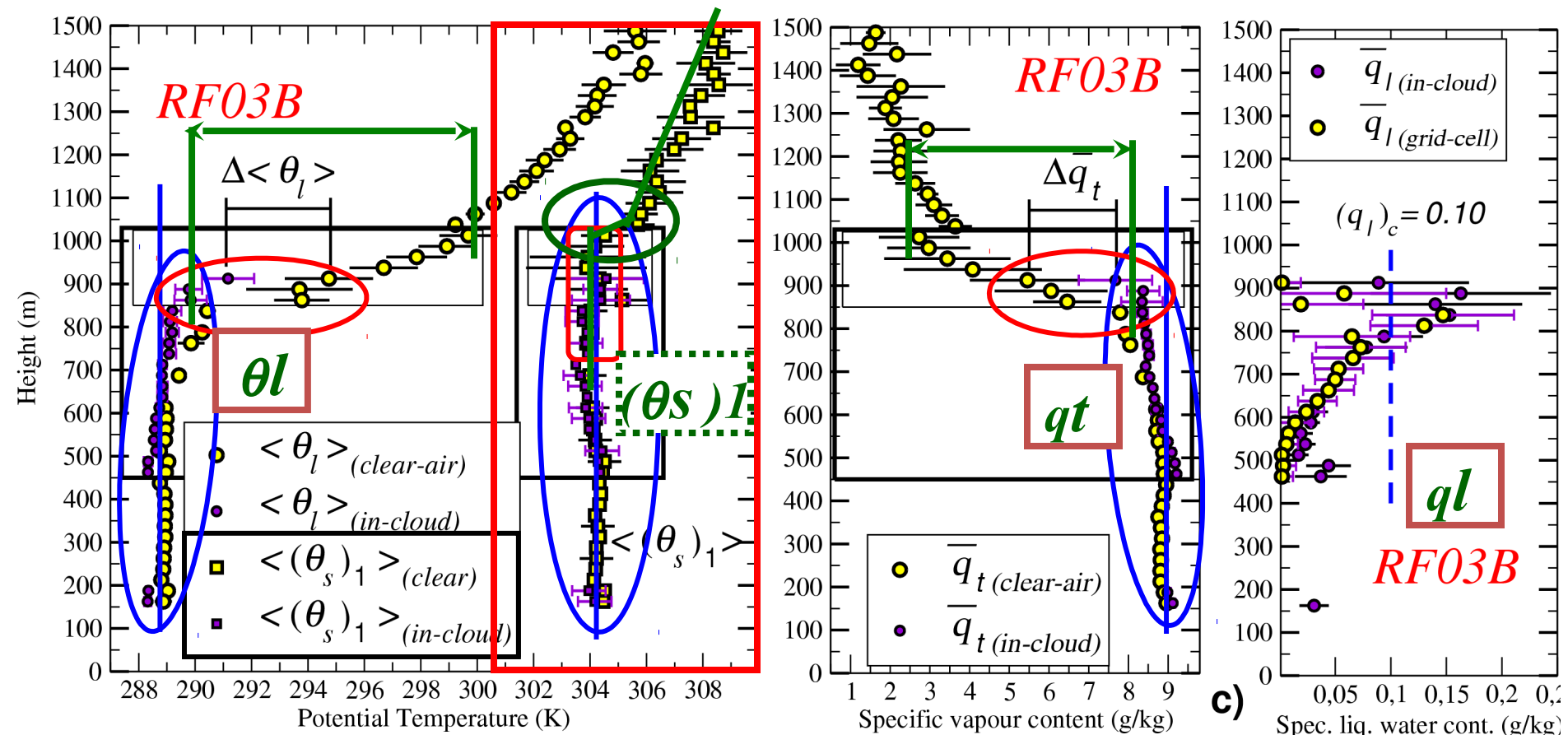


$Sc = \text{'cloud stew'} \Rightarrow \text{laboratory for conservation rules}$

"clear-air" \neq "cloud" (entrain. region)

Large jumps in θ_l and q_t (entrain. region)

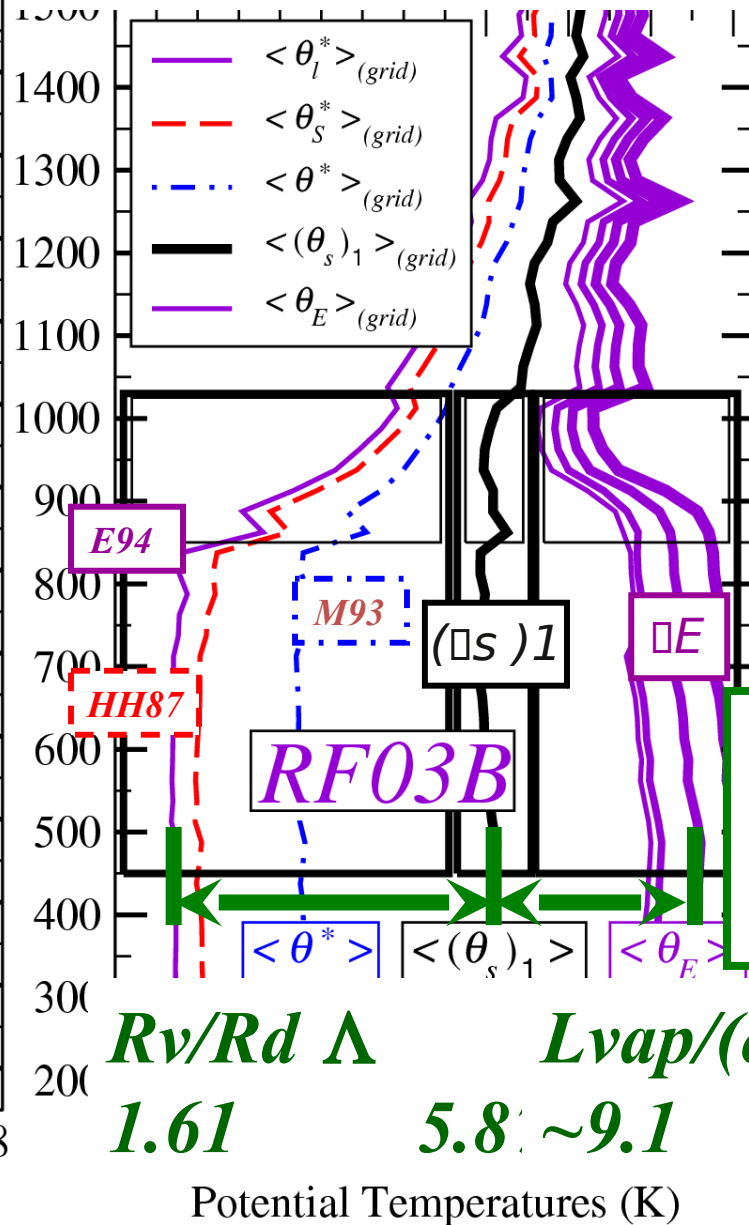
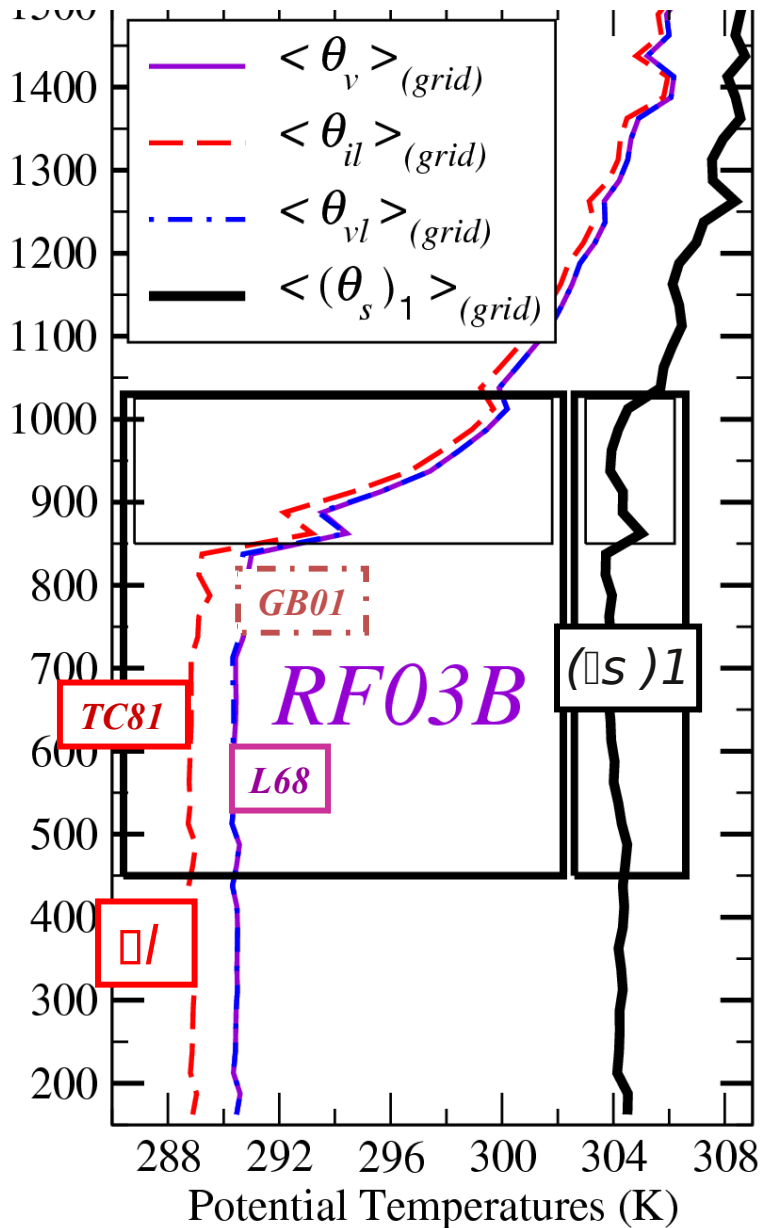
Applications / FIRE-I : [θ_l ; q_t ; q_l] RF03B-hom.



$(\theta_s)_1$ constant with z
 'clear-air' = 'cloud' ! for $(\theta_s)_1$
 No jump in $(\theta_s)_1$!

$$(\theta_s)_1 = \theta_l \exp[\Lambda q_t]$$

And observations tell us about the 'target' of mixing



But θ_s is so homogeneous that it cannot give any good indication about cloud amount!

$(\theta_s)_1 \approx 2/3 - 1/3$
 between θ_l & θ_E

Transport problems: which fluxes and variables?

Originally

$$MSE = c_{pd} T + L_v q_v + g z$$

Practical evolution

$$MSE = c_p T + L_v q_v + g z$$

Neither L_s counterpart, nor even any appearance of q_l ??

Stevens et al. (2003)

$$\frac{c_{pd}}{(\theta_l)} \overline{w' \theta_l'} \approx \frac{1}{(T)} \overline{w' S'_l}$$

$$S_l = c_{pd} T + g z - \overline{L_v} q_l$$

Asymmetric (MSE inheritance), no $q_t=1-q_d$ related part

In p -type coordinates, the new quantity S'_l is the exact counterpart of $c_{pd}T + g z$ for the fully dry case.

$$S'_{li} = (c_{pd} + (c_{pv} - c_{pd}) q_t) T + g z - L_v(T) q_l - L_s(T) q_i$$

$$\theta_{li} = \theta \cdot \exp \left(- \frac{L_{vap} q_l + L_{sub} q_i}{c_{pd} T} \right) \Leftrightarrow S_{hm} - c_{pd} T_Y q_t$$

$$q_t = q_v + q_l + q_i$$

Why has MSE a 'quasi-conservative' reputation?

Originally

$$MSE = c_{pd} T + L_v q_v + g z$$

S'l adaptation

$$MSE' = c_p' T + L_v(T) q_v + g z$$

$$MSE' = \left(c_{pd} + (c_{pv} - c_{pd})(q_v + q_l) \right) T + g z - L_v(T) q_l + L_v(T)(q_v + q_l)$$

So, if $q_i=0$, MSE' and Shm differ only by the last term

But $T_Y = 2362 \text{ K}$ & $L_v(T_0)/c_{pd}=2489 \text{ K} !!!$ (while $\Delta T_0=1603 \text{ K}$)

The close match between the two values is a coincidence. It explains why MSE' (or its MSE approximation) is nearly conservative (5% difference), in the 'warm' case.

But, as soon as we have ice phase, it collapses ($L_s(T_0)/c_{pd}=2821 \text{ K}$) => Use

Shm !

$$S'_{li} = \left(c_{pd} + (c_{pv} - c_{pd}) q_t \right) T + g z - L_v(T) q_l - L_s(T) q_i$$

$$S_{hm} = S'_{li} + c_{pd} T_Y q_t$$

[analogy with $(\theta_s)1$]

...and S'li for the Betts' transforms

May we use M11's findings in moist turbulence (apart from upgrading Betts' transforms & better measuring stability)?

- **The relevant issues are:**
 - **Finding a way to express how nature seems to tend to full mixing of θ_s (i.e. maximising turbulent energy conversion via the transport of qt). *Hints in Pauluis and Held (2002, Part I)?***
 - **Going around the fact that θ_s is a very bad tracer of cloudiness.**
 - **Doing both steps while remaining close to the present formalism for the computation of the buoyancy flux (the development of a formulation for the Brunt-Väisälä-Frequency (BVF) is an interesting intermediate step for that). *See Marquet and Geleyn, 2013, QJRMS.***
 - **Finding a consistent way to introduce that there is a part of the heat and moisture transports which is realised through the asymmetry between the situations inside and outside the clouds.**

The moist entropic potential temperature θ_s within its related Brunt-Väisälä Frequency expansion (1/2)

- For homogenous (non-saturated and fully-saturated) situations, one can compute the squared BVF by noticing that density is function of moist entropy ‘ s ’, total water content ‘ qt ’ and pressure ‘ p ’ only.
- Let us suppose that we know a ‘transition parameter’ (‘ C ’, which can be identified to a cloudiness or to a cloud efficiency) and let us define:

$$F(C) = 1 + C \left[\frac{L_v(T)}{C_p T} \frac{R}{R_v} - 1 \right] \quad M(C) \stackrel{\text{OLE}}{=} \frac{1 + D_C}{1 + D_C F(C)} \quad D_C = \frac{T}{p - e_s(T)} \frac{de_s(T)}{dT}$$

- $F(C)$ ensures the transition between the non-saturated case ($C=0$) where moisture acts only through expansion (Rv/R) and the fully-saturated one ($C=1$) where it acts only through latent heat release ($Lv(T)/(Cp.T)$).
- $M(C)$ cares for the linked change of adiabatic gradient, **without any need for a second transition variable.**
- Remarkably **DC does not depend on moisture amounts.**

A digression concerning vertical adiabatic lapse rates (1/2)

- We compare here the new formulation with the ‘classical’ ones of Durran and Klemp (1982) and of Emanuel (1994) by expressing the vertical adiabatic lapse rates $\Gamma = -dT/dz$.
- In the non-saturated case the correct solution is $\Gamma_{ns} = g/c_p$
- In the case of full saturation with respect to liquid water we have:

$$\Gamma_{sw} = (g/c_p) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}{1 + \left(\frac{R}{c_p} \right) \left(\frac{L_v(T)}{R_v \cdot T} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]} \quad (MG13)$$

Without any doubt, the more exact the derivation, the simpler the final result!

$$\Gamma_{sw} = (g(1 + r_t)/c_{pd}) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}{1 + \frac{c_{pv} \cdot r_{sw} + c_l \cdot r_l}{c_{pd}} + \left(\frac{R(1 + r_t)}{c_{pd}} \right) \left(\frac{L_v(T)}{R_v \cdot T} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]} \quad (DK82)$$

$$\Gamma_{sw} = (g(1 + r_t)/(c_{pd} + c_{pv} \cdot r_{sw})) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}{1 + \frac{c_l \cdot r_l}{c_{pd} + c_{pv} \cdot r_{sw}} + \left(\frac{R(1 + r_t)}{c_{pd} + c_{pv} \cdot r_{sw}} \right) \left(\frac{L_v(T)}{R_v \cdot T} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]} \quad (E94)$$

A digression concerning vertical adiabatic lapse rates (2/2)

- But we have a similar loss of simplicity when replacing the complex θ_s by its simple approximation $(\theta_s)_1$:

$$\Gamma_{sw} = (g/c_p) \frac{1 + \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}{1 + \left(\frac{R}{c_p} \right) \left(\frac{L_v(T)}{R_v \cdot T} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]} \quad (\text{MG13, } \theta_s)$$

$$\Gamma_{sw} = (g/c_{pd}) \left(\frac{R_d}{R} \right) \frac{1 + \left(\frac{R}{R_d} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]}{1 + \frac{L_v(0) \cdot q_l}{c_{pd} \cdot T} + \left(\frac{R}{c_{pd}} \right) \left(\frac{L_v(T)}{R_v \cdot T} \right) \left[\frac{L_v(T) \cdot r_{sw}}{R_d \cdot T} \right]} \quad (\text{MG13, } (\theta_s)_1)$$

- Remark: all the relevant computations were performed for reversible adiabatic $\left(r_{sw}(T, p) = (R_d/R_v) [e_{sw}(T)/(p - e_{sw}(T))] \right)$:

- In the irrev $q_{sw}(T, p) = (R_d/R_v) [e_{sw}(T)/(p - e_{sw}(T)(1 - R_d/R_v))]$ and p :

The moist entropic potential temperature θ_s within its related Brunt-Väisälä Frequency expansion (2/2)

- Going back to $F(C)$ and $M(C)$, for any atmospheric condition, one gets for the squared 'BVF' (MG13):

$$N^2(C)/g = M(C) \frac{1}{C_p} \frac{\partial s}{\partial z} + \frac{\partial \ln(1 - q_t)}{\partial z} + M(C) \left((1 + r_v) \frac{R_v}{R} F(C) - \frac{C_{pd}}{C_p} \Lambda \right) \frac{\partial q_t}{\partial z}$$

- Interpretation (loosely following PH02):

'Classical' TKE \Leftrightarrow TPE conversion

Total water lifting effect (TKE \Leftrightarrow PE)

Λ -scaled differential expansion and latent heat effects (TKE \Leftrightarrow ?)

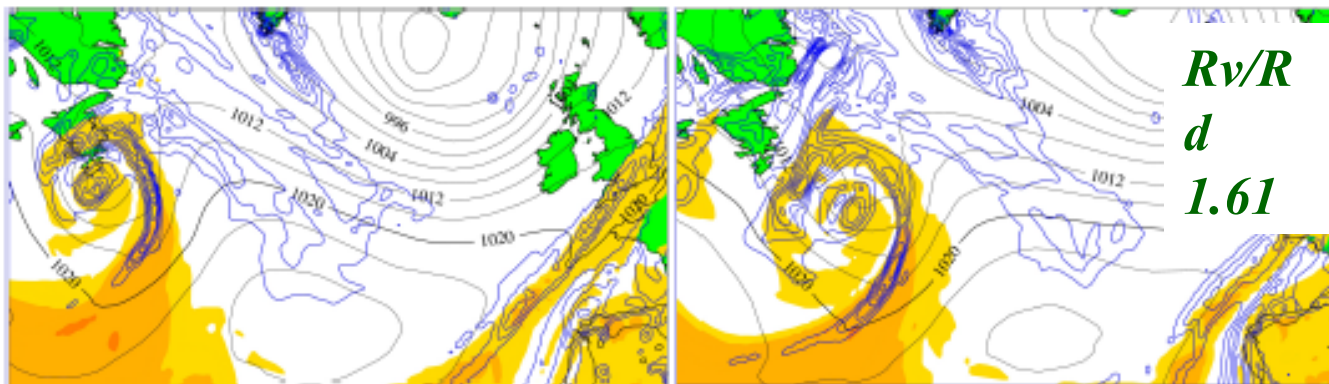
- The (sometimes neglected) 'water loading' second term corresponds to the third reason why the simplistic view of Betts' method is wrong.

Conclusions

- *They are too various and too interdependent to be listed and ranked.*
- *One just hopes to have made more evident the need and interest of treating thermodynamics more carefully and more purposefully in future modelling endeavours (see in particular Catry et al., 2007).*
- *The consequences of the M11 and MG13 papers for treatment of moist turbulence are still under investigation.*
- *There are more advanced consequences of the ‘specific moist’ view of atmospheric thermodynamics in two other areas (i) exergy (or, better said, available enthalpy) & (ii) moist potential vorticity with a state variable (θ_s) conserved in Lagrangian advection and in mixing.*
- *The next step would be to consider the potential of application to the deep convective situation (closure?), most probably with reference to the ideas of PH02.*

Moist PV with θ_v , θ_s , θ_e (900, 925, 950 hPa average)

PV of θ_v (nearly dry, all positive, density linked and hence invertible by definition)

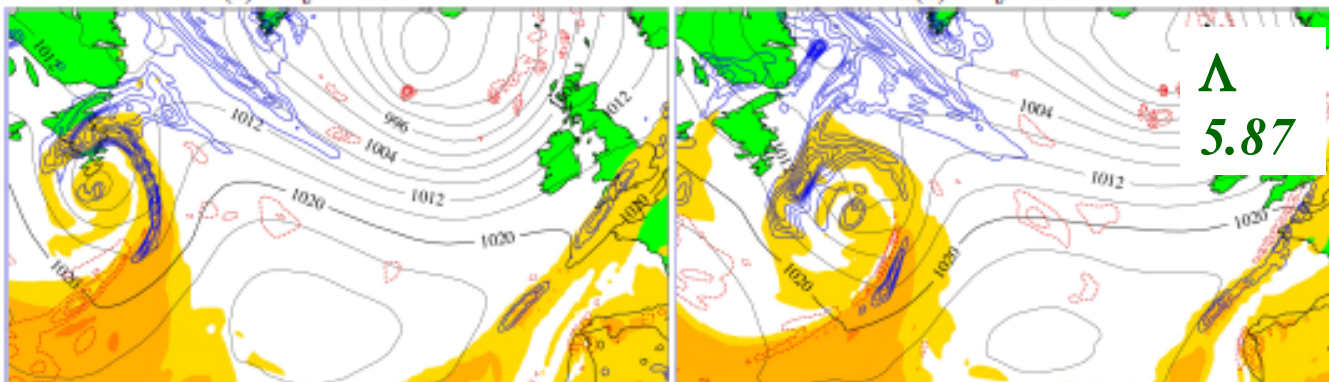


(a) $PV_v / 0$ UTC

(b) $PV_v / 12$ UTC

Rv/Rd
 d
 1.61

PV of θ_s (specific moist, negative only in key zones and perhaps approximately invertible)

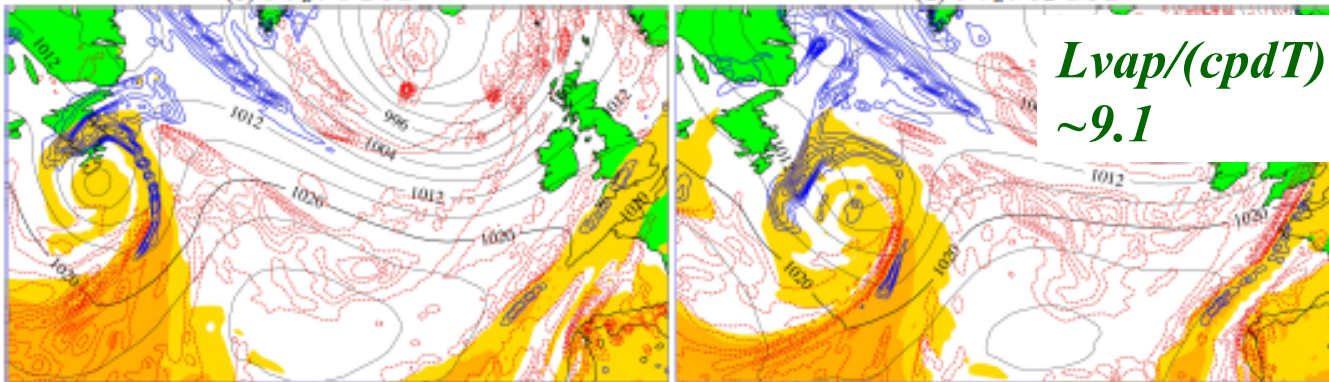


(c) $PV_s / 0$ UTC

(d) $PV_s / 12$ UTC

Λ
 5.87

PV of θ_e ('classically' non-specific moist, negative in wide zones and thus most probably non-invertible)

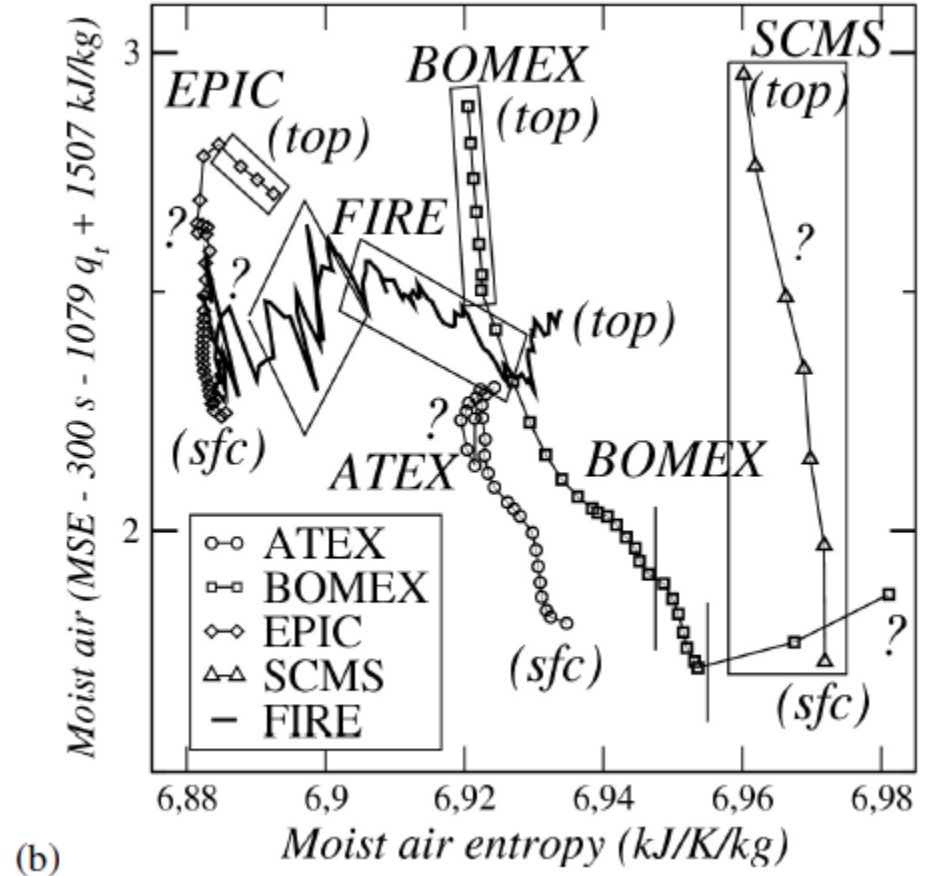
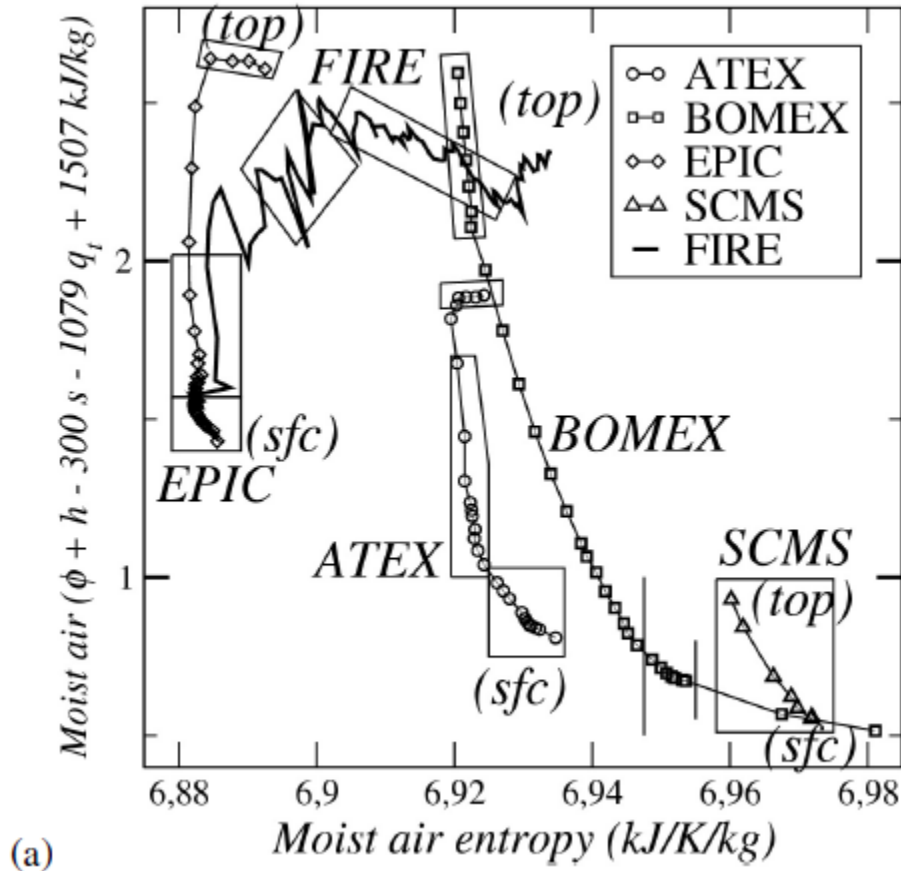


(e) $PV_e / 0$ UTC

(f) $PV_e / 12$ UTC

$Lvap/(cpdT)$
 ~ 9.1

Scaled exergy vs. entropy (reference temperature 300 K; units in kJ/kg equivalent to K) for various field experiments



Based on specific moist enthalpy

Based on moist static energy

The question marks on the right diagram indicate where the 'MSE' profiles seem more questionable than those of the 'h' solution