Part II
Initialisations and auxiliary tools

1 Energetics and conservation aspects

1.1 Basic hypotheses

- The atmosphere is composed of a mixture of two perfect gases, dry air and water vapour.
- The system is in local thermodynamic equilibrium (so we may use the state equation).
- Condensed phases of water may appear in the atmosphere:
  - their volume is zero;
  - they leave the system immediately (in one time step);
  - while falling, they exchange mass, momentum and energy with the layers they cross. The precipitation temperature is the same as the layer they cross, as well as their horizontal velocities. Their potential energy is converted into kinetic energy, dissipated into heat;
  - when leaving the system, they bring away mass, momentum, and energy from the atmosphere.

The fact that the condensed phases are evacuated in one time step means that the environmental mixing ratio of condensed waters is kept to zero; but it does not prevent that there may be some condensed water present locally, as the condensed water diagnosed inside the updraught (subscript $_u$), through the equation:

$$\frac{\partial(q_u + \ell_u)}{\partial \phi} = -\frac{\ell_u}{\mathsf{ECMNP}} \tag{1}$$

where ECMNP is the critical minimum thickness of precipitating clouds, and ℓ represents the condensed water specific contents.
The volume of the condensate is neglected everywhere, so we write

$$\ell \quad = \quad \frac{\rho_i + \rho_l}{\rho}$$

where ρ_i and ρ_l are the mass of ice and liquid water per unit volume, and the specific humidity is defined as

$$\rho_v = q\rho \qquad \text{or} \qquad q \equiv \frac{\rho_v}{\rho_a + \rho_v} \tag{2}$$

The precipitation flux ($kg\ m^{-2}s^{-1}$) crossing a layer of thickness $\triangle p$ in time $\triangle t$ can be seen as follows:

$$\left.\begin{array}{l} \mathcal{P} = \frac{m_{\text{prec}}}{S\triangle t} = \rho_{\text{prec}} \cdot w \\ w = \frac{\triangle p}{\rho g \triangle t} \end{array}\right\} \Longrightarrow \mathcal{P} = \frac{\rho_{\text{prec}}}{\rho}\frac{\triangle p}{g\triangle t} \tag{3}$$

This represents condensed water present in the layer crossed by a precipitation flux, but this water is evacuated in one time step. It does not take part to the definition of local q. It is supposed constant over the duration of the time step, even if there is precipitation evaporation into the layer, because the precipitation flux is fed continuously.

1.2 Variable mass option

Parameter NDPSFI $\equiv \delta_m$ controls mass conservation:

- $\delta_m = 0$: Total mass is conserved, water rained out is replaced by *dry* air, while the vapour produced by evaporating precipitation is compensated by a removal of dry air.
- $\delta_m = 1$: Total mass is not conserved, mass changes are controlled by the precipitation-evaporation budget at the surface. Condensation produces a local mass deficit, while precipitation evaporation produces a local mass increase.

1.3 Thermo-dynamical properties

The model considers the variation of the specific heat c_p and gas constant R with the specific moisture; and also the variation of the vaporisation and sublimation latent heats with temperature.
We have:

$$\begin{aligned} c_p &= c_{pa} + (c_{pv} - c_{pa})q + (c_{w|i} - c_{pa})\ell_{w|i} \\ &= c_{pa}(1 - q - \ell_{w|i}) + c_{pv}\ q + c_{w|i}\ \ell_{w|i} \end{aligned} \tag{4}$$

If we compare two states such that water substance is conserved:

$$q + \ell_{w|i} = q_0 + \ell_{w|i0} \tag{5}$$

we have:

$$\begin{aligned} c_p &= c_{p0} + c_{pv}(q - q_0) + c_{w|i}(\ell_{w|i} - \ell_{w|i0}) \\ &= c_{p0} + c_{pv}(q - q_0) + c_{w|i}(q_0 - q) \\ &= c_{p0} + (c_{pv} - c_{w|i})(q - q_0) \end{aligned} \tag{6}$$

This expression will be used in the updraught, where we consider intra-cloud moisture and condensed water. Since the model doesn't contain large scale condensed water, equation (6) is of less interest at large scale.

For the latent heat, we consider the following:

$$\begin{tikzcd} \mathrm{liq}(T) \arrow[r, "L(T)"] \arrow[d, "-c_w(T - T_0)"] & \mathrm{vap}(T) \\ \mathrm{liq}(T_0) \arrow[r, "L_0"] & \mathrm{vap}(T_0) \arrow[u, "c_{pv}(T - T_0)"'] \end{tikzcd}$$

And the dependency writes

$$\mathsf{FOLH}(\mathsf{T}, \delta) \equiv L(T) = L_0 + (c_{pv} - c_{w|i})(T - T_0) \tag{7}$$

with $\delta = 0$ for liquid water, $\delta = 1$ for ice. For T_0 we can take the triple point temperature T_t

This temperature dependence of the latent heat has little impact on short/medium range NWP integrations, but it provides the framework to have an exact description of all energy cycles in the atmosphere — including the Clausius-Clapeyron cycle (§2.1)— and it allows to construct a simpler Newton algorithm computing the saturation specific humidity function $q_{\mathrm{sat}}(T, p)$ for wet bulb (§3) and moist adiabat (see chapter on deep convection) calculations.

1.3.1 Local effective latent heat

State changes must take into account the hypotheses made around the condensed phases.

First let's consider *local intra-cloud* phase changes, i.e. the condensation of some cloud water vapour or evaporation of locally present liquid water. The heat produced is computed using the local effective latent heat, defined by:

$$\int_{p_t}^{p_b} \left[L_{\mathrm{eff}} \left(-g \frac{\partial \mathcal{P}}{\partial p} \right) + c_p \left(\frac{\partial T}{\partial t} \right)_{\mathcal{P}} \right] dp = 0 \tag{8}$$

where the boundaries p_t and p_b are the pressures at the top and the bottom of the modelled atmospheric system.
Condensation $-\triangle m_v$ at a model level l implies the following:

- Latent heat for state change at T: $L_{v-w|i}(T)\triangle m_v$
- Move the condensed water to the surface: $\triangle m_v c_{w|i}(T - T\mathrm{surf})$;

- If $\delta_m = 0$, move the same mass of dry air from the surface to level l: $\triangle m_v c_{pa}(T - T\text{surf})$;
- If $\delta_m = 1$, we must convert into heat the potential energy of the mass we removed: $\triangle m_v(\phi - \phi_{\text{surf}})$

The resulting local effective latent heat is then

$$L_{\text{eff}} = L(T) + \left\{(c_{w|i} - c_{pa}) + \delta_m c_{pa}\right\}(T - T_{\text{surf}}) + \delta_m(\phi - \phi_{\text{surf}}) \tag{9}$$

or using (7),

$$L_{\text{eff}} = L(T_{\text{surf}}) + \{(c_{pv} - c_{pa}) + \delta_m c_{pa}\}(T - T_{\text{surf}}) + \delta_m(\phi - \phi_{\text{surf}}) \tag{10}$$

Actual code writes

$$L_{\text{eff}} = L(T^l) + \left\{(c_w - c_{pa}) + (c_i - c_w)\mathsf{ZSNP}^l + \delta_m c_{pa}\right\}(T^l - T_{\text{surf}}) + \delta_m(\phi^l - \phi_{\text{surf}}) \tag{11}$$

where ZSNP is the solid fraction of the precipitation.

1.3.2 Precipitation flux latent heat

We want to express here the *total* amount of dry static energy born by the precipitation flux, i.e. the flux of dry static energy corresponding to the precipitation flux:

$$F_{s\mathcal{P}} \equiv -L_{\text{flux}}\mathcal{P} \tag{12}$$

We do not consider suspended condensed phases (LCONDWT=.FALSE.). Local specific moisture is linked to precipitation flux $\mathcal{P}(kg\ m^{-2}s^{-1})$ through (cfr. equation (6))

$$\left(\frac{\partial q}{\partial t}\right)_{\mathcal{P}} = -g(1 - \delta_m q)\frac{\partial \mathcal{P}}{\partial p} \tag{13}$$

Intuitively we can feel this as follows.

$$q = \frac{m_v}{m_v + m_a} \qquad g\frac{\triangle t}{\triangle p}\mathcal{P} = \frac{m_p}{m_v + m_a}$$

and we consider a variation μ (evaporation) of the condensed phase.

$$\triangle m_v = \mu = -\triangle m_p$$

With $\delta_m = 0$ this yields:

$$\triangle q = \frac{\mu}{m_v + m_a} = -g\frac{\triangle t}{\triangle p}\triangle\mathcal{P}$$

while with $\delta_m = 1$ we get:

$$\begin{aligned}\triangle q &= \frac{m_v + \mu}{m_v + m_a + \mu} - \frac{m_v}{m_v + m_a}\\ &= \frac{\mu}{m_v + m_a + \mu}(1 - q) = -g\frac{\triangle t}{\triangle p}\triangle\mathcal{P}(1 - q)\end{aligned}$$

The local tendency of dry static energy, due to $\mathcal{P}$:

$$\left(\frac{\partial s}{\partial t}\right)_{\mathcal{P}} = -g\frac{\partial F_{s\mathcal{P}}}{\partial p} - g\mathcal{P}\,[\text{pseudo} - \text{advection}] \tag{14}$$

includes

- the variation brought by the variation of $\mathcal{P}$ (evaporation/re-condensation), which is the s-flux we want to express,
- the part advected by $\mathcal{P}$ (pseudo-advection resulting of the void created by the precipitation).

If the mass is conserved, the pseudo-advection corresponds to the heat exchange between the precipitate and water vapour in its direct neighbourhood; otherwise, we have to take into account the heat flux associated to the mass leaving the system, the heat exchanged between moist air and the precipitation flux, as the corresponding mass is not replaced by dry air.

Now, definition of s implies

$$\left(\frac{\partial s}{\partial t}\right)_{\mathcal{P}} = c_p \left(\frac{\partial T}{\partial t}\right)_{\mathcal{P}} + T\left(\frac{\partial c_p}{\partial t}\right)_{\mathcal{P}} + \underbrace{\left(\frac{\partial \phi}{\partial t}\right)_{\mathcal{P}}}_{=0} \tag{15}$$

The local tendency of ϕ due to the precipitation flux is actually zero.
We may express the temperature tendency as:

$$c_p \left(\frac{\partial T}{\partial t}\right)_{\mathcal{P}} = gL(T)\frac{\partial \mathcal{P}}{\partial p} - g\delta_m \mathcal{P}\frac{\partial \phi}{\partial p} - g\mathcal{P}\frac{\partial T}{\partial p}(c_{w|i} - c_{pa} + \delta_m c_{pa}) \tag{16}$$

where

- the first term of the RHS represents the evaporation,
- the second term is the conversion of potential energy into heat when $\delta_m = 1$,
- the third term is a pseudo-advection term by the precipitation flux:
  - the liquid or solid precipitation exchanges heat with the layer to keep all the time the temperature of the environment;
  - if mass is conserved, an equivalent flux of dry air has to be moved upwards and get the layer temperature.

Note that from (8) we should verify:

$$\int_{p_t}^{p_b} c_p \left(\frac{\partial T}{\partial t}\right)_{\mathcal{P}} dp \quad = \quad \int_{p_t}^{p_b} gL_{\text{eff}}\frac{\partial \mathcal{P}}{\partial p}dp$$

or

$$\begin{aligned}
&\int_{p_t}^{p_{\text{surf}}} gL(T)\frac{\partial \mathcal{P}}{\partial p} - g\delta_m \mathcal{P}\frac{\partial \phi}{\partial p} - g\mathcal{P}\frac{\partial T}{\partial p}(c_{w|i} - c_{pa} + \delta_m c_{pa})dp \\
&\stackrel{?}{=} \int_{p_t}^{p_{\text{surf}}} \left[gL(T) + g\left\{(c_{w|i} - c_{pa}) + \delta_m c_{pa}\right\}(T - T_{\text{surf}}) + g\delta_m(\phi - \phi_{\text{surf}})\right]\frac{\partial \mathcal{P}}{\partial p}dp \\
&= \int_{p_t}^{p_{\text{surf}}} gL(T)\frac{\partial \mathcal{P}}{\partial p}dp + g\left\{(c_{w|i} - c_{pa}) + \delta_m c_{pa}\right\}\left\{\underbrace{\left[(T - T_{\text{surf}})\mathcal{P}\right]_{p_t}^{p_{\text{surf}}}}_{=0} - \int_{p_t}^{p_{\text{surf}}} \mathcal{P}\frac{\partial T}{\partial p}dp\right\} \\
&\quad + g\delta_m\left\{\underbrace{\left[(\phi - \phi_{\text{surf}})\mathcal{P}\right]_{p_t}^{p_{\text{surf}}}}_{=0} - \int_{p_t}^{p_{\text{surf}}} \mathcal{P}\frac{\partial \phi}{\partial p}dp\right\} \\
&= \text{QED.}
\end{aligned}$$

As we have

$$\frac{\partial c_p}{\partial t} = (c_{pv} - c_{pa})\frac{\partial q}{\partial t} \quad \Longrightarrow \quad \left(\frac{\partial c_p}{\partial t}\right)_{\mathcal{P}} = -g(c_{pv} - c_{pa})(1 - \delta_m q)\frac{\partial \mathcal{P}}{\partial p}$$

(15) becomes

$$\begin{aligned}
\left(\frac{\partial s}{\partial t}\right)_{\mathcal{P}} &= gL(T)\frac{\partial \mathcal{P}}{\partial p} - g\delta_m \mathcal{P}\frac{\partial \phi}{\partial p} - g\mathcal{P}\frac{\partial T}{\partial p}(c_{w|i} - c_{pa} + \delta_m c_{pa}) - g(c_{pv} - c_{pa})(1 - \delta_m q)T\frac{\partial \mathcal{P}}{\partial p} \\
&= gL(T)\frac{\partial \mathcal{P}}{\partial p} + g\mathcal{P}(\underline{c_{pv} - c_{w|i}})\frac{\partial T}{\partial p} - g\mathcal{P}\frac{\partial T}{\partial p}(\underline{c_{pv} - c_{w|i}} + c_{w_i} - c_{pa} + \delta_m c_{pa}) \\
&\quad - gT\frac{\partial \mathcal{P}}{\partial p}(c_{pv} - c_{pa})(1 - \delta_m q) - g\delta_m \mathcal{P}\frac{\partial \phi}{\partial p} \\
&= g\frac{\partial L(T)\mathcal{P}}{\partial p} - g(c_{pv} - c_{pa})(1 - \delta_m q)\frac{\partial \mathcal{P}T}{\partial p} \\
&\quad - g\delta_m \mathcal{P}\left\{\frac{\partial T}{\partial p}\left[c_{pa}(1 - q) + c_{pv}q\right] + \frac{\partial \phi}{\partial p}\right\} - g\mathcal{P}\frac{\partial T}{\partial p}(c_{pv} - c_{w|i})
\end{aligned}$$

Using $\left(\frac{\partial s}{\partial p}\right) = c_p \frac{\partial T}{\partial p} + T\frac{\partial c_p}{\partial p} + \frac{\partial \phi}{\partial p}$ and neglecting $\frac{\partial c_p}{\partial p} = (c_{pv} - c_{pa})\frac{\partial q}{\partial p}$ yields

$$\left(\frac{\partial s}{\partial t}\right)_{\mathcal{P}} = g\frac{\partial}{\partial p}\left[\mathcal{P}\left\{L(T) - (c_{pv} - c_{pa})T(1 - \delta_m q)\right\}\right] - g\mathcal{P}\left\{\frac{\partial T}{\partial p}(c_{pv} - c_{w|i}) + \delta_m \frac{\partial s}{\partial p}\right\} \tag{17}$$

Hence,

$$F_{s\mathcal{P}} = -\mathcal{P}\left\{L(T) - (c_{pv} - c_{pa})T(1 - \delta_m q)\right\} \tag{18}$$

yielding the flux latent heat:

$$L_{\text{flux}} = L(T) - (c_{pv} - c_{pa})T(1 - \delta_m q) \tag{19}$$

This value is computed by routine ACCLFP:

$$-L_{\text{flux}} \equiv \mathsf{PLH}\begin{matrix}\mathsf{L}\\ \mathsf{N}\end{matrix} = -\mathsf{FOLH}(T^{\bar{l}}, \begin{matrix}0\\ 1\end{matrix}) + (c_{pv} - c_{pa})T^{\bar{l}}(1 - \delta_m q^{\bar{l}})$$

1.3.3 Budget latent heat

L_{bud} represents the static energy brought to the *whole* vertical column by a *local* unit variation of q due to precipitation/evaporation effects or any external moisture input.
Physically, since the model doesn't have condensed water storage (LCONDWT=.FALSE.), every water drop appearing at a model level has either to be evaporated or to be moved to the ground.
When making a global energy budget, it cannot make a difference that such a drop condensed near the tropopause or in the PBL: it could occur that the water has done several courses around the cloud with phase changes in both directions, if we consider the downdraughts.
The energy lost by the atmosphere is equal to the dry static energy brought by the precipitation flux when it reaches the surface, i.e.

$$L_{\text{flux}}(\text{surf}) \cdot \mathcal{P}_s$$

If we assess the energy brought by the large scale moisture convergence for instance, the large scale brings water vapour at a given level into the vertical column. If this vapour condensates, somewhere into the column, the corresponding net precipitation reaching the surface is the only part of it that has released its latent heat into sensible heat in the energy budget of this column. Can we then conclude that the budget latent heat is equal to the surface precipitation flux latent heat ? Actually the part of the fed moisture that doesn't finish into precipitation, it is still available as latent heat, and the budget is the same...

$$L_{\text{bud}} = L(T_s) - (c_{pv} - c_{pa})(1 - \delta_m q_s)T_s = L_{\text{flux}}(\text{surf}) \tag{20}$$

L_{bud} will multiply a moisture flux (at any particular level) resulting either from advection or a local variation of the precipitation flux.

Remember that the values T_s and q_s intervening inside the latent heat expression correspond to the environment at the place where we decide to compute the state change, and it does not contradict the fact that the same latent heat has to be multiplied by a moisture flux occurring at a given level to obtain the corresponding heat (sensible and latent) brought by the large scale to the column.

The budget latent heat is relevant whenever we compute budgets between the whole vertical column and the environment, while the local effective latent heat must be used when we consider intra-cloud water phase changes. Actually, the budget latent heat may be quite different from the local value of the latent heat corresponding to the wet bulb characteristics (T_w, q_w), which are used implicitly when computing the saturated pseudo-adiabat: if we decided to use the budget latent heat to multiply the large scale moisture convergence in the convective cloud calculation, we would be at risk to change the cloud limits: for this reason, in this particular computation L_{eff} is used.
On the contrary, in the final budgets of the convection routine, the convective dry static energy flux for output is computed with the budget latent heat.

2 Thermodynamical functions

Include module FCTTRM contains 2 separate sets of thermo-dynamical function, as described below.

2.1 Absolute thermodynamical functions

Latent heats are derived from the triple point values: $T_t \equiv \mathsf{RTT}$, $L_{v-w}(T_t) \equiv \mathsf{LVTT}$, $L_{v_i}(T_t) \equiv \mathsf{LSTT}$. Vaporisation, sublimation and melting latent heats are then:

$$\begin{aligned}\mathsf{RLV} \equiv L_{v-w}(T) &= L_{v-w}(T_t) + (c_{pv} - c_w)(T - T_t)\\ \mathsf{RLS} \equiv L_{v-i}(T) &= L_{v-i}(T_t) + (c_{pv} - c_i)(T - T_t)\\ \mathsf{RLF} \equiv L_{w-i}(T) &= L_{v-w}(T) - L_{v-i}(T)\end{aligned}$$

The saturating vapour tension is given by Clausius-Clapeyron equation:

$$\frac{de_{\text{sat}}}{e_{\text{sat}}} = \frac{LdT}{R_v T^2} \tag{21}$$

Writing

$$\frac{L}{R_v} = \beta - \gamma T$$

we get readily:

$$\ln(e_{\text{sat}}(T)) = \alpha - \frac{\beta}{T} - \gamma \ln(T)$$

with α corresponding to $e_{\text{sat}}(T_t)$, and α, β, γ being different for liquid and ice phases.

The saturating vapour tensions with respect to liquid water and ice, are computed as:

$$\begin{array}{ll}\mathsf{ESW}(T) = \exp\left[\alpha_w - \frac{\beta_w}{T} - \gamma_w \ln T\right] & \mathsf{ESS}(T) = \exp\left[\alpha_i - \frac{\beta_i}{T} - \gamma_i \ln T\right]\\ \gamma_w = (c_w - c_{pv})/R_v & \gamma_i = (c_i - c_{pv})/R_v\\ \beta_w = L_{v-w}(T_t)/R_v + \gamma_w T_t & \beta_i = L_{v-w}(T_t)/R_v + \gamma_i T_t\\ \alpha_w = \ln(e_{\text{sat}}(T)) + \beta_w/T + \gamma_i T_t & \alpha_i = \ln(e_{\text{sat}}(T)) + \beta_i/T + \gamma_i T_t\end{array}$$

Checking temperature positivity through index

$$\delta_T \equiv \begin{cases} 0 & \text{if } T \geq T_t \\ 1 & \text{if } T < T_t \end{cases}$$

we can express the saturating vapour tension $\mathsf{ES(T)}$.

2.2 Model physics functions

Using a phase indicator

$$\delta \equiv \begin{cases} 0 & \text{referencing to water} \\ 1 & \text{referencing to ice} \end{cases}$$

we get the saturating vapour function

$$\begin{aligned}\mathsf{FOEW}(T,\delta) &\equiv e_{\text{sat}}(T,\delta) = \exp\left[\alpha_w + (\alpha_i - \alpha_w)\delta - \frac{\beta_w + (\beta_i - \beta_w)\delta}{T} - (\gamma_w + (\gamma_i - \gamma_w)\delta)\ln T\right]\\ \mathsf{FODLEW}(T,\delta) &\equiv \frac{\partial \ln e_{\text{sat}}}{\partial T} = \frac{\beta_w + (\beta_i - \beta_w)\delta - (\gamma_w + (\gamma_i - \gamma_w)\delta)T}{T^2}\end{aligned}$$

The saturating specific humidity is then

$$\begin{aligned}\mathsf{FOQS}(\frac{e_{\text{sat}}}{p}) &= \frac{e_{\text{sat}}/p}{1 + (R_v/R_a - 1)\max(0, 1 - e_{\text{sat}}/p)}\\ \mathsf{FODQS}(q_{\text{sat}}, \frac{e_{\text{sat}}}{p}, \frac{\partial \ln e_{\text{sat}}}{\partial T}) &\equiv \frac{\partial q_{\text{sat}}}{\partial T} = \frac{q_{\text{sat}} - q_{\text{sat}}^2}{1 - e_{\text{sat}}/p}\frac{\partial \ln e_{\text{sat}}}{\partial T}\end{aligned}$$

so that

$$q_{\text{sat}} = \begin{cases} \frac{e_{\text{sat}}/R_v}{(p - e_{\text{sat}})/R_a + e_{\text{sat}}/R_v} & \text{if } e_{\text{sat}}(T) \leq p \\ \frac{e_{\text{sat}}}{p} & \text{if } e_{\text{sat}}(T) \geq p \end{cases}$$

And finally the latent heat function

$$\mathsf{FOLH}(T,\delta) \equiv L(T,\delta) = L_{v-w}(T_t) + [L_{v-i}(T_t) - L_{v-w}(T-t)]\,\delta + [c_{pv} - c_w + (c_w - c_i)\delta]\,(T - T_t)$$

3 Wet bulb computation

Module ACTQSAT computes the wet bulb temperature and specific humidity.

$$dh = 0 \quad , \quad dp = 0 \quad \Longrightarrow \quad c_p dT + L dq = 0$$

with $c_p(q)$ and $L(T)$ given by (6) and (7):

$$\begin{array}{rclcrcl} c_p & = & c_{p0} + (c_{pv} - c_w)(q - q_0) & \Longrightarrow & dc_p & = & (c_{pv} - c_w)dq \\ L(T) & = & L_0 + (c_{pv} - c_w)(T - T_0) & \Longrightarrow & dL & = & (c_{pv} - c_w)dT \end{array}$$

$$\Longrightarrow c_p \frac{dL}{c_{pv} - c_w} + L \frac{dc_p}{c_{pv} - c_w} = 0 \Longrightarrow L c_p = L_0 c_{p0} = cste$$

hence

$$\left\{ \begin{array}{l} c_{p0}(T_f - T_0) + L_f(q_f - q_0) = 0 \\ c_{pf}(T_f - T_0) + L_0(q_f - q_0) = 0 \end{array} \right. \tag{22}$$

The wet bulb final state is saturated: $q_f = q_{\rm sat}(T_f)$, but as $q_{\rm sat}(T)$ is not linear, we use a Newton algorithm linearizing around the previous iteration k:

$$q_{k+1} = q_{\rm sat}(T_k) + \frac{\partial q_{\rm sat}(T_k)}{\partial T_k}(T_{k+1} - T_k) \tag{23}$$

with (22)

$$\begin{array}{l} c_{p0}\left[(T_{k+1} - T_k) + (T_k - T_0)\right] \\ \quad + \left[L_0 + (c_{pv} - c_w)\left((T_{k+1} - T_k) + (T_k - T_0)\right)\right] \left[(q_{\rm sat}(T_k) - q_0) + \dfrac{\partial q_{\rm sat}(T_k)}{\partial T_k}(T_{k+1} - T_k)\right] = 0 \end{array}$$

Dropping second order terms in $(T_{k+1} - T_k)$:

$$\begin{array}{l} \left[c_{p0}(T_k - T_0) + L_k(q_{\rm sat}(T_k) - q_0)\right] \\ \quad + (T_{k+1} - T_k)\left[c_{p0} + (c_{pv} - c_w)(q_{\rm sat}(T_k) - q_0) + L_k \dfrac{\partial q_{\rm sat}(T_k)}{\partial T_k}\right] = 0 \end{array} \tag{24}$$

Defining q_k and q_{k+1} with

$$c_{p0}(T_k - T_0) + L_k(q_k - q_0) = 0\,, \qquad c_{pk}(T_{k+1} - T_k) + L_{k+1}(q_{k+1} - q_k) = 0 \tag{25}$$

yields

$$\begin{array}{rcl} L_k(q_{\rm sat}(T_k) - q_k) + (T_{k+1} - T_k)\left\{c_{pk} + (c_{pv} - c_w)(q_{\rm sat}(T_k) - q_k) + L_k \dfrac{\partial q_{\rm sat}(T_k)}{\partial T_k}\right] & = & 0 \\ L_{k+1}(q_{\rm sat}(T_k) - q_k) + (T_{k+1} - T_k)\left[c_{pk} + L_k \dfrac{\partial q_{\rm sat}(T_k)}{\partial T_k}\right] & = & 0 \end{array}$$

$$(q_{\rm sat}(T_k) - q_k) = (q_{k+1} - q_k)\left[1 + \frac{L_k}{c_{pk}} \frac{\partial q_{\rm sat}}{\partial T_k}\right] \tag{26}$$

Starting from (T_0, q_0) the algorithm follows:

$$\begin{array}{rcl} (q_{k+1} - q_k) & = & \dfrac{q_{\rm sat}(T_k) - q_k}{1 + \frac{L_k}{c_{pk}} \frac{\partial q_{\rm sat}}{\partial T_k}} \\ c_{pk+1} & = & c_{pk} + (c_{pv} - c_w)(q_{k+1} - q_k) \\ T_{k+1} - T_k & = & -\dfrac{L_k}{c_{pk+1}}(q_{k+1} - q_k) \\ L_{k+1} & = & L_k + (c_{pv} - c_w)(T_{k+1} - T_k) \end{array}$$

converging to (T_w, q_w) after NBITER iterations.
Use of c_{pk+1} in the third statement is the only difference with the "intuitive" algorithm, but it is essential to ensure the scheme coherence.
Routine ACTQSAT receives as input the 3D fields of T, q, c_p and p, and returns the 3D fields of T_w, q_w, L, L/c_p, q_{sat}, RH, using:

$$
\begin{aligned}
L/c_p &= L(T_0)/c_p(q_0) \\
q &\equiv \frac{\rho_v}{\rho}, \qquad q_{\text{sat}} \equiv \frac{\rho_{v\text{sat}}}{\rho_{\text{sat}}} \qquad \Longrightarrow RH \equiv \frac{\rho_v}{\rho_{v\text{sat}}} = \frac{q\rho}{q_{\text{sat}}\rho_{\text{sat}}} = \frac{qR_{\text{sat}}}{q_{\text{sat}}R} = \frac{q(1+(R_v/R_a-1)q_{\text{sat}})}{q_{\text{sat}}(1+(R_v/R_a-1)q)}
\end{aligned}
$$

4 Initialisations

Initialisations are required for

- Chemistry:
  - Ozone: only in the CLIMATE version, is ozone a historic model variable; in other cases (LOZONE = .FALSE.) a climatologic profile is used:

$$ZQO3^{\bar{l}} = \frac{2a}{1+\sqrt{\left(b/p^{\bar{l}}\right)^3}} \;, \; a = 6.012 \cdot 10^{-2} \;, \; b = 3166\text{Pa}$$

  - CO_2: a constant profile is taken (namelist parameter QCO2).
  - Aerosols: an empiric profile is taken, using namelist parameters AERCS1, AERCS3, AERCS5.

$$
\begin{aligned}
\mathsf{ZDAR}^l &= \epsilon^{\bar{l}-1} - \epsilon^{\bar{l}} \\
\epsilon^{\bar{l}} &= \mathsf{AERCS1}\left(\frac{\overline{p}^{\bar{l}}}{\pi_{\text{ref}}}\right) + \mathsf{AERCS3}\left(\frac{\overline{p}^{\bar{l}}}{\pi_{\text{ref}}}\right)^3 + \mathsf{AERCS5}\left(\frac{\overline{p}^{\bar{l}}}{\pi_{\text{ref}}}\right)^5 \\
\left(\frac{\overline{p}^{\bar{l}}}{\pi_{\text{ref}}}\right) &= A(\eta) + B(\eta)
\end{aligned}
$$

  where $\overline{p}$ is the horizontally averaged pressure, as π_{ref} corresponds to average surface pressure.

- Critical moisture for ACNEBN is computed in CPG and APLPAR: see chapter VII.
- Moisture convergence for convection is computed in APLPAR: see chapter VI.
- Meteorological geopotential heights for wind, temperature and moisture PBL diagnostics.
- Flux latent heats are computed in ACCLFP (see §1.3.2).