Part III
Turbulent fluxes and PBL processes

1 Theoretical context

Interaction with earth surface influences strongly the flow up to a certain height above the surface, depending itself of the specific situation.
The no-slip boundary condition imposes that the velocity must vanish at the surface, causing an important vertical shear near the surface. Viscosity itself acts directly only in a thin layer of a few millimeters, while above it it becomes much smaller than the other terms of the momentum equation.
The relay is taken by turbulent eddies, first with very small spatial and temporal scales, but becoming wider with increasing height. Those shear-induced eddies, together with convective eddies caused by surface heating, are very effective at transferring momentum down to the surface and heat away from the surface - much faster than could be done by molecular diffusion alone (Kolmogorov's cascade).
The turbulent layer height can range from $30m$ to more than 3 km in highly convective conditions. Remember that a boundary layer of 1 km contains around 10% of the mass of the atmosphere. Above, in the free atmosphere and not too close to fronts, jet streams, and convective clouds, turbulence can generally be ignored, while the flow rejoins a geostrophic behaviour.

Turbulent eddies in the ***Planetary Boundary Layer*** **(PBL)** tend to have similar scales in the horizontal and the vertical, ranging thus between 10^{-3}m and 10^3m: those scales are not resolved in operational models, while these eddies are of critical importance for momentum, energy and moisture budgets at the surface. Momentum transport to the surface also affects dramatically the large scale flow, so the geostrophic approximation is no longer adequate.

Given the importance of buoyancy forces, density fluctuations cannot be ignored. *Boussinesq's approximation* replaces density everywhere by a constant value ρ_0 except in the buoyancy term of the vertical momentum equation.
We define then (within the grid box we are studying):

$$\rho \equiv \rho_0(z) + \widetilde{\rho}(x,y,z,t) \quad , \qquad \theta \equiv \theta_0(z) + \widetilde{\theta}(x,y,z,t) \quad , \qquad p \equiv p(z) + \widetilde{p}(x,y,z,t)$$

i.e. $\widetilde{\rho}$, $\widetilde{\theta}$, $\widetilde{p}$ represent departures from the basic state values ρ_0, θ_0, p_0.
As we have

$$\frac{\theta}{\theta_0} = \frac{T}{T_0}\left(\frac{p_0}{p}\right)^{\frac{R}{c_p}} = \frac{\rho_0}{\rho}\left(\frac{p_0}{p}\right)^{\frac{c_v}{c_p}} \approx \frac{\rho_0}{\rho}$$

and the hydrostatic equation for the basic state:

$$\frac{1}{\rho_0}\frac{\partial p_0}{\partial z} + g = 0$$

we can write the vertical equation

$$\begin{aligned}
\frac{dw}{dt} &= -g - \frac{1}{\rho}\frac{\partial p}{\partial z} + F_{rz} = -g\frac{1}{\rho}\left(\frac{\partial p_0}{\partial z} + \frac{\partial \widetilde{p}}{\partial z}\right) + F_{rz} \\
&= -\frac{1}{\rho}\frac{\partial \widetilde{p}}{\partial z} + g\left(\frac{\rho_0}{\rho} - 1\right) + F_{rz} \simeq -\frac{1}{\rho_0}\frac{\partial \widetilde{p}}{\partial z} + g\left(\frac{\theta}{\theta_0} - 1\right) + F_{rz} \\
\Longrightarrow \frac{dw}{dt} &= -\frac{1}{\rho_0}\frac{\partial \widetilde{p}}{\partial z} + g\frac{\widetilde{\theta}}{\theta_0} + F_{rz} = -\frac{1}{\rho_0}\frac{\partial p}{\partial z} + g\frac{\theta}{\theta_0} + F_{rz}
\end{aligned} \tag{1}$$

and the adiabatic thermodynamic equation

$$\frac{d\theta}{dt} = 0 \iff \frac{d\widetilde{\theta}}{dt} = -w\frac{d\theta_0}{dz} \tag{2}$$

In a turbulent fluid, locally measured field variables fluctuate rapidly in time as eddies of various scales pass the point. *Reynolds averaging* assumes that field variables ψ can be separated into slowly varying mean fields

$\overline{\psi}$ and rapidly varying turbulent components, ψ', so that $\psi = \overline{\psi} + \psi'$.
The mean of fluctuating components must vanish, but not the mean of the product of fluctuating components: for example, we have

$$\overline{w\theta} = \overline{(\overline{w} + w')(\overline{\theta} + \theta')} = \overline{w}\overline{\theta} + \overline{w'\theta'}$$

The average $\overline{w'\psi'}$ of the product of a turbulent velocity component by the turbulent part of a field ψ is named *"turbulent flux of ψ"* along the corresponding direction.

Applying Reynolds averaging in (1) and (2), and defining an "average material derivative":

$$\frac{\overline{D}}{Dt} \equiv \frac{\partial}{\partial t} + \overline{u}\frac{\partial}{\partial x} + \overline{v}\frac{\partial}{\partial y} + \overline{w}\frac{\partial}{\partial z}$$

we get after some calculations

$$\begin{aligned}
\frac{\overline{D}\overline{w}}{Dt} \equiv \frac{\partial \overline{w}}{\partial t} + \overline{\mathbf{V}}\cdot\nabla\overline{w} + \overline{w}\frac{\partial\overline{w}}{\partial z} &= -\frac{1}{\rho_0}\frac{\partial\overline{p}}{\partial z} + g\frac{\overline{\theta}}{\theta_0} - \left[\frac{\partial\overline{u'w'}}{\partial x} + \frac{\partial\overline{v'w'}}{\partial y} + \frac{\partial\overline{w'w'}}{\partial z}\right] + \overline{F}_{rz} \\
\frac{\overline{D}\overline{\overline{\theta}}}{Dt} \equiv \frac{\partial\overline{\overline{\theta}}}{\partial t} + \overline{\mathbf{V}}\cdot\nabla\overline{\overline{\theta}} + \overline{\overline{\theta}}\frac{\partial\overline{\overline{\theta}}}{\partial z} &= -\overline{w}\frac{d\theta_0}{dz} - \left[\frac{\partial\overline{u'\theta'}}{\partial x} + \frac{\partial\overline{v'\theta'}}{\partial y} + \frac{\partial\overline{\theta'w'}}{\partial z}\right]
\end{aligned}$$

As horizontal inhomogeneities (mountains, towns,...) are treated separately and often localised, the study of turbulent PBL supposes generally that turbulent fluxes are horizontally homogeneous, so only the z derivatives of the turbulent stresses are kept. The horizontal equations write:

$$\frac{\overline{D}\overline{u}}{Dt} = -\frac{1}{\rho_0}\frac{\partial\overline{p}}{\partial x} + f\overline{v} - \frac{\partial\overline{u'w'}}{\partial z} \quad , \qquad \frac{\overline{D}\overline{v}}{Dt} = -\frac{1}{\rho_0}\frac{\partial\overline{p}}{\partial y} - f\overline{u} - \frac{\partial\overline{v'w'}}{\partial z}$$

The acceleration of the mean flow is small compared to the Coriolis and pressure gradient terms, and explicit molecular diffusion terms can also be neglected. Using the geostrophic velocity, we get the final set of equations:

$$\begin{aligned}
f(\overline{v} - \overline{v}_g) - \frac{\partial\overline{u'w'}}{\partial z} = 0 \quad &, \qquad -f(\overline{u} - \overline{u}_g) - \frac{\partial\overline{v'w'}}{\partial z} = 0 \\
\frac{\overline{D}\overline{w}}{Dt} = -\frac{1}{\rho_0}\frac{\partial\overline{p}}{\partial z} + g\frac{\overline{\theta}}{\theta_0} - \frac{\partial\overline{w'w'}}{\partial z} \quad &, \qquad \frac{\overline{D}\overline{\theta}}{Dt} = -\overline{w}\frac{d\theta_0}{dz} - \frac{\partial\overline{\theta'w'}}{\partial z}
\end{aligned}$$

In the hydrostatic model, we do not need to consider the vertical equation, as the large scale vertical velocity will always be derived from the continuity equation.
In all subsequent developments, $\overline{\theta}$ will represent Reynolds' average of the potential temperature departure $\widetilde{\theta}$.
The point of the parameterization is thus to evaluate vertical turbulent fluxes of momentum $J_{\mathbf{V}} = -\rho\overline{\mathbf{V}'w'}$ and of thermodynamic quantities J_q, J_s behaving like $J_{\widetilde{\theta}} = -\rho\overline{\theta'w'}$. Their expressions will strongly differ following the atmosphere's vertical stability.

1.1 The Flux-Gradient (K-)theory

In neutral or stable (stratified) boundary layers, wind speed and direction vary significantly with height.
One traditionally assumes that the eddies act similarly to molecular diffusion, so the turbulent fluxes are proportional to the local gradient of the mean field:

$$J_\psi = \rho K_\psi \frac{\partial\psi}{\partial z}$$

or

$$\overline{\mathbf{V}'w'} = -K_m\left(\frac{\partial\overline{\mathbf{V}}}{\partial z}\right) \quad , \qquad \overline{\theta'w'} = -K_h\left(\frac{\partial\overline{\theta}}{\partial z}\right) \tag{3}$$

K_m and K_h are *eddy* exchange coefficients (*eddy viscosity, eddy diffusivity*); a big difference with the molecular coefficients is that K_ψ coefficients depend on the flow rather than on the physical properties of the fluid.
We have now to find ways to estimate those coefficients. In reality, K_ψ must vary rapidly near the ground: a classic approach distinguishes

- a *surface constant flux layer*, maintained entirely through vertical momentum transfer by turbulent eddies, and considered as neutral. The depth of this layer depends on stability but is generally less than 10% of the boundary layer.
- above this, a layer where K_m remains constant.

This old frame is no longer needed as we'll see below.

1.2 Neutral surface layer: Prandtl mixing length

Prandtl's mixing length hypothesis assumes that a fluid parcel displaced vertically will carry its original properties over a characteristic distance ξ' (taken > 0 upwards), before mixing with its surroundings. In the analogy with the molecular mechanism, this displacement creates a turbulent fluctuation proportional to the gradient of the mean property:

$$\begin{aligned} \mathbf{V}' &= -\xi' \frac{\partial \overline{\mathbf{V}}}{\partial z} \quad , \qquad \theta' = -\xi' \frac{\partial \overline{\theta}}{\partial z} \\ \Longrightarrow -\overline{\mathbf{V}'w'} &= \overline{w'\xi'} \frac{\partial \overline{\mathbf{V}}}{\partial z} \quad , \qquad -\overline{\theta' w'} = \overline{w'\xi'} \frac{\partial \overline{\theta}}{\partial z} \end{aligned}$$

As the horizontal and vertical scales of the eddies should be comparable:

$$|w'| \sim |\mathbf{V}'| \quad \Longrightarrow \quad w' \simeq \xi' \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right|$$

(the absolute value comes from that w' should always have the same sign as ξ').
We have then

$$\begin{aligned} -\overline{\mathbf{V}'w'} &= \overline{\xi'^2} \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right| \frac{\partial \overline{\mathbf{V}}}{\partial z} = l_m^2 \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right| \frac{\partial \overline{\mathbf{V}}}{\partial z} \quad , \qquad -\overline{\theta' w'} = l_m l_h \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right| \frac{\partial \overline{\theta}}{\partial z} \\ K_m &= l_m^2 \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right| \quad , \qquad K_h = l_h l_m \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right| \end{aligned}$$

The mixing length l measures the average eddy size.
Near the surface, this size is limited by the distance to the surface: this is addressed by choosing an expression in the form

$$l_m = \kappa(z + z_0) \quad , \quad l_h = \kappa(z + z_{0H}) \quad , \quad \text{or} \quad l_m = \frac{\kappa(z + z_0)}{1 + \frac{\kappa(z+z_0)}{\lambda_m}} \quad , \quad l_h = \frac{\kappa(z + z_{0H})}{1 + \frac{\kappa(z+z_{0H})}{\lambda_h}} \tag{4}$$

where

- $\kappa \sim 0.4$ is a universal constant called *von Karman's constant*;
- λ_m, λ_h are asymptotic mixing length values;
- z_0 is the surface roughness length, which could be seen as the distance from the actual surface where the average horizontal velocity vanishes, corresponding in our coordinate system to $z = 0$.
  This length depends on the characteristics of the surface.
- Similarly, z_{0H} is a roughness length for thermal processes, namely the distance from the actual surface where the average departure $\widetilde{\theta}$ vanishes (so $\theta = \theta_0$).
  As we have a single vertical coordinate system, it is better to consider z_{0H} as defining the minimum eddy size at $z = 0$, as $l_h(0) = \kappa z_{0H}$.

For a neutral surface layer close to the surface, the kinematic turbulent momentum flux can be expressed in terms of a *friction* or *scaling velocity* u_*:

$$u_*^2 \equiv \left|\overline{u'w'}\right|_{\text{surf}} \sim 0.1 \; [\text{m}^2\text{s}^{-2}] \Longrightarrow u_* \sim 0.3 \; [\text{ms}^{-1}] \tag{5}$$

If Coriolis and pressure gradient forces are to balance the momentum flux divergence and considering $\delta z \sim 10m$

$$\frac{\delta(u_*^2)}{\delta z} \leq 10^{-3} m s^{-2} \Longrightarrow \delta(u_*^2) \leq 10^{-2} \; [\text{m}^2\text{s}^{-2}]$$

hence a change less than 10% of the momentum flux in the lowest $10m$. Therefore, it is acceptable to assume a constant turbulent flux in the lowest meters of the atmosphere:

$$K_m \frac{\partial \overline{u}}{\partial z} = l_m^2 \left| \frac{\partial \overline{\mathbf{V}}}{\partial z} \right| \frac{\partial \overline{u}}{\partial z} = u_*^2$$

With $l=\kappa(z+z_0)$ we get a logarithmic wind profile:

$$\frac{\partial \overline{u}}{\partial z}=\frac{u_*}{\kappa(z+z_0)}\Longrightarrow \overline{u}=\frac{u_*}{\kappa}\ln(1+\frac{z}{z_0}) \tag{6}$$

with $\overline{u}=0$ for $z=0$, where the eddy size is equal to κz_0.
So the lower boundary flux in neutral conditions, can be expressed in the form:

$$u_*^2\equiv|\overline{u'w'}|=\left(\frac{\kappa}{\ln(1+z/z_0)}\right)^2|\overline{u}|^2\equiv C_{nM}|\overline{u}|^2 \tag{7}$$

where C_{nM} is a drag coefficient for neutral conditions. For the thermic quantities, we get:

$$\begin{aligned} K_h\frac{\partial\overline{\theta}}{\partial z} &= l_m l_h\left|\frac{\partial \overline{\mathbf{V}}}{\partial z}\right|\frac{\partial\overline{\theta}}{\partial z}=l_h u_*\frac{\partial\overline{\theta}}{\partial z}=u_*\theta_* \\ \Longrightarrow\frac{\partial\overline{\theta}}{\partial z} &= \frac{\theta_*}{l_h}=\frac{\theta_*}{\kappa(z+z_{0H})}\Longrightarrow\overline{\theta}=\frac{\theta_*}{\kappa}\ln(1+\frac{z}{z_{0H}}) \qquad (8)\\ u_*\theta_* &= \frac{\kappa^2}{\ln(1+\frac{z}{z_0})\ln(1+\frac{z}{z_{0H}})}|\overline{u}||\overline{\theta}|\equiv C_{nH}|\overline{u}||\overline{\theta}| \qquad (9)\end{aligned}$$

1.3 Stable or Unstable surface layer: Monin-Obukhov similarity theory

The cases where the surface layer is stable or unstable, could be derived from the neutral case through Monin-Obukhov's similarity theory.

1.3.1 Surface layer

We modify (6) and (8) by multiplying respectively by empirical functions ϕ_m and ϕ_h:

$$\begin{aligned} \frac{\partial\overline{u}}{\partial z} &= \frac{u_*}{\kappa(z+z_0)}\phi_m(\frac{z}{L}) \quad , \qquad u_*^2=\left|\overline{w'u'}\right| \qquad (10)\\ \frac{\partial\theta}{\partial z} &= \frac{\theta_*}{\kappa(z+z_{0H})}\phi_h(\frac{z}{L}) \quad , \qquad \theta_*u_*=-\overline{w'\theta'} \qquad (11)\\ L &= \frac{\overline{\theta}u_*^2}{\kappa g\theta_*}\propto\frac{\text{Reynolds stress contribution}}{\text{buoyancy contribution}} \qquad (12)\end{aligned}$$

L is the Monin-Obukhov length, coming from a comparison of the relative importance of the two sources of turbulence: writing

$$\begin{aligned} \text{buoyancy} &\propto \frac{g}{\overline{\theta}}\frac{\triangle\overline{\theta}}{\triangle z}=\frac{g}{\overline{\theta}}\frac{\theta_*}{l_h}\sim\frac{g}{\overline{\theta}}\frac{\theta_*}{\kappa(z+z_0)}\\ \text{Reynolds stress shear} &\propto \left(\frac{\triangle u}{\triangle z}\right)^2=\frac{u_*^2}{l_m^2}\sim\frac{u_*^2}{\kappa(z+z_0)}\end{aligned}$$

and both sources (mechanical and thermal) are equal at $(z+z_0)=L$.
With neutral stability, we'll have $L\to\infty$ and $\phi_m(0)=1$, while the heat flux vanishes, through $\theta_*=0$.

Integrating (10), between the roughness length z_0 and height z:

$$\begin{aligned} \int_{u_0=0}^{u}du &= \frac{u_*}{\kappa}\int_{z_0}^{z_0+z}\frac{dz}{z}-(1-\phi_m)\frac{dz/L}{z/L}\\ \Longrightarrow u(z) &= \frac{u_*}{\kappa}(\ln\frac{z_0+z}{z_0}-\psi_m(\frac{z}{L})+\psi_m(\frac{z_0}{L})) \qquad (13)\\ \triangle\theta\equiv\theta(z)-\theta_0 &= \frac{\theta_*}{\kappa}(\ln\frac{z_0+z}{z_0}-\psi_h(\frac{z}{L})+\psi_h(\frac{z_0}{L})) \qquad (14)\\ \psi_m(\frac{z}{L}) &= \int_{t=z_0/L}^{t=(z_0+z)/L}(1-\phi_m(t))d\ln(t) \qquad \psi_h(\frac{z}{L})=\int_{t=z_0/L}^{t=(z_0+z)/L}(1-\phi_h(t))d\ln(t) \qquad (15)\end{aligned}$$

Substituting (13) and (14) in (12):

$$L = \frac{\overline{\theta}\overline{u}^2}{g\triangle\theta} \frac{\ln(1+\frac{z}{z_0}) - \psi_h(\frac{z}{L}) + \psi_h(\frac{z_0}{L})}{\left[\ln(1+\frac{z}{z_0}) - \psi_m(\frac{z}{L}) + \psi_m(\frac{z_0}{L})\right]^2} \tag{16}$$

and we recognize a bulk Richardson number $\mathcal{R}i_B$:

$$\mathcal{R}i \equiv \frac{g}{\theta} \frac{\frac{\partial\theta}{\partial z}}{\left|\frac{\partial \mathbf{V}}{\partial z}\right|^2} \quad \rightarrow \quad \mathcal{R}i_B = \frac{g\triangle\theta}{\overline{\theta}\overline{u}^2} z \tag{17}$$

comparing buoyancy and shear forces, and often used as a stability index. Using the implicit relationship (16) in (13) and (14) allows us to write:

$$u_*^2 = C_{nM}|\overline{u}|^2 F_m(\frac{z}{z_0}, \mathcal{R}i_B) \quad , \qquad u_*\theta_* = C_{nH}|\overline{u}|\triangle\theta F_h(\frac{z}{z_0}, \mathcal{R}i_B)$$

with the drag coefficients in neutral conditions

$$C_{nM} = \left(\frac{\kappa}{\ln(1+z/z_0)}\right)^2 \quad , \qquad C_{nH} = \frac{\kappa^2}{\ln(1+z/z_0)\ln(1+z/z_{0H})}$$

Louis [1979] computed numerically the functions F_m and F_h, starting from ϕ_m and ϕ_h functions proposed by Businger et al. [1971], and fitted analytical curves for different conditions, with the form

$$\begin{aligned} F &= 1 - \frac{b\mathcal{R}i_B}{1+c\sqrt{|\mathcal{R}i_B|}} && \text{for the unstable case} \\ F &= \frac{1}{(1+b'\mathcal{R}i_B)^2} && \text{for the stable case} \end{aligned}$$

Final results are given in §2.1.1, including some enhancements added in subsequent tunings [Louis et al., 1981].

1.3.2 Similarity theory for fluxes above the surface layer

Above the surface layer, the eddy fluxes are computed as diffusive fluxes, following the K-theory. To keep continuity with the surface fluxes, the dependence of K with stability is assumed the same as that of the surface fluxes.

$$K_m = l^2 \left|\frac{\triangle\overline{\mathbf{V}}}{\triangle z}\right| F(\mathcal{R}i) \quad , \qquad \mathcal{R}i = \frac{g\triangle z\triangle\theta}{\overline{\theta}(\triangle\overline{V})^2}$$

where functions F are the same as above and Richardson number is now based on the layer thickness $\triangle z$.

2 Model implementation

In this section we no longer write the bars over Reynolds-averaged values, as all model grid-point variables are of this kind.
The diffusion equation writes

$$\frac{\partial\psi}{\partial t} = \frac{1}{\rho}\frac{\partial}{\partial z}\rho K_\psi \frac{\partial\psi}{\partial z} = -g\frac{\partial J_\psi}{\partial p} \quad , \qquad J_\psi = \frac{\rho g K_\psi}{\Delta\phi}\Delta\psi \equiv -K'_\psi \Delta\psi \tag{18}$$

The parameterization has to provide the exchange coefficients $K_\psi(m^2/s)$ or actually $K'_\psi(kg\ m^{-2}s^{-1})$, and also an expression for the flux at the surface.
We write:

$$\begin{aligned} J_\psi &= 0 && && \text{at } p = p_{top} \\ J_\psi &= \rho K_\psi \tfrac{\partial\psi}{\partial z} && K_\psi = g\, l^2 \left|\tfrac{\partial \mathbf{V}}{\partial\phi}\right| f(\mathcal{R}i) && \text{at the different model levels} \\ J_\psi &\rightarrow \rho C_\psi \left|\mathbf{V}(z)\right| (\psi(z) - \psi_s) && && \text{as } z \rightarrow 0 \end{aligned} \tag{19}$$

where C_ψ is the surface exchange coefficient corresponding to the actual stability conditions (see below).

2.1 ACHMT: Surface turbulence parameterization

The routine focuses on the layer between the surface and the lowest model level.

2.1.1 Surface exchange coefficient

C_ψ being dimensionless, to get a variable with dimension $\delta p/g\Delta t[kg\ m^{-2}s^{-1}]$, we store PCDROV, PCHROV as:

$$C'_\psi = \rho_s\, C_\psi\, |\mathbf{V}_L|$$

where $_L$ is the lowest model level. Coefficient C_ψ depends upon static stability.
Model key LDZ0H activates the use of a different roughness length z_{0H} for thermic phenomena.

Expressions of C_ψ are given by

- Neutral case ($\mathcal{R}i \sim 0$):

$$\begin{aligned} C_{nM} &= \left(\frac{\kappa}{\ln(1+z/z_0)}\right)^2 \equiv \mathsf{PCDN} \\ C_{nH} &= \frac{\kappa^2}{\ln(1+z/z_0)\ln(1+z/z_{0H})} \equiv \mathsf{ZCDNH} \end{aligned}$$

  so the value is the same in the case the roughness length is the same for momentum and thermic processes.

- Stable case ($\mathcal{R}i > 0$):

$$\begin{aligned} \mathsf{PCD} \equiv C_M &= \left(\frac{1}{1+2b\frac{\mathcal{R}i}{\sqrt{1+d\mathcal{R}i}}}\right)\cdot C_{nM} < C_{nM} \\ \mathsf{PCH} \equiv C_H &= \left(\frac{1}{1+3b\mathcal{R}i\sqrt{1+d\mathcal{R}i}}\right)\cdot C_{nH} < C_{nH} \end{aligned}$$

- Unstable case ($\mathcal{R}i < 0$):

$$\begin{aligned} \mathsf{PCD} \equiv C_M &= \left(1-\frac{2b\mathcal{R}i}{1+3bc_mC_{nM}\sqrt{-\mathcal{R}i(1+z/z_0)}}\right)\cdot C_{nM} > C_{nM} \\ \mathsf{PCH} \equiv C_H &= \left(1-\frac{3b\mathcal{R}i}{1+3bc_hC_{nH}\sqrt{-\mathcal{R}i(1+z/z_{0H})}}\right)\cdot C_{nH} > C_{nH} \end{aligned}$$

where

- $\kappa \equiv 0.4$ is the von Karman constant,
- $b \equiv$ EDB determines the exchange coefficient "near neutrality";
- $\begin{cases} c_m \equiv \mathsf{EDC} \equiv c_h & \text{if not } \mathsf{LDZ0H} \\ c_m = c_{m0}(1+z/z_0)^{(x_m-0.5)} & \text{and} \quad c_h = c_{h0}(1+z/z_0)^{(x_h-0.5)} \quad \text{if } \mathsf{LDZ0H} \end{cases}$

  EDC determines the coefficients in asymptotic unstable regime, c_{m0}, c_{h0}, x_m, x_h are given by third degree polynomials with coefficients in array GCZ0H(0:3,4), calibrating the free convection regime;
- $d \equiv$ EDD determines the exchange coefficients in asymptotic stable regime.
- The (bulk) Richardson number $\mathcal{R}i$ compares the buoyancy to the vertical shear. As we have

$$\begin{aligned} \theta = T\left(\frac{p_0}{p}\right)^{\frac{R}{c_p}} \Longrightarrow \frac{1}{\theta}\frac{\partial\theta}{\partial z} &= \frac{1}{T}\frac{\partial T}{\partial z} + \frac{g}{c_pT} \\ \frac{\partial s}{\partial z} &= c_p\frac{\partial T}{\partial z} + g \end{aligned}$$

we may write

$$\mathcal{R}i = \frac{\frac{g}{\theta}\frac{\partial\theta}{\partial z}}{\left|\frac{\partial \mathbf{V}}{\partial z}\right|^2} \sim \frac{\frac{g}{c_pT}\frac{\partial s}{\partial z}}{\left|\frac{\partial \mathbf{V}}{\partial z}\right|^2} = \frac{\triangle\phi_L\frac{\triangle s}{c_pT}}{|\mathbf{V}_L|^2} \equiv \frac{\mathsf{ZSTA}}{|\mathbf{V}_L|^2} \tag{20}$$

In ACHMT we want to estimate a drag coefficient which, multiplied by the de-centered vertical gradient between the surface and the lowest level, must yield a flux at the surface.
Systematically we attach more importance to the position of the resulting flux than to the position of the gradient computation.
Therefore, to compute the mean of RT at the surface, we should bring back the value at the upper level to the lower interface level: as this represents merely a correction, we do it following a dry adiabatic.

We write this way:

$$\frac{\triangle s}{c_pT} = \frac{c_{pL}T_L + \phi_L - c_{ps}T_s - \phi_s}{(c_{pL}T_L + (\phi_L - \phi_s) + c_{ps}T_s)/2} \simeq \frac{R_LT_L - R_sT_s + \triangle\phi_LR_a/c_{pa}}{(R_LT_L + \triangle\phi_LR_a/c_{pa} + R_sT_s)/2}$$

because we have $\phi_s = 0$ and making the approximation

$$\frac{c_{pa}}{c_{pv}} \approx \frac{R_a}{R_v}$$

of the influence of moisture on buoyancy[1].

So the buoyancy is estimated at the mid-level between surface and the lowest model level. When the surface is very cold, some retroaction loop could appear, with a reinforcement of the stability preventing any heating by the atmosphere, leading to a very cold radiative equilibrium (in the polar night). To avoid this, we introduce a limitation on the Richardson number, replacing it by

$$\mathcal{R}i' = \frac{\mathcal{R}i}{(1 + \alpha\mathcal{R}i/\mathcal{R}i_{cr})^{1/\alpha}}$$

in the stable case, where $\alpha = 1$ for momentum and $\alpha = 3$ for moisture and temperature (but setting USURID $= 0$ resets $\alpha \equiv 1$).
$\mathcal{R}i_{cr}$ is applied through parameter USURIC and its lowest level multiplier USURICL:

$$\mathsf{ZSTA} = \frac{\mathsf{ZSTA}}{1 + \max(0, \mathsf{ZSTA})\frac{\mathsf{USURIC}\cdot\mathsf{USURICL}}{|\mathbf{V}_L|^2}}$$

A more complete description is given below, when handling the higher levels.

- Stability is diagnosed with

$$\delta_{\text{stab}} \equiv \mathsf{PSTAB} = \begin{cases} 1 & \text{if } \mathsf{ZSTA} > 0 \\ 0 & \text{otherwise} \end{cases}$$

2.1.2 Brunt-Vaisäla frequency

The moist static or Brunt-Vaisäla frequency is normally

$$N_e^2 \equiv \frac{g}{\theta_e}\frac{\partial\theta_e}{\partial z} \qquad \text{or} \qquad N_w^2 \equiv \frac{g}{\theta_w}\frac{\partial\theta_w}{\partial z} \tag{21}$$

using either the potential equivalent temperature θ_e or the wet bulb potential temperature θ_w. Both potential temperatures represent the temperature got by a dry air parcel transformed adiabatically from the original pressure level towards $1000hPa$; for θ_e, the dry parcel starts from the equivalent temperature of the parcel under study, obtained by following the dry, then moist pseudo-adiabat, until the parcel gets dry; for θ_w, the dry parcel starts with the wet bulb temperature of the parcel under study, obtained by adding water at constant pressure until saturation.

[1]For an adiabatic transform: $c_vdT + pdV = 0 = c_vdT + dRT - RT\frac{dp}{p} \Rightarrow \frac{c_p}{R}\frac{dT}{T} = \frac{dp}{p}$ or $\frac{T_1}{T_2} = \left(\frac{p_1}{p_2}\right)^{R/c_p}$ and we use to follow a dry adiabatic (R_a/c_{pa}) as long as there is no saturation.

Present calculation supposes the surface layer is not saturated, and uses the potential temperature (or dry static energy) instead:
ACHMT outputs the surface value into

$$\mathsf{PNBVNO(KLEV)} \equiv \left(\frac{N_s}{\rho g}\right)^2 = \frac{\mathsf{ZSTA}}{(\rho_s \triangle\phi)^2} = \frac{\mathsf{ZSTA}(R^{\overline{L}} T^{\overline{L}})^2}{(p_s \triangle\phi)^2}$$

which may be negative in the unstable case. We use here the surface density ρ_s, while ZSTA has been computed at a medium level between the surface and the lowest full model level L.
The value of ZSTA used here is taken before its modification limiting the Richardson number, as this limitation has no relevance in other contexts.

2.1.3 Surface moisture computation

We estimate two weighting coefficients, HU for the saturating moisture and HQ for the air moisture contributions to the surface moisture:

$$q_s = \mathsf{HU}\ q_{\text{sat}}(T_s, p_s) + \mathsf{HQ}\ q_L \tag{22}$$

When ISBA is not active (LSOLV=.FALSE.), we write:

$$\begin{aligned} \mathsf{HU} &= (1-P_n)f(\mathcal{W}) + P_n & \qquad \mathsf{HQ} = (1-\mathsf{HU})\cdot \mathsf{veg} \\ f(\mathcal{W}) &= \frac{1-\cos(\pi\mathcal{W})}{2} & \qquad \mathcal{W} \equiv W_s/W_{s\,\max} \end{aligned}$$

where

- $W_s \equiv$ PWS (+ the frozen part $W_{si} =$ PWSI under LSNV) and $W_{s\,\max} \equiv$ WSMX are the surface reservoir and its capacity,
- veg is the vegetation fraction,
- $P_n \equiv$ PNEIJ is the fraction of snow covered ground, computed from the snow mass per unit surface PSNS, the land-sea mask, and the critical value WCRIN.

So as soon as there is snow, $q_s = q_{\text{sat}}$; with no snow and an empty surface reservoir, $q_s = q_L$, while if the reservoir is not empty, $q_s \geq q_L$.
Now in the case of dew: $q_L > q_{\text{sat}}(T_s, p_s)$, we write:

$$\mathsf{HU} = (1-\mathsf{veg})((1-P_n)f(\mathcal{W}) + P_n) + \mathsf{veg} \qquad \mathsf{HQ} = 0$$

so on bare soil, nothing is changed, while on vegetation we have immediately saturation.

The determination of HU and HQ in the ISBA scheme, is explained in the chapter over the soil processes.

2.1.4 PBL parameters at standard meteorological heights

Module ACHMT is called under LDHMT, to compute [Geleyn, 1988] the wind at level PDPHIV $= gz_{\mathbf{V}}$ and T, q, and the relative humidity at level PDPHIT $\equiv gz_T$, both levels situated in principle between the lowest model level and the surface.
As the surface ($z = 0$) wind is zero, we write:

$$u(z) = \alpha_d(z)u_L \quad , \qquad v(z) = \alpha_d(z)v_L$$

while for moisture and dry static energy:

$$\begin{aligned} q(z) &= q_s + \alpha_h(z)(q_L - q_s) \quad , \qquad s(z) = s_s + \alpha_h(z)(s_L - s_s) \\ s(z) &= c_pT(z) + \phi(z) \quad , \qquad c_p(q) = c_{pa} + (c_{pv} - c_{pa})q(z) \\ \Rightarrow T(z) &= \frac{c_p(q_s)T_s + (\phi_s - \phi(z)) + \alpha_h(z)(c_p(q_L)T_L - c_p(q_s)T_s + (\phi_L - \phi_s))}{c_p(q(z))} \end{aligned}$$

Coefficients α_i (i in $[h, d]$) are expressed

$$\alpha_i = \frac{1}{b_i} \ln[1 + \frac{z}{z_L}(e^{b_{ni}} - 1) - f_i(z)] \qquad 0 \le \alpha \le 1$$

$$b_{nd} = \ln(1 + z/z_0) \quad , \quad b_d = \frac{\kappa}{\sqrt{C_M}} \quad , \quad b_{nH} = \ln(1 + z/z_{0H}) \quad , \quad b_H = \frac{\kappa\sqrt{C_M}}{C_H}$$

$$f_i(z) = \begin{cases} \frac{z}{z_L}(b_{ni} - b_i) & \text{stable case} \\ \ln(1 + \frac{z}{z_L}(e^{b_{ni} - b_i} - 1)) & \text{unstable case} \end{cases}$$

Relative humidity is obtained from $q(z)$ with

$$H_r(z) \equiv \frac{e}{e_{\text{sat}}} = \frac{p(z)q(z)\frac{R_a}{R_v}}{e_{\text{sat}}(1 + q(z)(\frac{R_v}{R_a} - 1))}$$

because

$$q \equiv \frac{\rho_v}{\rho_a + \rho_v} = \frac{R_a}{R_v} \frac{e}{(p - e) + e\frac{R_a}{R_v}} = \frac{R_a}{R_v} \frac{1}{\frac{p}{e} + (\frac{R_a}{R_v} - 1)}$$

2.2 ACCOEFK: Atmospheric turbulence parameterization

In the atmosphere, we express the exchange coefficient

$$K_\psi = g\, l_m l_\psi \left| \frac{\partial \mathbf{V}}{\partial \phi} \right| f(\mathcal{R}i)$$

- The mixing length l_ψ is l_h for energy, l_m for momentum, and its vertical profile depends on 3 parameters:
  - $\lambda_m \equiv$ ALMAV: asymptotic mixing length for the wind, $\lambda_h \equiv \lambda_m\sqrt{\frac{3d}{2}}$ for energy, with parameter $d \equiv$ EDD determining C_M and C_H in asymptotic stable regime (see below).
  - $Z \equiv 1/$UHDIFV: scale height for the decrease of l_m,
  - $\beta \equiv$ BEDIFV: shaping coefficient for the vertical diffusion profile.

$$l_\psi(z) = \frac{\kappa(z + z_0)}{1 + \frac{\kappa(z+z_0)}{\lambda}} \left(\beta + \frac{1 - \beta}{1 + \frac{(z+z_0)^2}{Z^2}} \right) \tag{23}$$

  $\kappa \equiv 0.4$ is the von Karman constant, z_0 the surface roughness length.
  The last parenthesized term (23) is local variable ZPFD in the code. So l is increasing from the ground ($l \approx \kappa z_0$), passes a maximum before decreasing in the free atmosphere to the asymptotic value $\beta\lambda$.

- the shaping functions F respectively for wind and thermodynamical variables are taken as
  - Stable case:

$$F_m(\mathcal{R}i) = \frac{1}{1 + 2b\mathcal{R}i/\sqrt{1 + d\mathcal{R}i}}$$
$$F_h(\mathcal{R}i) = \frac{1}{1 + 3b\mathcal{R}i\sqrt{1 + d\mathcal{R}i}}$$

  - Unstable case:

$$F_m(\mathcal{R}i) = 1 - \frac{2b\mathcal{R}i}{1 + 3bc\sqrt{\frac{|\mathcal{R}i|}{27}} \left(\frac{l_m}{z+z_0}\right)^2}$$
$$F_h(\mathcal{R}i) = 1 - \frac{3b\mathcal{R}i}{1 + 3bc\sqrt{\frac{|\mathcal{R}i|}{27}} \left(\frac{l_h}{z+z_0}\right)^2}$$

with $b \equiv \mathsf{EDB}$, $c \equiv \mathsf{EDC}$, $d \equiv \mathsf{EDD}$.

- The Richardson number $\mathcal{R}i$ is computed with the same approximation as in section (2.1.1): we write

$$\begin{aligned}\frac{\triangle s + c_{pa}\mathsf{ZAUX}}{c_pT} &\simeq \frac{R_jT_j - R_{j+1}T_{j+1} + (\phi_j - \phi_{j+1})R_a/c_{pa} + R_a\mathsf{ZAUX}}{(R_jT_j + R_{j+1}T_{j+1})/2} \\ &= \frac{\triangle(RT) + \gamma\triangle\phi + R_a\mathsf{ZAUX}}{(RT)_{\bar{j}}} \\ &\equiv \mathsf{ZSTA}/\triangle\phi\end{aligned}$$

noting $\triangle\psi \equiv \psi_j - \psi_{j+1}$ and $\gamma \equiv R_a/c_{pa}$.

ZAUX is a correction applied under key LCVPP, in case of **shallow convection**:

> *we call* shallow convection *the process in which vertical displacements associated to local turbulent fluxes induce saturation.*

$$\mathsf{ZAUX} = \min(0, \triangle(q - q_{\mathrm{sat}}))\frac{L_{\bar{j}}}{c_{p\bar{j}}}\delta^h \qquad \text{with} \qquad \delta^h = \begin{cases} 1 & \text{if } h_j \le h_{j+1} \\ 0 & \text{otherwise}\end{cases}$$

Actually, ZAUX is divided by namelist parameter GRCVPP allowing to reduce shallow convection; and δ^h is computed with

$$\max\left(0,\ \mathrm{sign}\left\{1, -R_a\frac{L_{\bar{j}}}{c_{p\bar{j}}}\left(\triangle q - \mathsf{GCCSV}\triangle q_{\mathrm{sat}}\frac{p_{\bar{j}}}{p_{\overline{L}}}\right) - (\triangle(RT) + \gamma\triangle\phi)\right\}\right)$$

where parameter GCCSV allows choice of the vertical stability criterion. $\mathsf{GCCSV} \cdot p/p_{surf}$ passes from a test on the moist static energy gradient to a test of the same used in the modified Richardson number for the shallow convection itself. Setting $\mathsf{GCCSV} = 1$ increases the occurrence of shallow convection. L/c_p is actually computed by routine ACTQSAT.

There is no shallow convection effect if the moist static energy is increasing upwards (stable atmosphere); buoyancy is reinforced (more negative) when moving a parcel upwards makes it closer to the saturation, and reduced if it makes it dryer.
We have this way

$$\mathcal{R}i = \frac{g}{c_pT}\frac{\frac{\partial s}{\partial z} + L\min\left(0, \frac{\partial q}{\partial z} - \frac{\partial q_{\mathrm{sat}}}{\partial z}\right)\delta^h}{\left|\frac{\partial \mathbf{V}}{\partial z}\right|^2} = \frac{\mathsf{ZSTA}}{|\triangle\mathbf{V}|^2}$$

- As in ACHMT, we introduce a limitation on the Richardson number:

$$\text{if } \mathcal{R}i > 0 \text{ then} \qquad \mathcal{R}i \qquad \leftarrow \qquad \mathcal{R}i' \equiv \frac{\mathcal{R}i}{(1 + \alpha\mathcal{R}i/\mathcal{R}i_{cr})^{1/\alpha}} \tag{24}$$

The critical value $\mathcal{R}i_{cr}$ is based on parameters USURIC, USURICL, USURICE:

$$1/\mathcal{R}i_{cr}(z) = \mathsf{USURIC}\cdot(1 + (\mathsf{USURICL} - 1)\left(\frac{l_h(z)}{\kappa(z + z_0)}\right)^{\mathsf{USURICE}})$$

with $l_h(z)$ from (23).

In (24), if $\alpha > 0$, in the stable cases very near to the neutrality, the operational $\mathcal{R}i'$ tends to zero as in the case $\mathcal{R}i_{cr} = 0$. Theoretical considerations have shown that the values $\alpha = 1$ for momentum and $\alpha = 3$ for temperature and humidity have the desired asymptotic features: the heat flux tends to an asymptotic value and the operational $\mathcal{R}i'$ is independent of the real Richardson number when $\mathcal{R}i \to \infty$. We distinguish then a coefficient $\alpha' = 1$ for momentum, and

$$\alpha'' = \frac{3\mathcal{R}i + \mathcal{R}i_d}{\mathcal{R}i + \mathcal{R}i_d}$$

for temperature and humidity. But a realistic simulation of storm activity requires big values $\mathcal{R}i_d \sim 100$ while to avoid inversion erosion, small values $\mathcal{R}i_d \sim 10$ are necessary. Experiments have lead to introduce a vertical variation of $\mathcal{R}i_d$, as for $\mathcal{R}i_{cr}$. Its vertical profile is determined by the asymptotic values in the upper atmosphere and an exponent characterizes the vertical variation:

$$\frac{1}{\mathcal{R}i_d} = \mathsf{USURID}\left(1 + \left(\frac{Z}{z + z_0}\right)^2\right)^{\mathsf{USURIDE}}$$

where $Z \equiv 1/\mathsf{UHDIFV}$ as above. Setting $\mathsf{USURID} = 0$ removes its effect, leading to $\alpha \equiv 1$.

- The Brunt-Vaisäla frequency is obtained as

$$\mathsf{PNBVNO} \equiv \left(\frac{N}{\rho g}\right)^2 = \frac{\mathsf{ZSTA}}{(\rho_{\bar{j}}\Delta\phi)^2} = \frac{\mathsf{ZSTA}\cdot(R_{\bar{j}}T_{\bar{j}})^2}{(p_{\bar{j}}\Delta\phi)^2}$$

again using a value of ZSTA not yet modified by USURICs.

The diffusion coefficients are returned as

$$\begin{aligned}\mathsf{PKTROV(JLON,JLEV)} &\equiv K'_H = -\frac{\rho g K_H}{\Delta\phi} && [\mathrm{kg\ m^{-2}s^{-1}}] \text{ for moisture and energy}\\ \mathsf{PKUROV(JLON,JLEV)} &\equiv K'_{\mathbf{V}} = -\frac{\rho g K_{\mathbf{V}}}{\Delta\phi} && [\mathrm{kg\ m^{-2}s^{-1}}] \text{ for horizontal momentum}\end{aligned}$$

2.3 ACDIFUS: Vertical turbulent diffusion

We got the equations:

$$J_\psi = \begin{cases} -K'\Delta\psi & \text{above the lowest level}\\ -C_{M|H}(\psi_L - \psi_s) & \text{at the ground}\end{cases}$$

with ground ($z = 0$) boundary conditions:

$$\begin{aligned}\mathbf{V} = \mathbf{V}_s \equiv 0 \quad &, \qquad p = p_s\\ q_s &= \mathsf{HU}q_{\mathrm{sat}}(T_s, p_s) + \mathsf{HQ}q_L\\ \frac{\partial T_s}{\partial t} &= C_s(\sum F_{\mathrm{energy}}) + \frac{2\pi}{\tau}(T_p - T_s) \qquad (25)\end{aligned}$$

C_s is the inverse of the ground inertia, $\tau = 86400$ is a characteristic period (24h), T_p is the deep soil temperature, T_s is the surface temperature, q_s the surface moisture has been expressed in ACHMT.

ACDIFUS computes the roughness length over the sea, to input to ACHMT at the next time step, as:

$$z_0 = \underbrace{\frac{1}{g}C_K u_*^2}_{\text{Charnock}} + \underbrace{z_{0c}F_m(\mathcal{R}i)}_{\text{gustiness}} \qquad (26)$$

The second term aims to simulate the sensible and latent heat fluxes occurring by very weak wind in convective situations (surface evaporation), which also impacts slightly on the surface friction. $\mathcal{R}i < 0 \Rightarrow F_m(\mathcal{R}i) > 1$, leads to an increased roughness length.
$C_K \equiv \mathsf{VCHRNK}$ and $z_{0c} \equiv \mathsf{VZ0CM}$ are empirical coefficients.
u_* is the friction velocity, derived from the velocity at the lowest model level $\mathbf{V}_L$.

2.3.1 Diffusion from the surface and in the atmosphere

2.3.1.1 Momentum

$$\begin{aligned}\psi_i^+ - \psi_i^- &= -g\frac{\Delta t}{\delta p_i}[F_{\psi_i} - F_{\psi_{i-1}}] = -g\frac{\Delta t}{\delta p_i}[K_i(\psi_i^+ - \psi_{i+1}^+) - K_{i-1}(\psi_{i-1}^+ - \psi_i^+)]\\ &= -w_{i,i}(\psi_i^+ - \psi_{i+1}^+) + w_{i-1,i}(\psi_{i-1}^+ - \psi_i^+)\\ \text{and}\qquad \psi_L^+ - \psi_L^- &= -g\frac{\Delta t}{\delta p_L}[F_{\psi_L} - F_{\psi_{L-1}}] = -g\frac{\Delta t}{\delta p_L}[C_{ML}(\psi_L^+ - \psi_s^+) - K_{L-1}(\psi_{L-1}^+ - \psi_L^+)]\\ &= -x_L(\psi_L^+ - \psi_s^+) + w_{L-1,L}(\psi_{L-1}^+ - \psi_L^+)\end{aligned}$$

where $w_{i,j} \equiv gK_i\triangle t/\delta p_j$ and $x_L = gC_{ML}\frac{\triangle t}{\delta p_L}$.
Matricial form becomes

$$\begin{bmatrix} 1+w_{1,1} & -w_{1,1} & 0 & \cdots & 0 \\ -w_{1,2} & 1+w_{1,2}+w_{2,2} & -w_{2,2} & \ddots & \vdots \\ 0 & \cdots & & & \\ \vdots & \ddots & & & \\ \vdots & & & & -w_{L-1,L-1} \\ 0 & \cdots & 0 & -w_{L-1,L} & 1+w_{L-1,L}+x_L \end{bmatrix} \left\{ \begin{array}{c} \psi_1^+ \\ \psi_2^+ \\ .. \\ \psi_{n-1}^+ \\ \psi_L^+ \end{array} \right\} = \left\{ \begin{array}{c} \psi_1^- \\ \psi_2^- \\ .. \\ \psi_{L-1}^- \\ \psi_L^- + \psi_s x_L \end{array} \right\}$$

and the surface momentum must be zero so $\psi_s x_L = 0$.
Coefficients write:

$$\begin{array}{lll} a_{i,i} = 1 + w_{i-1,i} + w_{i,i} & a_{1,1} = 1 + w_{1,1} & a_{L,L} = 1 + w_{L-1,L} + x_L \\ a_{i,i+1} = -w_{i,i} & a_{i,i-1} = -w_{i-1,i} & \end{array}$$

Gauss elimination proceeds as follows:

$$[A]\left\{\psi^+\right\} = \left\{\psi^-\right\} \iff [M]\,[E]\,[A]\left\{\psi^+\right\} = [M]\,[E]\left\{\psi^-\right\}$$

where $[M]$ is a diagonal normalisation matrix, $[E]$ is a bi-diagonal elimination matrix, such that $[M]\,[E]\,[A]$ is bi-diagonal with a unity diagonal. This yields:

$$\begin{array}{llll} e_{i,i} = a_{i+1,i+1} & e_{i,j+1} = -a_{i,j+1} & m_{i,j} = \dfrac{1}{a_{i+1,i+1}a_{i,i} - a_{i,j+1}a_{i+1,j}} & \forall i < L \\ & m_{L,L}e_{L,L}a_{L,L} = 1 & & \end{array}$$

and we can now solve the sequence of arithmetic equations starting from $i = 1$.

2.3.1.2 Moisture and dry static energy

Evolution of s_L, T_s, q_L are coupled through the latent heat fluxes depending on T_s, which evolution is given by (25). Therefore we will solve both implicit systems simultaneously, adding a linearised equation for T_s. (25) writes:

$$\begin{aligned} \frac{\partial T_s}{\partial t} &= \frac{2\pi}{\tau}(T_p - T_s^+) \\ &+ C_s \left\{ (F_\dagger' - \epsilon\sigma T_s^4) + F_\odot'(1-\alpha) - \rho C_H \left|\mathbf{V}\right| \left[c_{ps}T_s + \phi_s - (c_pT+\phi)_L^+ + L_s(q_s - q_L^+) \right] \right\} \end{aligned}$$

$\epsilon \equiv$ PEMIS is the surface emissivity.
The thermal radiation flux $F_\dagger\prime \to F_\dagger \equiv$ PFRTH is corrected for the surface radiation, and the same correction is then applied at all levels to avoid modifying the tendencies of T linked to it.
Note that the solar flux input to the routine PFRSO $\equiv F_\odot = F_\odot'(1-\alpha)$ is a net flux, i.e. the difference of the up and down components.

We use then

$$\begin{aligned} q_s &= \mathsf{HU}\ q_{\mathrm{sat}}(T_s) + \mathsf{HQ}\ q_L \\ c_{ps} &= c_{pa} + (c_{pv} - c_{pa})q_s \\ c_{ps}^+ &= c_{ps}^- + (c_{pv} - c_{pa})(q_s^+ - q_s^-) = c_{ps}^- + (c_{pv} - c_{pa})\left[\mathsf{HU}(q_{\mathrm{sat}}(T_s^+) - q_{\mathrm{sat}}(T_s^-)) + \mathsf{HQ}(q_L^+ - q_L^-)\right] \end{aligned}$$

For surface latent heat, we use the *budget latent heat*, supposing mass conservation ($\delta_m = 0$). We get:

$$\begin{aligned} L_s(T) &= L(T_s) - (c_{pv} - c_{pa})(1 - \delta_m q_s)T_s \\ &= L_{T=0} + (c_{pv} - c_{w|i})T_s - (c_{pv} - c_{pa})T_s = L_{T=0} + (c_{pa} - c_{w|i})T_s \\ \Longrightarrow L_s^+ &= L_s^- + (c_{pa} - c_{w|i})(T_s^+ - T_s^-) \end{aligned}$$

linearization uses:

$$\left(T_s^+\right)^4 = \left(T_s^-\right)^4 + 4\left(T_s^-\right)^3(T_s^+ - T_s^-) \quad , \qquad q_{\mathrm{sat}}(T_s^+) = q_{\mathrm{sat}}(T_s^-) + \left(\frac{\partial q_{\mathrm{sat}}}{\partial T_s}\right)^-(T_s^+ - T_s^-)$$

hence

$$c_{ps}^{+} = c_{ps}^{-} + (c_{pv} - c_{pa}) \left[\mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} (T_s^{+} - T_s^{-}) + \mathsf{HQ} (q_L^{+} - q_L^{-}) \right]$$

$$\begin{aligned}
\frac{\partial T_s}{\partial t} &= \frac{2\pi}{\tau}(T_p - T_s^{+}) \\
&\quad + C_s \left\{ (F_\dagger' - 4\epsilon\sigma {T_s^{-}}^{3} T_s^{+} + 3\epsilon\sigma {T_s^{-}}^{4}) + F_\odot'(1-\alpha) \right. \\
&\quad -\rho C_H |\mathbf{V}| \left\{ c_{ps}^{-} T_s^{+} + (c_{pv} - c_{pa}) \left[\mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} (T_s^{+} - T_s^{-}) + \mathsf{HQ}(q_L^{+} - q_L^{-}) \right] T_s^{+} + \phi_s \right. \\
&\quad \left.\left. -(c_p T + \phi)_L^{+} + \left(L_s^{-} + (c_{pa} - c_w)(T_s^{+} - T_s^{-}) \right) \left[\mathsf{HU}\ q_{\text{sat}}(T_s^{-}) + \mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} (T_s^{+} - T_s^{-}) + \mathsf{HQ}\ q_L^{+} - q_L^{+} \right] \right\} \right\} \\
\frac{T_s^{+} - T_s^{-}}{\triangle t} &= \frac{2\pi}{\tau} T_p + C_s \left\{ (F_\dagger' + 3\epsilon\sigma {T_s^{-}}^{4}) + F_\odot'(1-\alpha) \right\} \\
&\quad -\frac{2\pi}{\tau} T_s^{+} - C_s 4\epsilon\sigma {T_s^{-}}^{3} T_s^{+} \\
&\quad -C_s \rho C_H |\mathbf{V}| \left\{ \phi_s - (c_p T + \phi)_L^{+} + c_{ps}^{-} T_s^{+} \right. \\
&\quad +(c_{pv} - c_{pa}) \mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} (T_s^{+} - T_s^{-}) T_s^{+} \\
&\quad +(c_{pa} - c_w) \mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} (T_s^{+} - T_s^{-})^2 \\
&\quad +(c_{pv} - c_{pa}) \mathsf{HQ} (q_L^{+} - q_L^{-}) T_s^{+} \\
&\quad +(c_{pa} - c_w) \mathsf{HU} q_{\text{sat}}(T_s^{-})(T_s^{+} - T_s^{-}) \\
&\quad +(c_{pa} - c_w)(\mathsf{HQ} - 1) q_L^{+} (T_s^{+} - T_s^{-}) \\
&\quad +L_s^{-} \mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} T_s^{+} \\
&\quad \left. +L_s^{-} \left[\mathsf{HU} \left(q_{\text{sat}}(T_s^{-}) - \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} T_s^{-} \right) + (\mathsf{HQ} - 1) q_L^{+} \right] \right\}
\end{aligned}$$

and we suppress second order terms in $(T_s^{+} - T_s^{-})$:

$$\begin{aligned}
& T_s^{+} \left[1 + \frac{2\pi}{\tau}\triangle t + C_s \triangle t \left\{ 4\epsilon\sigma {T_s^{-}}^{3} + \rho C_H |\mathbf{V}| \left(c_{ps}^{-} + L_s^{-} \mathsf{HU} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} + (c_{pa} - c_w)(q_s^{-} - q_L^{-}) \right) \right\} \right] \\
&= T_s^{-} + \frac{2\pi \triangle t}{\tau} T_p \\
&\quad + C_s \triangle t \left\{ F_\dagger' + F_\odot'(1-\alpha) + 3\epsilon\sigma {T_s^{-}}^{4} + \rho C_H |\mathbf{V}| \left[(\phi + c_p T)_L^{+} - \phi_s + L_s^{-} \mathsf{HU} (T_s^{-} \frac{\partial q_{\text{sat}}}{\partial T_s^{-}} - q_{\text{sat}} T_s^{-}) \right. \right. \\
&\quad \left.\left. + T_s^{-} \left[(c_{pa} - c_w)(q_s^{-} - q_L^{-}) + (c_{pv} - c_{pa}) q_s^{-} \right] + \left[L_s^{-}(1 - \mathsf{HQ}) - (c_{pv} - c_{pa}) T_s^{-} \right] q_L^{+} \right] \right\}
\end{aligned} \tag{27}$$

The whole system writes then

$$\begin{bmatrix}
1 + w_{1,1} & -w1,1 & & & (0) \\
-w_{1,2} & 1 + w_{1,2} + w_{2,2} & -w_{2,2} & & \\
& & & & \\
& & \left[(A) \right] & & \\
& & & & \\
& & & & -w_{1,2} \\
(0) & & & -w_{1,1} & 1 + w_{1,1}
\end{bmatrix}
\left\{ \begin{array}{c} s_1^{+} \\ s_2^{+} \\ .. \\ \left\{ \begin{array}{c} s_L^{+} \\ T_s^{+} \\ q_L^{+} \end{array} \right\} \\ .. \\ q_2^{+} \\ q_1^{+} \end{array} \right\}
=
\left\{ \begin{array}{c} s_1^{-} \\ s_2^{-} \\ .. \\ \left\{ \begin{array}{c} B \end{array} \right\} \\ .. \\ q_2^{-} \\ q_1^{-} \end{array} \right\}$$

and we *move* a term in $\mathsf{HQ}\ q_L T_s^{+}$ in order to get a really tri-diagonal matrix for $[A]$ (term 0^* below), so we can apply Gaussian elimination, with $2L + 1$ lines.

$$[A] = \begin{bmatrix} -w_{L-1,L} & 1+w_{L-1,L}+w_{L,L} & -w_{L,L}\mathsf{CTVS} & 0^* & 0 \\ 0 & -\mathsf{CSVT} & 1+\mathsf{CTVT} & -\mathsf{CQVT} & 0 \\ 0 & 0 & -w_{L,L}\mathsf{CTVQ} & 1+w_{L-1,L}+w_{L,L}\mathsf{CQVQ} & -w_{L-1,L} \end{bmatrix}$$

$$\{B\} = \begin{Bmatrix} s_L^- + w_{L,L}\mathsf{RHSS} \\ T_s^- + \mathsf{RHST} \\ q_L^- + w_{L,L}\mathsf{RHSQ} \end{Bmatrix}$$

C?V? and RHS? coefficients are obtained by identification with equation (27) and the surface fluxes components given by:

$$\begin{aligned} J_q &= \rho C_H|\mathbf{V}|\left\{(1-\mathsf{HQ})q_L^+ - \mathsf{HU}\frac{\partial q_{\rm sat}}{\partial T_s^-}T_s^+ - \mathsf{HU}\left[q_{\rm sat}(T_s^-) - \frac{\partial q_{\rm sat}}{\partial T_s^-}T_s^+\right]\right\} \\ J_s &= \rho C_H|\mathbf{V}|\left\{s_L^+ - c_{ps}^-T_s^+ - (c_{pv}-c_{pa})\mathsf{HU}\left(T_s^-\frac{\partial q_{\rm sat}}{\partial T_s^-} + q_{\rm sat}(T_s^+ - T_s^-)\right) - \phi_s\right\} \\ J_{\rm latent} &= L_s^- J_q - \rho C_H|\mathbf{V}|\left\{(c_{pv}-c_w)(q_s^- - q_L^-)(T_s^+ - T_s^-)\right\} \\ J_{\rm sens} &= J_s + \rho C_H|\mathbf{V}|\left\{(c_{pv}-c_{pa})(q_s^- - q_L^-)(T_s^+ - T_s^-)\right\} - (c_{pv}-c_{pa})T_s^- J_q \end{aligned}$$

Actual formulae are:

$$\begin{aligned} \mathsf{CTVQ} &= \mathsf{HU}\frac{\partial q_{\rm sat}}{\partial T_s} \\ \mathsf{CQVQ} &= 1-\mathsf{HQ} \\ \mathsf{CTVS} &= c_{ps} + (c_{pv}-c_{pa})T_s\mathsf{CTVQ} \\ \mathsf{CSVT} &= \rho C_{Hs}|\mathbf{V}|\, C_s\Delta t \\ \mathsf{CQVT} &= \mathsf{CQVQ}C_s\Delta t\left[\rho C_{Hl}|\mathbf{V}|L_s - \rho C_{Hs}|\mathbf{V}|(c_{pv}-c_{pa})T_s\right] \\ \mathsf{CTVT} &= \frac{2\pi}{\tau}\Delta t + C_s\Delta t\left\{4\epsilon\sigma T_s^3 + \mathsf{ZDLDQ} + \rho C_{Hs}|\mathbf{V}|c_{ps} + \rho C_{Hl}|\mathbf{V}|L_s\mathsf{CTVQ}\right\} \\ \mathsf{ZDLDQ} &= (q_s - q_L)\left\{\rho C_{Hl}|\mathbf{V}|\left(\mathsf{ZPN}(c_{pv}-c_i) + (1-\mathsf{ZPN})(c_{pv}-c_w)\right) - \rho C_{Hs}|\mathbf{V}|(c_{pv}-c_{pa})\right\} \end{aligned}$$

where C_{Hs} and C_{Hl} are surface exchange coefficients for sensible and latent heat. Right-hand side coefficients write:

$$\begin{aligned} \mathsf{RHSQ} &= \mathsf{HU}(q_s - T_s\frac{\partial q_{\rm sat}}{\partial T_s}) \\ \mathsf{RHSS} &= \phi_L - (c_{pv}-c_{pa})T_s\mathsf{CTVQ}T_s \\ \mathsf{RHST} &= \frac{2\pi}{\tau}\Delta t T_p + C_s\Delta t\left\{(F_{\odot L} + F_{\dagger L} + (4\epsilon\sigma T^3 + \mathsf{ZDLDQ})T\right. \\ &\quad \left. -\rho C_{Hl}|\mathbf{V}|L_s\mathsf{RHSQ} - \rho C_{Hs}|\mathbf{V}|(\phi_L - (c_{pv}-c_{pa})\mathsf{HU}T_s q_s)\right\} \end{aligned}$$

Atmospheric fluxes for q and s are then obtained following the same principles as for momentum.

2.3.2 Diffusion inside the ground

Refer to the full description in part V.
Routine ACDIFUS computes the heat flux $F_{\rm sp}$ between the surface and the $n+1 = \mathsf{NCSS}+1$ inner-ground levels, following:

$$F_{\rm sp}^1 = \frac{\omega_0}{C_T\Delta x_0(\Delta x_0 - \Delta x_1)}(T_s^+ - T_p^1) \qquad (28)$$

$$F_{\rm sp}^k = \frac{\omega_0}{C_T\Delta x_0(\Delta x_{k-1} - \Delta x_k)}(T_p^{k-1} - T_p^k) \qquad k = 2\ldots n \qquad (29)$$

$$F_{\rm sp}^{n+1} \equiv 0 \qquad (30)$$

where

- C_T is a thermal coefficient,
- $\mathsf{SODELX}(0:\mathsf{NCSS}) \equiv \Delta x_k$ are the reduced thicknesses of the underground layers.
  If ISBA scheme is not active (LSOLV=.FALSE.), the same expressions could be used, replacing $\Delta x_0 = 1,\ \Delta x_k = 0,\ k = 2\ldots n$.
- $\omega_0 \equiv 2\pi/86400$ is the diurnal pulsation.

2.4 Anti-fibrillation scheme

Anti-fibrillation is an additional feature of the vertical diffusion scheme to avoid temporal oscillations (called "fibrillations") for long time steps.
The problem occurs because the vertical diffusion coefficients are computed from the state of the atmosphere at $t - \triangle t$, while the split-implicit algorithm makes them act to get a balanced solution at a pseudo $t + \triangle t$ time.
This is not important when the atmosphere is strongly unstable, as the exchange coefficient is big enough for the final state not to depend too much on its precise value.
But near the neutral state, the exchange coefficients vary very quickly with stability, and fibrillations may develop alternating one step with rather strong coefficients and weak gradients followed by one step with strong gradients and feeble coefficients: for the leapfrog scheme, this leads to a $4\triangle t$ oscillation, the physical time step being twice the dynamical time step. It wears also a spatial signature in the vertical, and sometimes also in the horizontal.
A time shift of the right-hand side of the implicit vertical diffusion equations (over-relaxation split-implicit scheme) results in a stable scheme; to avoid degrading too much the accuracy, Girard and Delage [1990] proposed to make this time-shift flow-dependent.

$$\frac{\partial \psi}{\partial t} = \frac{1}{\rho}\frac{\partial}{\partial z}\rho K_\psi \frac{\partial \psi}{\partial z} = -g\frac{\partial J_\psi}{\partial p} \quad , \qquad J_\psi = \frac{\rho g K_\psi}{\triangle \phi}\triangle\psi \equiv -K'_\psi \triangle \psi$$

is replaced by

$$\frac{\partial \psi}{\partial t} = -g\frac{\partial}{\partial p}\left[(1-\beta)K'_\psi\triangle\psi + \beta K'_\psi \triangle \psi^+\right]$$

In preceding sections, we set $\beta \equiv 1$ everywhere, through implicit discretization. With the anti fibrillation scheme, β is made flow-dependent (but independent of the variable ψ: actually ACCOEFK returns 2 sets of coefficients: PXTROV for T and q and PXUROV for the velocities, but they are equal).
When activated, β remains 1 everywhere there is no risk of fibrillation, while it can take as big values as necessary wherever the danger appears.
The problem was studied through stability analysis.
Rewriting previous equation in numerical form in z coordinate:

$$\frac{\psi^+ - \psi}{\triangle t} = \frac{\partial}{\partial z}\left[(1-\beta)\left(K_\psi \frac{\partial \psi}{\partial z}\right) + \beta\left(K_\psi\frac{\partial \psi^+}{\partial z}\right)\right]$$

yields

$$\left[1 - \triangle t \frac{\partial}{\partial z}\left(\beta K_\psi \frac{\partial}{\partial z}\right)\right]\left(\frac{\psi^+ - \psi}{\triangle t}\right) = K_\psi \frac{\partial^2 \psi}{\partial z^2} + \frac{\partial K_\psi}{\partial z}\frac{\partial \psi}{\partial z}$$

In the RHS, we need an expression of $\frac{\partial K_\psi}{\partial z}$, using the complete expressions of the exchange coefficients. The calculation yields respectively:

$$\left[1 - \triangle t \frac{\partial}{\partial z}\left(\beta K_m \frac{\partial}{\partial z}\right)\right]\left(\frac{\mathbf{V}^+ - \mathbf{V}}{\triangle t}\right) = K_m(2-2\alpha_m)\frac{\partial^2 \mathbf{V}}{\partial z^2} + \frac{K_m \alpha_m}{\Lambda}\frac{\partial^2\theta}{\partial z^2} \quad (31)$$

$$\left[1 - \triangle t \frac{\partial}{\partial z}\left(\beta K_h \frac{\partial}{\partial z}\right)\right]\left(\frac{\theta^+ - \theta}{\triangle t}\right) = K_h(1+\alpha_h)\frac{\partial^2 \theta}{\partial z^2} + K_h\Lambda(1-2\alpha_h)\frac{\partial^2\mathbf{V}}{\partial z^2} \quad (32)$$

with

$$\alpha_m = \frac{\mathcal{R}i}{f_\mathbf{V}}\frac{df_\mathbf{V}}{d\mathcal{R}i} \quad , \qquad \alpha_h = \frac{\mathcal{R}i}{f_H}\frac{df_H}{d\mathcal{R}i} \quad , \qquad \Lambda = \frac{\partial \theta}{\partial z}/\frac{\partial \mathbf{V}}{\partial z} \quad (33)$$

Linearization is performed around a stationnary state, to get equations for the small perturbations. Seeking oscillating solutions yields a characteristic equation that has to be solved.

$$F(\tau,\beta) = A(\beta)\tau^2 + B(\beta)\tau + C = 0 \qquad \text{with} \qquad \tau \equiv (e^{\omega\triangle t} - 1)$$

The solution was complicated by the fact that K_m and K_h have different expressions in Arpège.
The original implementation simplified the characteristic equation, which implied the correction of all points for which $\mathcal{R}i > 0$ and no point for which $\mathcal{R}i < 0$.

But a more detailed inspection of the equation shows that the points which really need a correction are those with moderate positive or negative $\mathcal{R}i$, roughly $-0.2 \leq \mathcal{R}i \leq 0.5$. It worked nevertheless because roughly 99% of model points where the turbulent scheme is not cancelled by convective activity satisfy $\mathcal{R}i > 0$.
The complete scheme proposed by BÉNARD et al. [1999] solves this problem; to keep access to the two versions of the scheme, the namelist parameter XMULAF has to be given negative values (XMULAF $= -1.75$ to select the complete scheme, and positive values to select the simplified one.
The additional anti-fibrillation parameter added for shallow convection: XMUCVPP, is presently set to 0. with the new scheme. With this we compute

$$\begin{aligned} \mathsf{ZSTAD} &= \triangle\phi(\triangle(RT) + \kappa\triangle\phi + \mathsf{XMUCVPP} \cdot R_a \cdot \mathsf{ZAUX}) \\ \mathcal{R}i' &= g\frac{|\mathsf{ZSTAD}|}{|\mathbf{V}_L|^2} \end{aligned}$$

This value of $\mathcal{R}i'$ replaces $\mathcal{R}i$ in all computations of anti-fibrillation coefficients.