Beyond 'Dufour et Van Mieghem 1975', contribution of the Third Law to the thermodynamic of moist atmospheric open systems

Jean-François GELEYN

CNRM, Météo-France, Toulouse

(many thanks to P. Marquet, B. Catry, and M. van Ginderachter , the people who did most of the work reported here)

Centenary of IRM, Brussels, 26/9/2013

Introduction (1/2)

- **Idea behind this talk: clean thermodynamics does not need to be too complicated and it has nice applications in meteorology.**

This was already recognised by Dufour and van Mieghem, back in 1975, in a textbook that remained a reference for many years (a landmark work, so to say).

- **But reaching this advantageous situation requires a good deal of consistency.**

If the book had such a lasting influence, it is indeed because the authors were very meticulous (one could say 'anomalously' with respect to their time).

- **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!**

It is here that, retrospectively, we start seeing weaknesses.

Introduction (2/2)

- **But sometimes practical implementation decisions do have some level of arbitrariness => the transversal issues, like for instance conservation properties, should in principle be treated through global constraints.**

In line with the years where they developed all their research, D&vM gave more importance to local phenomenology than to global budget aspects (the idea of systematically solving partial differential evolution equations with computers was not -yet- a paradigm).

- **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).**

We shall now see, with this specific example, how they were both right and wrong.

Split of the presentation

- **<u>A more specific (hindsighted) view of the Dufour and van Mieghem book</u>**

- **<u>Rules (and the importance of following them)</u>:**
  - **Additivity**
  - **Conservation of theoretical invariants**
  - **Related consistency in discretisation**

- **<u>Conditions of application</u>:**
  - **Simplifying (and structuring) hypotheses**
  - **Ancillary computations**

- **<u>A practical modern view of the three Laws of thermodynamics for the moist atmosphere</u>**

- **<u>Examples of (potential) applications</u>**

Retrospective view of the D&vM book (1/3)

- **The development of their equations surprises today. On the one hand they obeyed a sometimes superfluous gradation (dry air, moist air, moist air with one condensed phase, moist air with two condensed phases; hail vs. graupel; …) while on the other hand they were careful to deal with 'true' problems (distinction between temperatures of the various phases, open vs. closed systems).**
- **They found several 'tricks' in order to claim that applications of the First and Second Laws of thermodynamics are equivalent. Yet this is only true when there are no variations of the total water content q_t. In this way, they also avoided mentioning the Third Law.**

Retrospective view of the D&vM book (2/3)

- **They recognised when they were at odds with some other theory (like with respect to 'Normand 1921' for the definition of the wet-bulb temperature). But they did not see that their discrepancy was self-contradicting: the advantage of their solution only appears when variations of q_t are accounted for.**
- **They went around the problem of the non-equivalence of enthalpic and entropic considerations by using averaged amounts of water contents along 'trajectories'. Why not! But they justified it by saying that anyhow there was an asymmetry between the properties of incoming parcels and outgoing ones in 'open' systems. They were obviously not so fond of the Green-Ostrogradsky interpretation of diffusion!**

Retrospective view of the D&vM book (3/3)

- **In their defence, the first correct interpretation of the (important) role of the flux of total water came with Lalas and Einaudi (1974) which they probably did not read before printing their book.**
- **A recent paper by Pelkowski and Frisius (2011) (about the density of 'cloudy air') arrives at similar conclusions (to the ones concerning moist entropy): (i) among the rare authors to deal with a key issue, (ii) very rigorous methodology, but (iii) not so appropriate conclusions.**

Additivity rule

- **When having a complete parameterisation system, one must combine the outputs of individual computations in terms of evolutions of the main-model's variables.**
- **In the case of water species, things are simple thanks to the intrinsic linearity of the tendency equations.**
- **But for energy-linked quantities ($c_pT+\Phi$, $(u^2+v^2)/2$, …), this is not anymore true.**
- **One must then realise that tendencies ARE NOT ADDITIVE: $\delta(c_pT) \neq c_p\,\delta T + \sum T(\partial c_p/\partial q_x)\,\delta q_x$!**
- **Only fluxes (with physical meaning) ARE ADDITIVE.**

This gives a central role to the Green-Ostrogradsky theorem

Moist specific enthalpy conservation

- In a **barycentric** multi-phasic system (prognostic $q_{v/l/i}$) the 'Betts-type static energy' equivalent of the moist specific enthalpy is $S'_{li} = \left(c_{pd} + (c_{pv} - c_{pd})q_t\right)T + g\,z - L_v(T)\,q_l - L_s(T)\,q_i$ with $q_t = q_v + q_l + q_i$
- Using $c_p = c_v + R$ and the above, plus some manipulations, one gets a Green-Ostrogradsky form for the evolution of 'c_pT' (with P' & P''' the vertical integrals of phase changes with respect to vapour, and P_l & P_i the precipitation fluxes):

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

$$\hat{c} = \frac{c_{pd}q_a + c_{pv}q_v + c_lq_l + c_iq_i}{1 - q_r - q_s}$$

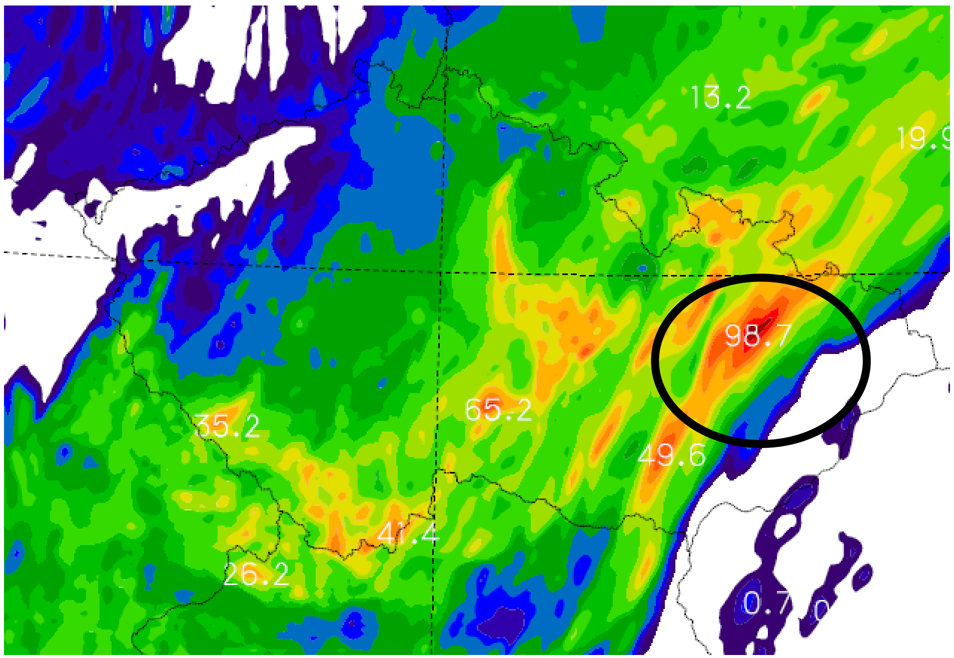
Recent Belgian contribution's slide (BC+MvG)

Impact of (no) enthalpy conservation (1/2)

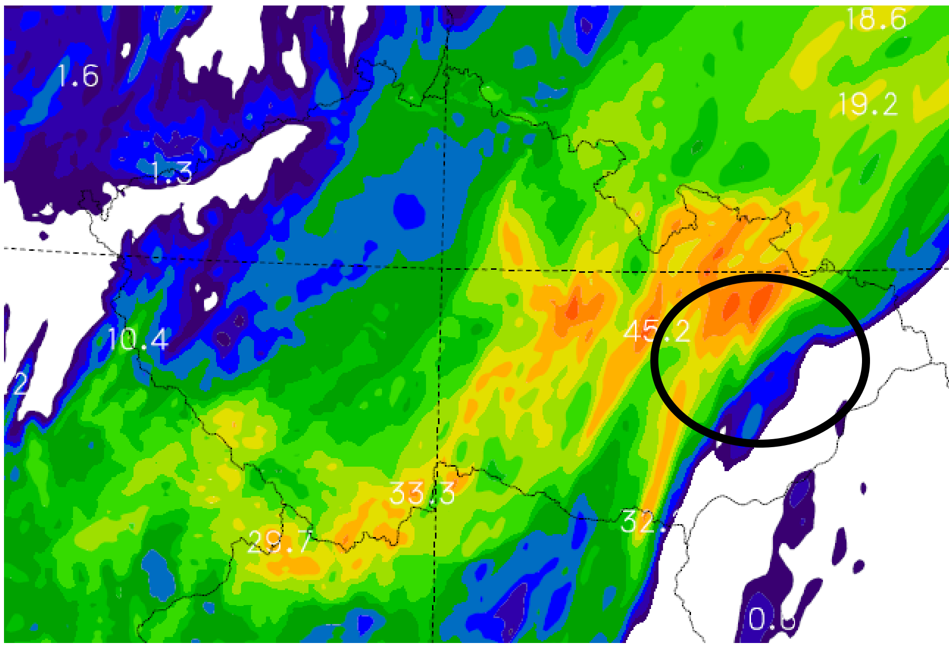
- It is sometimes customary to say that neglecting the time variation of c_p (or c_v, or R) during the ‘physical time-step’ (under the influence of phase changes) has little impact.
- We shall now see that this is not true at all at the ‘convection permitting scales’.
- The trick, given the compact shape 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 (2/2)

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

Courtesy of R. Brožková

‘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 => $p/(\rho.T)=R_d.q_d+R_v.q_v=R$)**
- **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!

Short reminder

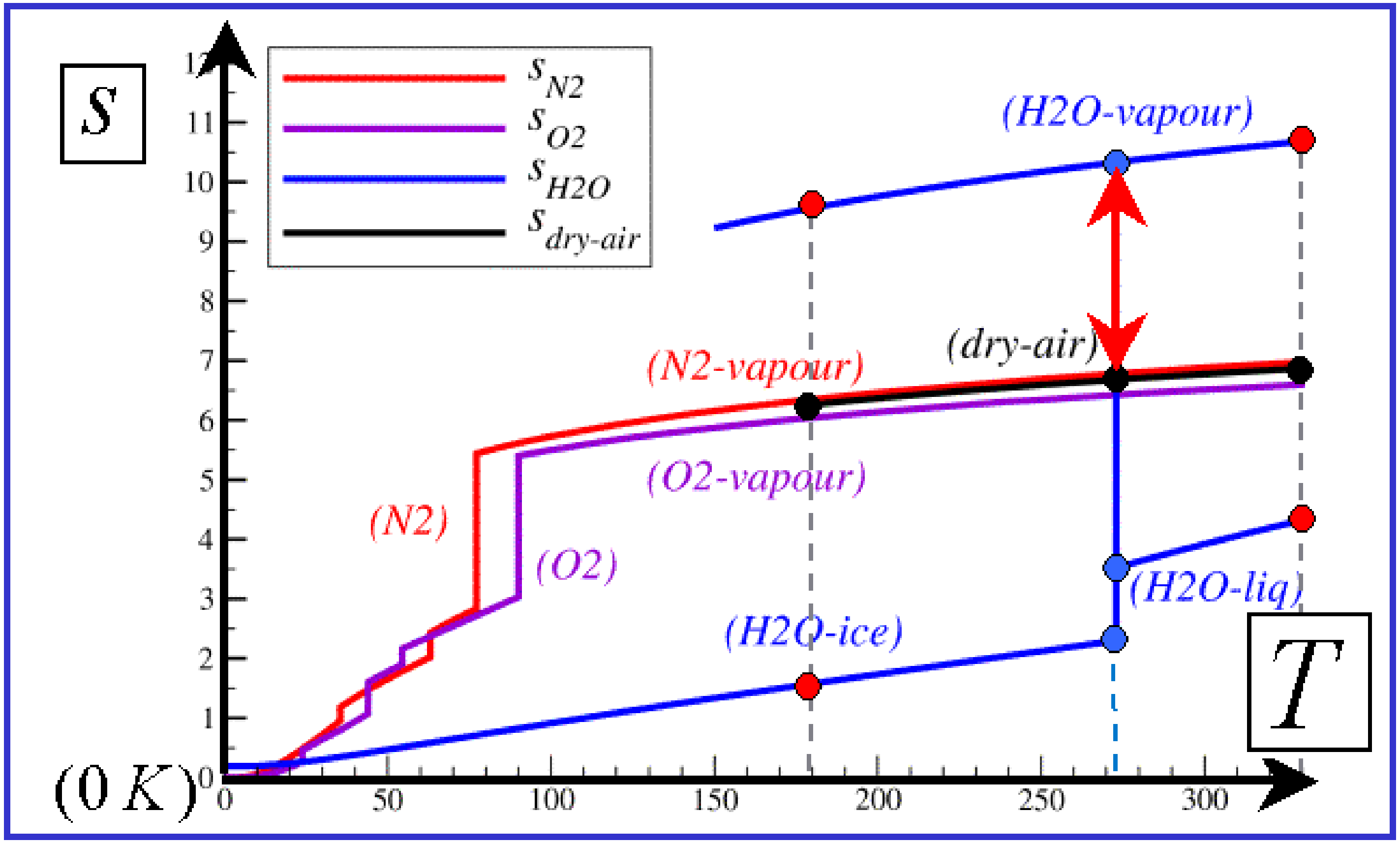
- **<u>First Law of thermodynamics</u>: Conservation of energy (heat Q + work W)**

- **<u>Second Law of thermodynamics</u>: For a closed system, where the change of entropy S due to a heat source is the ratio of the latter to the temperature T (dQ=T.dS):**
  - **Irreversibility (diabatism) implies increase of entropy;**
  - **Adiabatism equals conservation of specific entropy.**

- **<u>Third Law of thermodynamics</u>: 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).**

Practical application of the Third Law

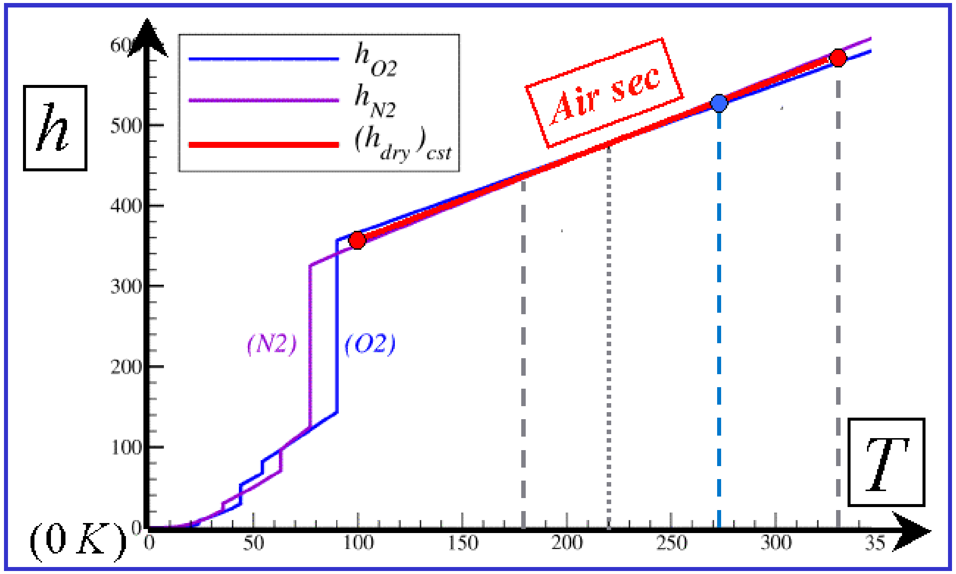


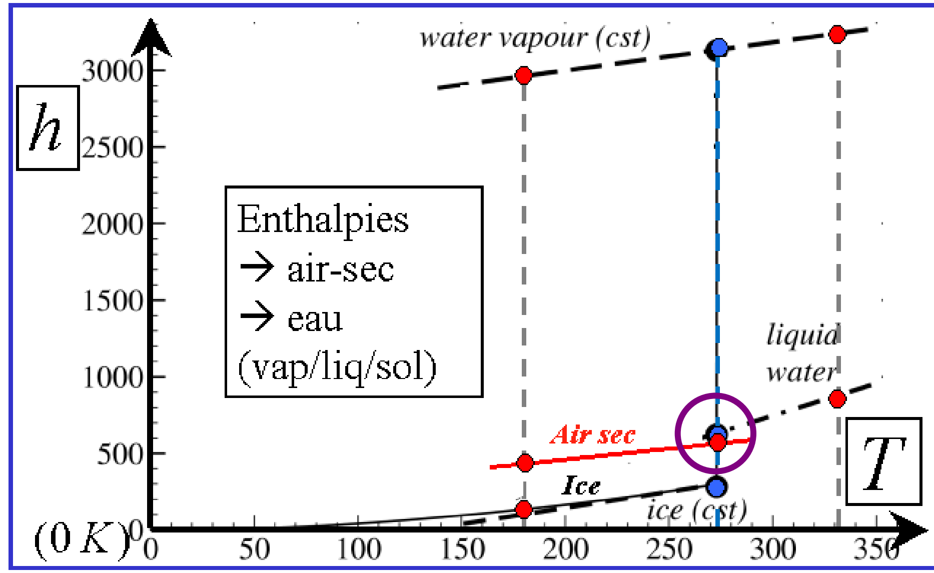
Entropy diagram (in kJ/K/kg) for N_2, O_2, H_2O and for a 1000 hPa pressure

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

Courtesy of P. Marquet

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' (the one that makes the so-called 'MSE' roughly conservative, in case of water condensate, but not in case of ice condensate)

Courtesy of P. Marquet

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 compute : $$\rho\, T\, \frac{d\,s}{dt} = \rho\, \left(\dot{Q}_i + \dot{D} \right) - \rho \left[\mu_k \, \frac{d_i\, q_k}{dt} \right] - \boldsymbol{J}_k \, . \boldsymbol{\nabla}(h_k) - T\, s_k \, (\boldsymbol{\nabla} . \boldsymbol{J}_k)$$

Entropy = state function → measurable at each point: $\boxed{s = q_d\, s_d + q_v\, s_v + q_l\, s_l + q_i\, s_i}$

$$s_d = (s_d)_r + c_{pd} \ln(T/T_r) - R_d \ln[\, p/(p_d)_r \,]$$
$$s_v = (s_v)_r + c_{pv} \ln(T/T_r) - R_v \ln[\, e/e_r \,]$$
$$s_l = (s_l)_r + c_l \ln(T/T_r)$$
$$s_i = (s_i)_r + c_i \ln(T/T_r)$$

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

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

$$s_{ref} = \text{Cste} \qquad \boxed{s \leftrightarrow \theta_s ?}$$

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

Marquet, 2011, QJRMS

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

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

$$s_{ref} \approx \; 1138.56 \, \mathrm{J \, K^{-1} \, kg^{-1}}$$

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

$$\boxed{\times \; \left(\frac{T}{T_r}\right)^{\lambda \, q_t} \left(\frac{p}{p_r}\right)^{-\kappa \, \delta \, q_t} \times \; \left(\frac{r_r}{r_v}\right)^{\gamma \, q_t} \frac{\left(1 + \eta \, r_v\right)^{\kappa \, (1 + \, \delta \, q_t)}}{\left(1 + \eta \, r_r\right)^{\kappa \, \delta \, q_t}}}$$

$(\theta_s)_1$

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

θ_s complicated ?

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

3-phase Betts ?

$$q_t = q_v + q_l + q_i$$

$$(\theta_s)_1 = \theta_{li} \, \exp\left(\Lambda \, q_t\right)$$

Marquet, 2011, QJRMS

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

+ ***absolute*** **values of partial entropies →**

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

The 3rd Law …

+ ***similar*** **computations for moist enthalpy →**

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

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

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

$$c_{pd}\, T_h = [\,c_{pd} + (c_{pv} - c_{pd})\, q_t\,] T - L_{vap}\, q_l - L_{sub}\, q_i + c_{pd}\, T_{\Upsilon}\, q_t$$
$$= S_{hm} - g\, z$$

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))

Computations of $s \rightarrow \theta_s \leftrightarrow T_h$: 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 3[rd] Law …

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

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

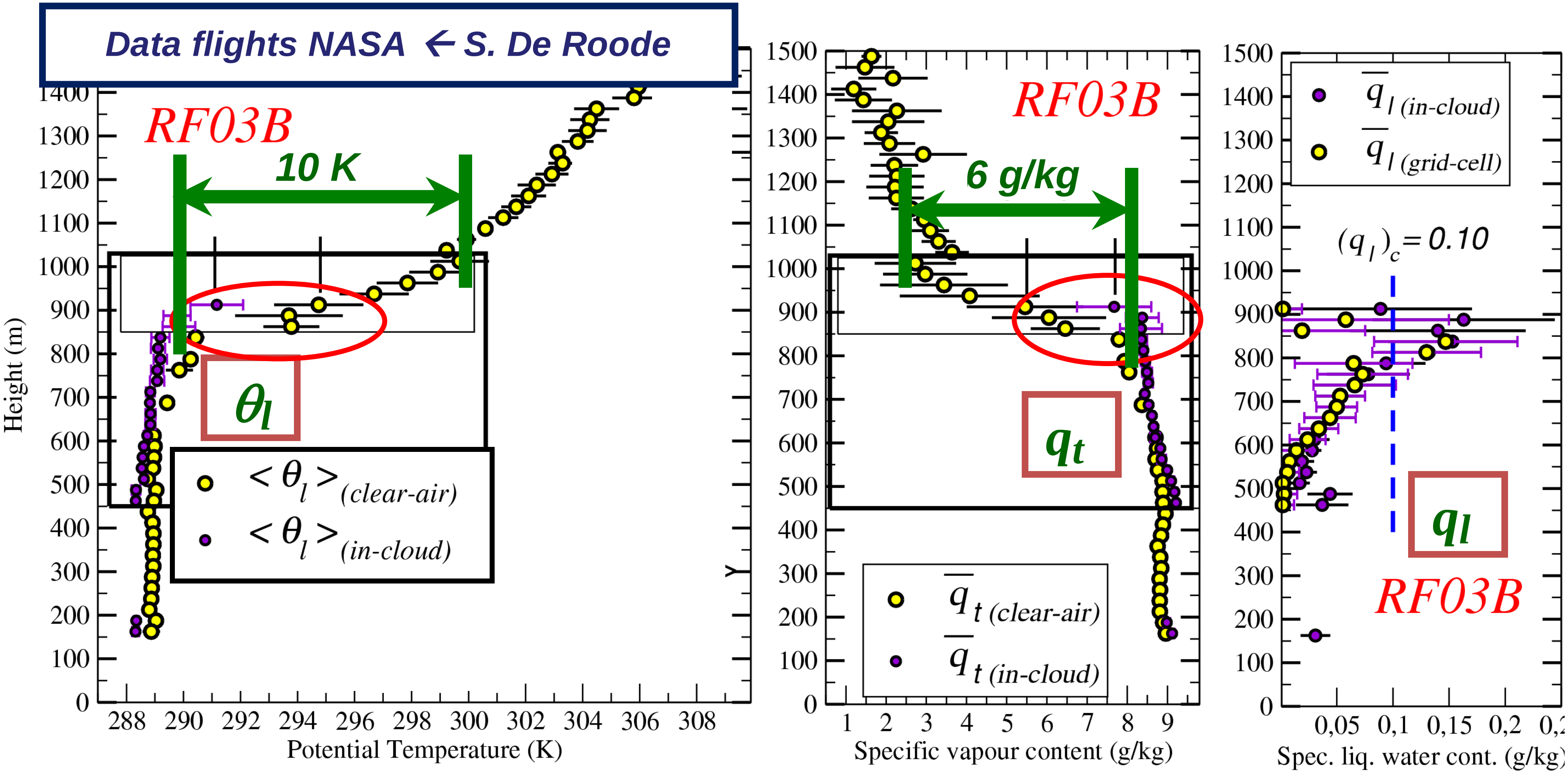
$$h_{ref} \approx 256\ kJ\,kg^{-1}$$

$$c_{pd}\, T_h = [\, c_{pd} + (c_{pv} - c_{pd})\, q_t \,] T - L_{vap}\, q_l - L_{sub}\, q_i + c_{pd}\, T_{\Upsilon}\, q_t$$
$$= S_{hm} - g\, z$$

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

Restricting to the conservation law for $c_p T$ brings back to S'_{li}

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



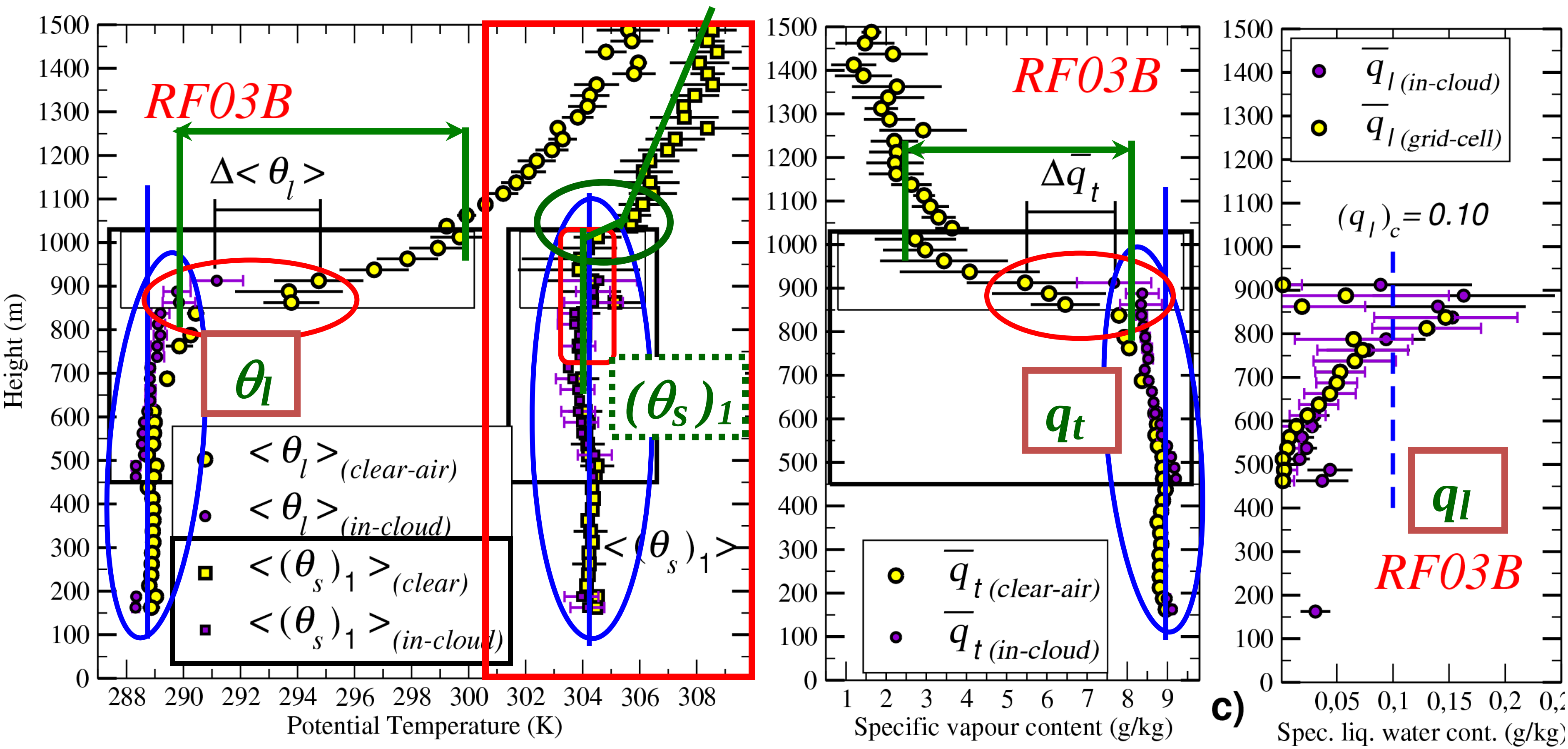
Sc = 'cloud stew' => laboratory for conservation rules

"clear-air" ≠ "cloud" (entrain. region)

Large jumps in θ_l and q_t (entrain. region)

Marquet, 2011, QJRMS

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



$(\theta_s)_1$ constant with z

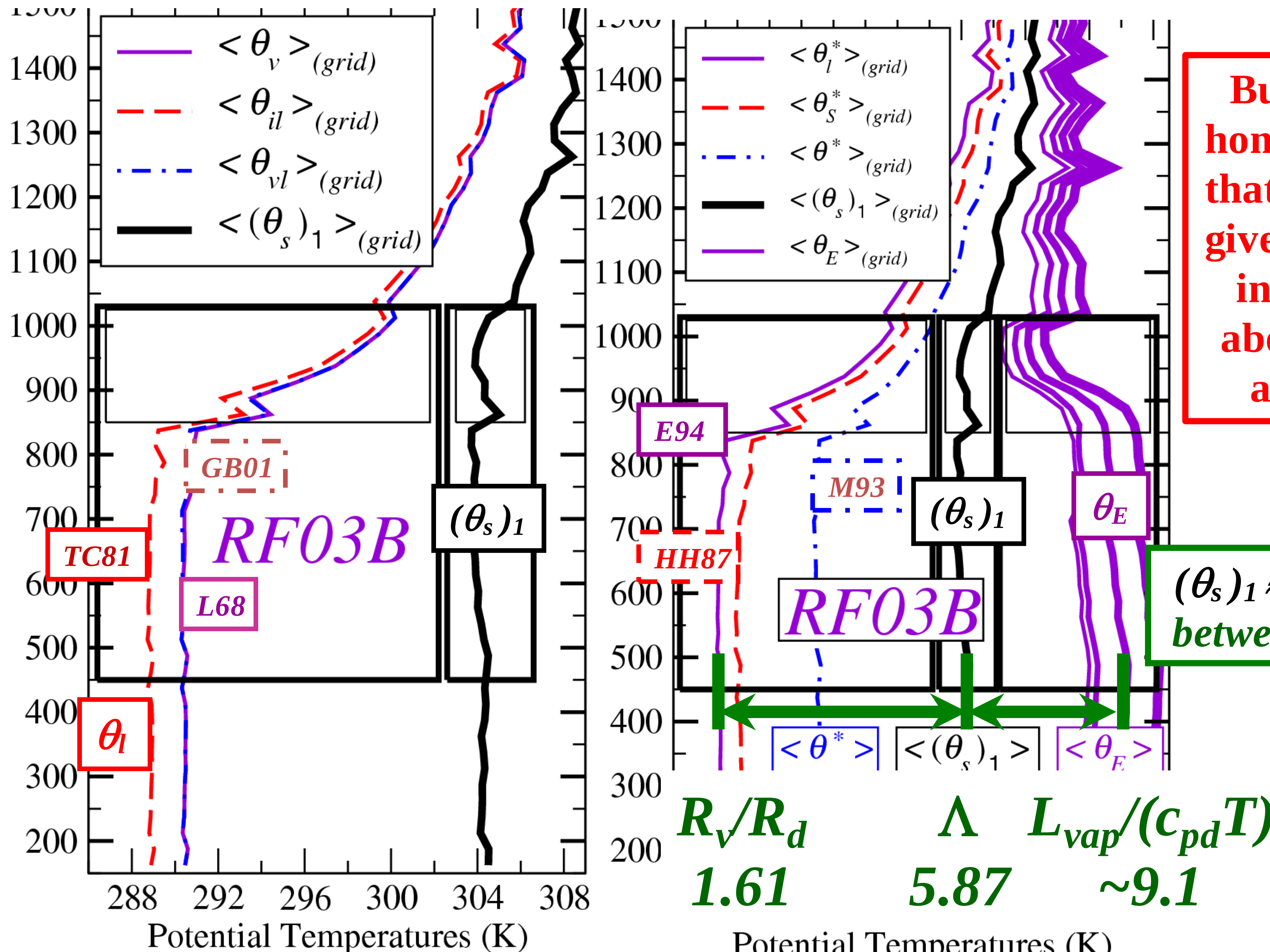
"clear-air" = "cloud" ! for $(\theta_s)_1$

No jump in $(\theta_s)_1$!

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

Marquet, 2011, QJRMS

And observations tell us about the 'target' of mixing



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

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

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

- We compare here the new formulation (Marquet and Geleyn, 2013) with the 'classical' ones of Durran and Klemp (1982) and of Emanuel (1994) by expressing the vertical adiabatic lapse rates ***Γ=-dT/dz*** .
- In the non-saturated case the correct solution is $\boldsymbol{\Gamma_{ns}=g/c_p}$
- In the case of full-saturation with respect to liquid water we have:

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

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

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

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

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

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

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

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

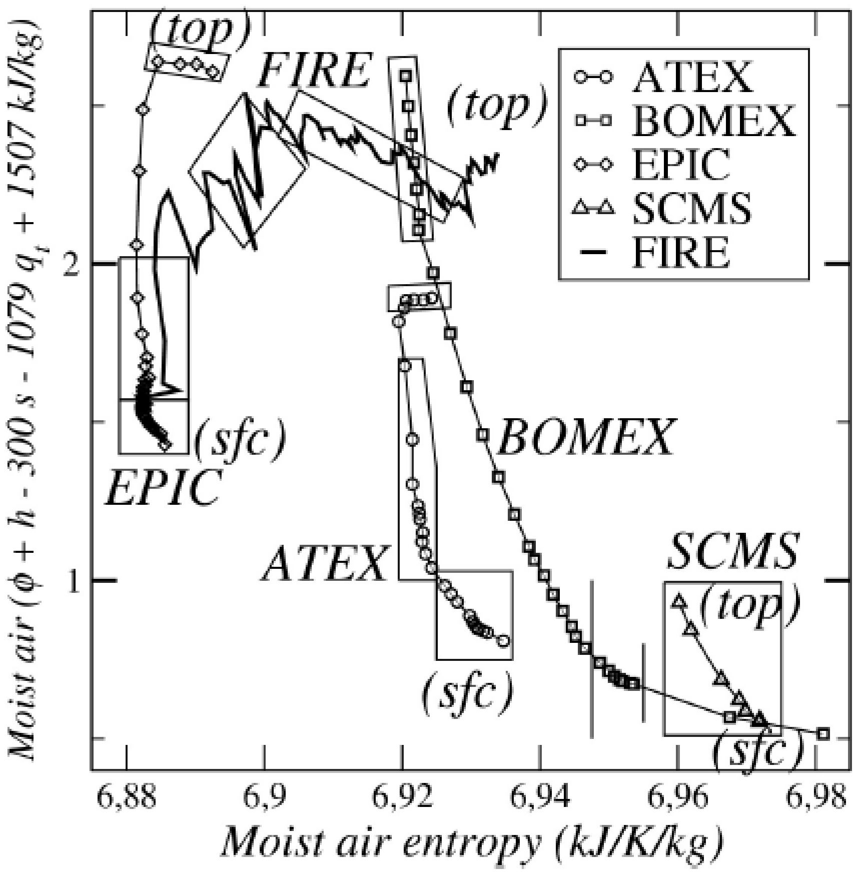
- Remark: all the relevant computations were performed for reversible adiabatic conditions (no precipitation) where we have:

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

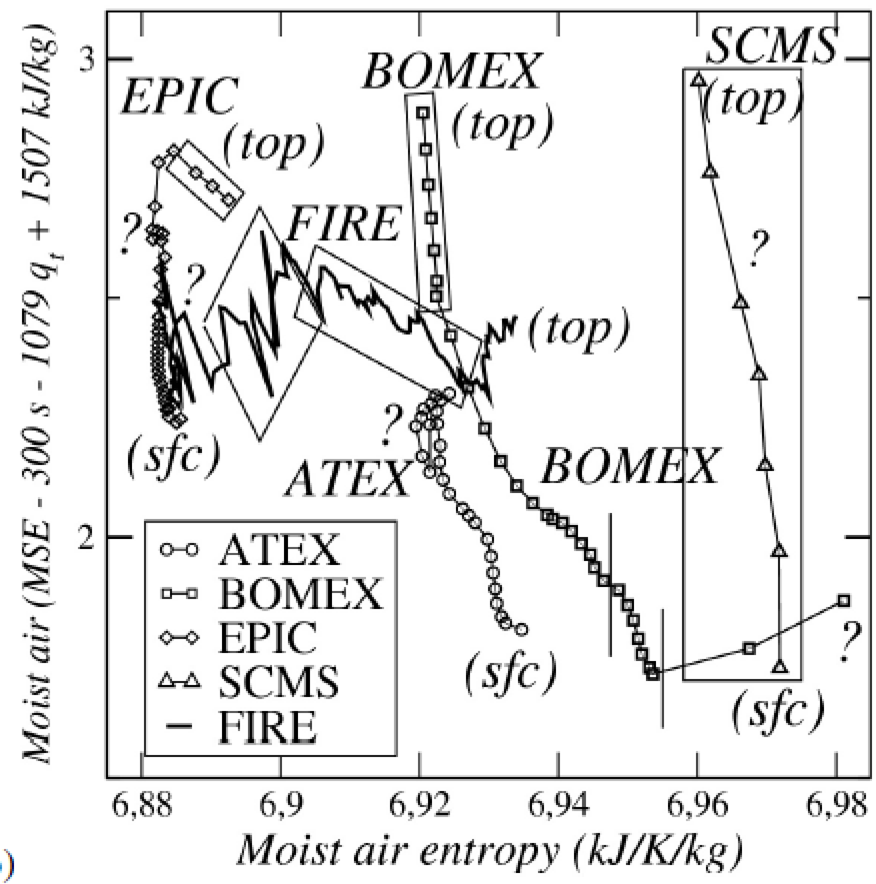
- In the irreversible case we would have instead as function of $\boldsymbol{T}$ and $\boldsymbol{p}$:

$$q_{sw}(T,p) = (R_d/R_v)\left[e_{sw}(T)/\left(p-e_{sw}(T)(1-R_d/R_v)\right)\right]$$

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



(a)



(b)

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

Courtesy of P. Marquet

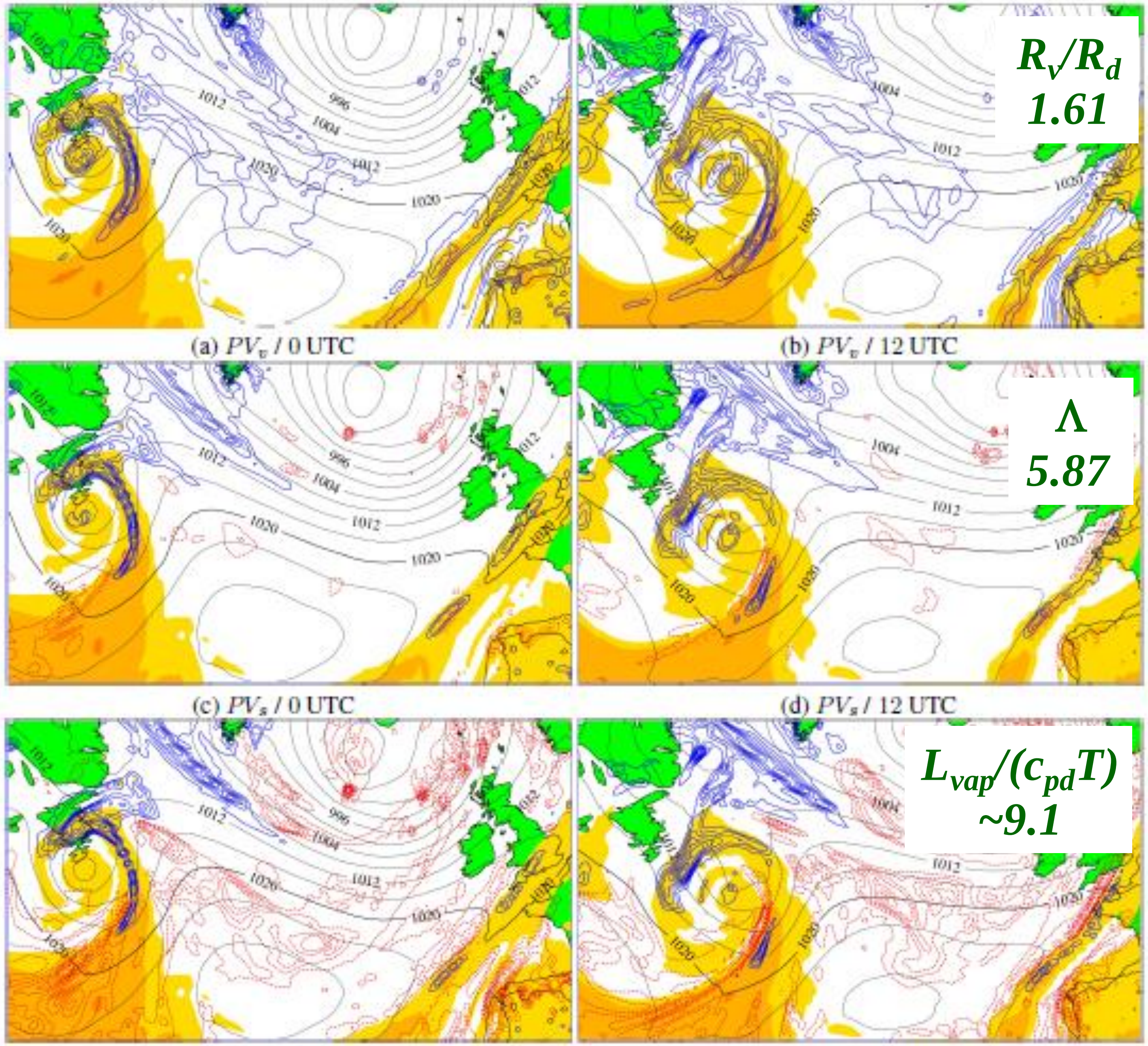
Moist PV with θ_v, θ_s, θ_e (900, 925, 950 hPa average)

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

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

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

Courtesy of P. Marquet



(a) PV_v / 0 UTC

(b) PV_v / 12 UTC

(c) PV_s / 0 UTC

(d) PV_s / 12 UTC

(e) PV_e / 0 UTC

(f) PV_e / 12 UTC

Conclusions

- ***Going back to the Dufour and van Mieghem book, what happened in the past 38 years? Well:***
  - ***We still need the careful handling of complex equations to find compact and rather simple algorithms;***
  - ***The respective roles of the three Laws are now better understood and it is clearly counterproductive to try and 'hide' these distinctions behind artificial simplifications;***
  - ***One automatically thinks globally in line with the solution of budget PDEs by super-computing means.***
- ***On top of that, in this talk:***
  - ***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);***
  - ***There are 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.***