The parametrisation of the turbulent diffusion fluxes in the presence of cloud ice and droplets: synthesis and application to Aladin

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An air parcel moved by diffusive vertical transport experiences variations of pressure an temperature; these variations affect the saturation pressure, entraining condensation/evaporation processes. When the temperature of the parcel is below the triple point, the condensed phase composition can also change. These processes are diabatic and the local variations of the temperature have a feedback on the local saturation pressure. If the condensate amounts become significant, microphysical processes may start, entraining precipitation.

In this context, it becomes a very rough approximation to represent the turbulent diffusion by a mere adiabatic transport.

To handle this problem, some authors like Deardorff [1976] promoted the use of conservative variables, i.e. variables which would be conserved along the transport. This may be done to a certain extent by using a set of hypotheses, which will appear in the further development.

First, we restrict to non precipitating cases. In this case, the total water:

$$q_t = q_v + q_i + q_\ell$$

is conserved (q_v, q_i, q_ℓ are the specific contents of water vapour, cloud ice particles and cloud droplets). In dry adiabatic motions, the potential temperature θ is conserved:

$$\theta = T\left(\frac{p_0}{p}\right)^{R/c_p} \qquad \text{with } R = R_a + r_v R_v \approx R_a + q_v R_v \text{ and } c_p = c_{pa} + r_v c_{pv} \approx c_{pa} + q_v c_{pv} \tag{1}$$

where r_v and q_v are respectively the mixing ratio and the specific contents of water vapour, T the temperature, p the pressure, $p_0 = 1000hPa$, R_a and R_v are the perfect gas constants for dry air and water vapour, c_{pa} and c_{pv} their specific heats.

θ is related to the dry static energy $s = c_pT + \phi$ (with ϕ the geopotential) by

$$\frac{\partial s}{\partial p} = c_p\frac{\partial T}{\partial p} - \frac{RT}{p} = \frac{c_pT}{\theta}\frac{\partial \theta}{\partial p} \tag{2}$$

using the perfect gas law and the hydrostatic hypothesis.

When saturation and condensation/evaporation are likely, θ is no longer conserved. Betts [1973] defined the liquid-water potential temperature θ_ℓ as

$$\theta_\ell \equiv \theta - \underline{\left(\frac{\theta}{T}\frac{L_v}{c_p}\right)}q_\ell \tag{3}$$

A similar expression may be written for an ice potential temperature θ_i, assuming a single solid condensate and using L_s, the sublimation latent heat.

Deardorff [1976] proposes some paths to generalize this to the simultaneous presence of cloud ice and droplets, as an "ice-liquid" potential temperature:

$$\theta_{li} = \theta - \frac{\theta}{T}(\frac{L_v}{c_p}q_\ell + \frac{L_s}{c_p}q_i) \tag{4}$$

we have

$$\frac{\partial \theta_{li}}{\partial p} = \frac{\partial \theta}{\partial p} - \frac{1}{c_p}\left(\frac{p_0}{p}\right)^{R/c_p}\left(L_v\frac{\partial q_\ell}{\partial p} + L_s\frac{\partial q_i}{\partial p}\right) + \frac{R}{c_p^2 p}\left(\frac{p_0}{p}\right)^{R/c_p}(L_v q_\ell + L_s q_i)$$

$$\Longrightarrow \frac{c_pT}{\theta}\frac{\partial \theta_{li}}{\partial p} = \frac{c_pT}{\theta}\frac{\partial \theta}{\partial p} - L_v\frac{\partial q_\ell}{\partial p} - L_s\frac{\partial q_i}{\partial p} + \frac{RLq_c}{c_p p} \approx \frac{\partial(s - L_v q\ell - L_s q_i)}{\partial p}.$$

(were we used a bulk $Lq_c = L_v q_\ell + L_s q_i$). Hence

$$s_{li} = s - L_v q_\ell - L_s q_i = c_p T + \phi - L_v q_\ell - L_s q_i \equiv c_p T_{li} + \phi \tag{5}$$

is an alternative candidate for a conservative variable.

Now we should assess more closely to what extents these variables may be considered conservative. Deardorff [1976] says that assuming no precipitation, no freezing/melting , no radiative transfer, θ_ℓ is conservative to the extent that the underlined factor in Eq. 3 is relatively constant in comparison with q_ℓ.
Actually, the latent heats depend mainly on temperature:

$$L_v(T) = L_{v0} + (c_{pv} - c_w)(T - T_0), \qquad L_s(T) = L_{s0} + (c_{pv} - c_i)(T - T_0),$$

while the specific heat vary with the phase composition:

$$c_p(q_v, q_\ell, q_i) = c_{pa} + (c_{pv} - c_{pa})q_v + (c_w - c_p a)q_\ell + (c_i - c_{pa})q_i$$

Differentiating Eq. 3,

$$\triangle\theta_\ell = \triangle\theta - \left(\frac{\theta}{T}\frac{L_v}{c_p}\right)\triangle q_\ell - q_\ell \triangle\left(\frac{\theta}{T}\frac{L_v}{c_p}\right)$$

Let's consider an imaginary motion where q_ℓ keeps a constant positive value (for instance the water is put into a watertight bag while the air keeps dry). One could think that in the absence of other exchange of mass or heat (conduction, radiation, molecular diffusion...) with the environment the dry air particle then follows an adiabatic transformation: there is no phase transition to act as a heat source or sink. But if the pressure is changed, the final temperature of the parcel is also changed, and the water in the bag must be brought to this temperature, which will modify θ: for this, the variation of $L_v(T)$ in the last term may play its role.
Now let's suppose that the bag were isolated: in this case, the last term still contains the variation of θ/T: one then needs the hypothesis that this variation is negligible, else we loose the conservative character of θ_ℓ. This justifies Deardorff's statement.
The expression for s_{li} in Eq.5 is simpler than the one for θ_{li}. Considering the same imaginary experiment as above (constant condensates), we only have the variations of the latent heats with the temperature, which correspond to bringing the condensates to the final temperature of the parcel. It appears that unlike θ_{li}, no approximation is required to consider that s_{li} is conservative. The last equality in Eq. 5 means that the parcel behaves like a dry parcel at temperature T_{li}. It looks as if we evaporated all the condensates before the motion, and re-condensed them at the end. This supposes that no other process acts on the way of the parcel, i.e.

- no exchange of substance with environment: no entrainment, no molecular diffusion, no precipitation;
- no exchange of heat: no conduction at the interface, no radiative effect.

These basic assumptions limit the motions where s_{li} is conserved to short and quick motions, like turbulent diffusion or parts of the processes of shallow clouds, excluding deep convection, as well as radiative and microphysical processes.
Our goal here is to handle the turbulent vertical diffusion.
The idea is to compute the turbulent diffusion of the two quasi-conservative variables: q_t and s_{li}, and the to find back corresponding diffusion fluxes for s, q_v, q_ℓ and q_i.
The definition of q_t and s_{li} give two relations: to close the system, we need two additional relations, for instance binding the contents of ice and droplets to the two conservative variables.
The partition between vapour and condensates depends on the local saturation. The model variables represent mean grid-box values: turbulent diffusion acts on the local values, which may vary significantly

within the grid box. We use Reynolds' decomposition of the local values between a mean component and a perturbation:

$$\psi = \overline{\psi} + \psi^{'}, \qquad \overline{\psi'} \equiv 0$$

where the overbar denotes the space averaging.
There can be condensation in parts of a grid box while the mean grid box values are not saturated. Condensation is loosely bound to saturation: it depends on the presence of condensation nuclei, and oversaturation may be observed. Practically, in the limits of the diffusion processes, it appears too ambitious to introduce such microphysical details, as long as the development will be based on vague statistical estimations of the subgrid variability. So the simplest is to assume that the condensation occurs as soon as the saturation is reached. The condensation may be expressed on base of the saturation vapour specific content. DEARDORFF [1976] or BOUGEAULT [1981] show that to a very good approximation, the dependence of q_s to the pressure can be neglected compared to the variation with temperature. So we may linearise the Clausius-Clapeyron equation as

$$\frac{\partial q_{s\ell}}{\partial T} = q_{s\ell} \frac{L_v}{R_v T^2}, \qquad \frac{\partial q_{si}}{\partial T} = q_{si} \frac{L_s}{R_v T^2} \tag{6}$$

around a temperature T_{li}:

$$q_{s\ell}(T) = q_{s\ell}(T_{li}) + \left.\frac{\partial q_{s\ell}}{\partial T}\right|_{T_{li}} (T - T_{li}) \qquad q_{si}(T) = q_{si}(T_{li}) + \left.\frac{\partial q_{si}}{\partial T}\right|_{T_{li}} (T - T_{li}) \tag{7}$$

This linearisation (computing the derivative at a given temperature) suggests to also suppress the quadratic terms in the expression of the perturbations of s_{li}, i.e. to use the values $L_s(\overline{T})$ and $L_v(\overline{T})$.
The saturation also depends on the phase to which condensation occurs.
Below the triple point, there still exists a condensation in the form of droplets when the ice forming nuclei are scarce. One often parametrizes this as a mixed phase present between two temperatures, say 0^{o}C and -40^{o}C, where statistically the ice fraction decreases in function of the temperature. In our scheme (based on Lopez 2001), the ice fraction of the cloud condensates follows

$$\frac{q_i}{q_c} = \alpha_i(T) = 1 - \exp\left(- \frac{(T_t - \min(T_t, T))^2}{2(T_t - T_x)^2} \right) \tag{8}$$

where $q_c = q_\ell + q_i$, $T_t = 273.15$ is the triple point temperature and T_x is the temperature of the maximum difference between the saturation vapour pressures with respect to ice and to liquid. Since α_i represents a statistical partition, we should only consider a mean value for a given grid box, $\alpha_i(\overline{T})$.
With the two hypothesis: prescribed $\alpha_i(\overline{T})$ and no oversaturation, we can express the local condensate contents as

$$q_c \equiv q\ell + q_i = \max(0, q_t - q_s), \qquad q_s = \alpha_i(\overline{T}) q_{si}(T) + (1 - \alpha_i(\overline{T})) q_{s\ell}(T).$$

Applying Eq. 7 around T_{li} and $\overline{T_{li}}$,

$$q_{si}(T) = q_{si}(T_{li}) + \left.\frac{\partial q_{si}}{\partial T}\right|_{T_{li}} (T - T_{li}) = q_{si}(\overline{T_{li}}) + \left.\frac{\partial q_{si}}{\partial T}\right|_{\overline{T_{li}}} (T^{'}_{li}) + \left.\frac{\partial q_{si}}{\partial T}\right|_{T_{li}} \frac{s - s_{li}}{c_p}$$

$$q_{s\ell}(T) = q_{s\ell}(T_{li}) + \left.\frac{\partial q_{s\ell}}{\partial T}\right|_{T_{li}} (T - T_{li}) = q_{s\ell}(\overline{T_{li}}) + \left.\frac{\partial q_{s\ell}}{\partial T}\right|_{\overline{T_{li}}} (T^{'}_{li}) + \left.\frac{\partial q_{s\ell}}{\partial T}\right|_{T_{li}} \frac{s - s_{li}}{c_p}$$

Using $s - s_{li} = L_v q_\ell + L_s q_i$, we note

$$\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}} = (1 - \alpha_i(\overline{T})) \left.\frac{\partial q_{s\ell}}{\partial T}\right|_{T_{li}} + \alpha_i(\overline{T}) \left.\frac{\partial q_{si}}{\partial T}\right|_{T_{li}}$$

and

$$q_s(\overline{T_{li}}) = \alpha_i(\overline{T}) q_{si}(\overline{T_{li}}) + (1 - \alpha_i(\overline{T})) q_{s\ell}(\overline{T_{li}}).$$

Then, in case of saturation

$$q_\ell(1+\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}}\frac{L_v(\overline{T})}{c_p})+q_i(1+\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}}\frac{L_s(\overline{T})}{c_p})=q_t-q_s(\overline{T_{li}})-\left.\frac{\partial q_s}{\partial T}\right|_{\overline{T_{li}}}\frac{s_{li}^{'}}{c_p}.$$

We assume that the ice fraction is the same for the local condensates (or the perturbations) as for the mean grid box condensates: $\alpha_i(\overline{T})$:

$$q_i=\alpha_i(\overline{T})q_c, \qquad q_\ell=(1-\alpha_i(\overline{T}))q_c.$$

This hypothesis is justified because α_i represents a statistics and we have no access to the actual local values of the ice fraction. The simple temperature dependence in Eq. 8 is a crude simplification of much more complex processes.
Hence

$$\left\{(1+\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}}\frac{L_v(\overline{T})}{c_p})(1-\alpha_i(\overline{T}))+(1+\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}}\frac{L_s(\overline{T})}{c_p})\alpha_i(\overline{T})\right\}q_c=q_t-q_s(\overline{T_{li}})-\frac{1}{c_p}\left.\frac{\partial q_s}{\partial T}\right|_{\overline{T_{li}}}s_{li}^{'}$$

Noting

$$\begin{aligned} a&=\left\{(1+\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}}\frac{L_v(\overline{T})}{c_p})(1-\alpha_i(\overline{T}))+(1+\left.\frac{\partial q_s}{\partial T}\right|_{T_{li}}\frac{L_s(\overline{T})}{c_p})\alpha_i(\overline{T})\right\}^{-1}\\ b&=\frac{1}{c_p}\left.\frac{\partial q_s}{\partial T}\right|_{\overline{T_{li}}}\end{aligned}\tag{9}$$

we get

$$q_c=\max\left\{0,a(\overline{q_t}-q_s(\overline{T_{li}}))+a(q_t^{'}-bs_{li}^{'})\right\}\tag{10}$$

Which can be expressed [Smith, 1990] as a function of the subgrid variability:

$$q_c(\zeta)=\max\left\{0,Q_c+\zeta\right\}, \qquad \zeta\equiv a(q_t^{'}-bs_{li}^{'}), \qquad Q_c=a(\overline{q_t}-q_s(\overline{T_{li}}))$$

Assuming $G(\zeta)$ to be the probability density distribution of ζ in the grid box, the cloud fraction f and the mean condensate are given by

$$f=\int_{-Q_c}^{\infty}G(\zeta)d\zeta, \qquad \overline{q_c}=\int_{-Q_c}^{\infty}(Q_c+\zeta)G(\zeta)d\zeta$$

The Smith scheme assumes a symmetric triangular distribution $G(\zeta)$. positive for $-\sigma_\zeta\sqrt{6}<\zeta<\sigma_\zeta\sqrt{6}$, with a maximum $1/(\sigma_\zeta\sqrt{6})$ at $\zeta=0$, where

$$\sigma_\zeta=a\sqrt{\overline{q_t^{'2}}-2b\overline{q_t^{'}s_{li}^{'}}+b^2\overline{s_{li}^{'2}}}$$

is the standard deviation of ζ.
To compute the moments for the vertical diffusion, with $w=\overline{w}+w^{'}$, we need to choose a joint distribution $G'(\zeta,w^{'})$, so that

$$\overline{w'q_c'}=\overline{wq_c}-\overline{w}\;\overline{q_c}=\int_{-\infty}^{+\infty}\int_{-Q_c}^{\infty}w^{'}(Q_c+\zeta)G(\zeta,w^{'})d\zeta dw^{'}$$

Mellor [1977] has shown that assuming a Gaussian joint distribution for w' and ζ, the resulting correlation is given by

$$\overline{w'q_c'}=Na(\overline{w'q_t'}-b\,\overline{w's_{li}'}), \qquad N=\int_{-Q_c}^{\infty}G(\zeta)d\zeta\tag{11}$$

where N is the cloud fraction. BOUGEAULT [1982] questioned the hypothesis of a joint Gaussian distribution, while proposing to keep the relation

$$\overline{m'q_c'} = \overline{m'\zeta}\frac{\overline{q_c'\zeta}}{\sigma_\zeta^2} \qquad \overline{q_c'\zeta} = \int_{-\infty}^{\infty} q_c'(\zeta)G(\zeta)d\zeta$$

valid for any variable m following Mellor's development, i.e. to extent this result to non Gaussian distributions.
He then uses a set of distributions characterized by a skewness factor A_s and the normalized generalized condensate $Q_1 = Q_c/\sigma_\zeta$. The different integrations yield then different functions, written as

$$N = F_0(Q_1, A_s), \qquad \frac{\overline{q_c}}{\sigma_\zeta} = F_1(Q_1, A_s), \qquad \frac{\overline{\zeta q_c'}}{\sigma_\zeta^2} = F_2(Q_1, A_s)$$

This implies to replace the factor N in Eq. 11 by F_2.
BECHTOLD et al. [1995] express

$$\frac{\overline{\zeta q_c'}}{\sigma_\zeta^2} = N(1 + f_{NG})$$

where f_{NG} is the non-Gaussian contribution to the flux.
So we can compute the vertical turbulent diffusion flux of condensate based on the fluxes of the quasi-conservative variables. In the expression of a, we can compute the derivatives at $\overline{T_{li}}$ instead of T_{li}. Finally, the vertical turbulent diffusion flux for the vapour, the condensed phases and the dry static energy are given by

$$\begin{aligned}
\overline{w'q_v'} &= \overline{w'q_t'} - \overline{w'q_c'} \\
\overline{w'q_i'} &= \alpha_i(\overline{T})\overline{w'q_c'} \\
\overline{w'q_\ell'} &= (1 - \alpha_i(\overline{T}))\overline{w'q_c'} \\
\overline{w's'} &= \overline{w's_{li}'} + L_s(\overline{T})\overline{w'q_i'} + L_v(\overline{T})\overline{w'q_\ell'} = \overline{w's_{li}'} + \left[(1 - \alpha_i(\overline{T})L_v(\overline{T}) + \alpha_i(\overline{T})L_s(\overline{T})\right]\overline{w'q_c'}
\end{aligned} \tag{12}$$

This way, the vertical variation of α_i (melting or freezing) contributes to the vertical divergence of $\overline{w's'}$, inducing a local heating or cooling.
In all these relations, the different local coefficients act on the total flux and *not* on the local increments. The situation is not the same as for the so-called "physical fluxes" which cumulate the local tendencies and are used as an interfacing tool in the Aladin model. For instance when we accumulate the local increments of condensate into a condensation flux the associated heat exchange is proportional to the local increment while the pre-existing part of the flux is simply transported further.
On the contrary, the diffusion flux is the expression of the local gradients. The equations of the fluxes describe the cause of the motion, not its effect. For instance

- a vertical gradient of the ice fraction between two layers will induce a diffusive motion, affecting the local tendency.
- A vertical gradient of temperature also implies a gradient of $L(T)$ affecting the dry static energy, because moving a parcel would require to heat or cool the condensates in the parcel.

Hence the latent heat in the conservative variables is associated to the flux and applies to the totality of the flux, which may absorb or release some latent heat locally. The variations of the latent heats correspond to bringing the condensates to the local temperature.
The variations of the phase partition are a diagnostic, not the expression of a phase change in a motion: the fluxes being proportional to gradients, those gradients include the one of α_i.
In conclusion, using equations 11 and 12 we have a coherent treatment of the turbulent fluxes, with no need to represent directly the condensation and evaporation processes occurring during the diffusion. The turbulent flux of dry static energy in Eq. 12 is equal to the flux of liquid-ice static energy as soon as the condensate fluxes are zero.
The central hypotheses of the presented formulation are

- the linearization of the Clausius-Clapeyron equation separately for saturation with respect to ice and to liquid water;
- Take all the time the latent heats and the ice fraction at the mean grid box temperature i.e. also in the expression of the perturbations of the condensates and static heat.

The use of conservative variables seems appropriate for the vertical turbulent diffusion process. For horizontal advection, it remains simpler to transport directly the condensate variables and make an *adiabatic* readjustment towards $\alpha_i(T)$, immediately after advection. In this case as well as for deep convection, we cannot ignore the effects of radiation, mixing or microphysical processes so that we no longer may assume the conservation of total water or liquid-ice static energy.

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