

AtmoData Scientific documentation

Version 1 for AtmoData 1.1

CEREA – ENPC / EDF R&D
Hervé Njomgang, Vivien Mallet and Luc Musson-Genon

Contents

Introduction	5
Notations	7
1 Meteorology	9
1.1 Conversion of coordinates	9
1.1.1 ECMWF	9
1.1.2 MM5	9
1.2 Basic meteorology	10
1.2.1 Potential temperature	10
1.2.2 Virtual temperature	10
1.2.3 Specific humidity	10
1.2.4 Relative humidity	10
1.2.5 Winds	11
1.2.6 Module of Winds	11
1.2.7 Richardson number	11
1.2.8 Planetary boundary layer height	12
1.3 Clouds	12
1.3.1 Critical relative humidity	12
1.3.2 Cloud Fraction	13
1.3.3 Cloudiness	13
1.3.4 Clouds basis height	14
1.4 Attenuation	14
1.4.1 “RADM” parameterization	14
1.4.2 ESQUIF parameterization	15
2 Vertical diffusion	15
2.1 Louis’ parameterization	16
2.2 Troen’s & Mahrt’s parameterization	16
2.2.1 K_z	16
2.2.2 $PBLH$	17
3 Deposition velocities	18
3.1 \mathbf{R}_a	18
3.1.1 Diagnosis with the drag coefficient	18
3.1.2 Using the momentum flux	19
3.1.3 Using the heat flux	20
3.2 \mathbf{R}_b	20
3.2.1 Diagnosis with the drag coefficient	20
3.2.2 Using the friction velocity	20
3.3 \mathbf{R}_c	21
3.3.1 Wesely’s parameterization	21

3.3.2	Zhang's parameterization	22
4	Surface emissions	24
4.1	Anthropogenic emissions	24
4.2	Biogenic emissions	25

Introduction

AtmoData ([6]) is a library for data processing and parameterizations in atmospheric chemistry and physics. This document describes the parameterizations and the miscellaneous physical functions available in the library.

Apart from this scientific documentation, additional resources are available on AtmoData website at <http://www.enpc.fr/cerea/atmodata/>: a more complete introduction, the latest version of this scientific documentation, a user's guide and the reference documentation.

In case you want to refer to AtmoData in a publication, a conference, a poster or so, please include the reference [6]: Vivien Mallet and Bruno Sportisse, *Data processing and parameterizations in atmospheric chemistry and physics: the AtmoData library*, Submitted to Atmospheric Environment, 2005.

Notations

Variables

A	Attenuation
CF	Cloud fraction
CH	Clouds basis height
CRH	Critical relative humidity
D_s	Molecular diffusivity of the species s
E_s	Emission for the species s
EF_s	Emission factor for the species s
ER_s	Emission rate for the species s
f_h	Heat flux
f_m	Momentum flux
f_s	Reactivity of species s
h	Relative humidity
H_s	Henry constant for species s
J	Photolysis rate
K_z	Vertical diffusion
l	Mixing length
LMO	Monin-Obukhov length
LUC	Land use coverage
LWC	Liquid water content
LWP	Liquid water path
N	Cloudiness
P	Pressure
PAR	Photosynthetically active radiation
PBL	Planetary boundary layer
$PBLH$	Planetary boundary layer height
P_i	Partial pressure for species #i
P_i^{sat}	Saturation pressure for species #i
q	Specific humidity
Q_0	Surface sensible heat flux
Ri	Richardson number
Ri_c	Critical Richardson number
SR	Solar radiation
T	Temperature
Tr	Cloud transmissivity
T_v	Virtual temperature
V	Meridional wind

W	Wind module
U	Zonal wind
u_*	Surface friction velocity
V_d	Deposition velocity
w_*	Convective velocity scale
Z	Zenith angle
Z_r	Roughness height
θ	Potential temperature
λ	Asymptotic mixing length
ρ	Mass density
τ	Cloud optical depth

Coordinates

F_i	Value of field F at node i along longitude
$F_{i_{interf}}$	Value of field F at interface i along longitude
F_j	Value of field F at node j along latitude
$F_{j_{interf}}$	Value of field F at interface j along latitude
F_k	Value of field F at node k along altitude
$F_{k_{interf}}$	Value of field F at interface k along altitude
z	Altitude
σ	Ratio of pressure on surface pressure

Note: z_k is dedicated to the altitudes of *nodes*; so $z_k \neq 0$ and $z_{0_{interf}} = 0$.

Constants

c_p	Specific heat capacity at constant pressure	$\frac{7}{2}r$
c_p	Specific heat capacity at constant volume	$\frac{5}{2}r$
g	Standard gravity	$9.80665 \text{ m} \cdot \text{s}^{-1}$
M_{air}	Molar mass of air	$28.96 \text{ g} \cdot \text{mol}^{-1}$
M_{vapor}	Molar mass of vapor	$18 \text{ g} \cdot \text{mol}^{-1}$
P_0	Standard pressure	$101,325 \text{ Pa}$
r	Molar gas constant for dry air	$287.0 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
r_{vap}	Molar gas constant for vapor	$461.5 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
R	Gas constant	$8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
T_0	Standard temperature	273.15 K
κ	Von Kármán constant	0.4

1 Meteorology

1.1 Conversion of coordinates

1.1.1 ECMWF

In the ECMWF model, the vertical coordinates are hybrid σ -P levels. The pressure at level k is computed as follows:

$$P_k = \alpha_k P_{surf} + \beta_k P_{ref} \quad (1)$$

where P_{ref} is a reference pressure, and α_k and β_k are hybrid coefficients.

To convert the pressure into meters, one uses the following formula:

$$z_{n+1} = z_n + \frac{rT}{P} \ln \frac{P_n}{P_{n+1}} \quad (2)$$

where index n denotes the level and $z_0 = 0\text{m}$. This formula can be easily derived from the *hydrostatic approximation* and the *perfect gas law*, assuming that the atmosphere is *isotherm* within two layers.

```
ComputePressure, ComputeHeight,  
ComputeInterfHeight, ComputeMiddleHeight
```

1.1.2 MM5

In MM5, the pressure at level k is given by

$$P_k = \sigma_k P_{surf} \quad (3)$$

Then formula (2) can also be used to convert the pressure to altitudes.

```
ComputeHeight, ComputeInterfHeight, ComputeMiddleHeight
```

For horizontal coordinates, MM5 uses three projections:

- Lambert Azimuthal Equal Area,
- Lambert Conformal Conic, and
- Mercator.

AtmoData provides classes to perform coordinate transformations from these projections to latitude/longitude coordinates, and vice versa. Note that AtmoData does not manipulate directly the three MM5 coordinates but it handles MM5 indices instead, which is more convenient.

```
LonlatToMM5LccInd, LonlatToMM5MercInd,  
LonlatToMM5StereInd, MM5LccIndToLonlat,  
MM5MercIndToLonlat, MM5StereIndToLonlat
```

1.2 Basic meteorology

1.2.1 Potential temperature

The potential temperature is computed with:

$$\theta = T \left(\frac{P}{P_{\text{ref}}} \right)^{-\frac{r}{c_p}} \quad (4)$$

Another formula (equivalent):

$$\theta = T \left(\frac{P}{P_{\text{ref}}} \right)^{\frac{1-\gamma}{\gamma}} \quad (5)$$

where $\gamma = \frac{c_p}{c_v}$, $c_p = c_v + r$ for a perfect gas and, usually, $P_{\text{ref}} = 100,000\text{Pa}$.

ComputePotentialTemperature

1.2.2 Virtual temperature

$$T_v = T \left(1 - q + \frac{r_{\text{vap}}}{r} q \right) \quad (6)$$

where q is the specific humidity (cf. 1.2.3). So

$$T_v = T (1 + 0.608q) \quad (7)$$

ComputeVirtualTemperature

1.2.3 Specific humidity

Definition:

$$q = \frac{\rho_{\text{vapor}}}{\rho_{\text{vapor}} + \rho_{\text{air}}} \quad (8)$$

It is not computed by AtmoData, but computed by meteorological models.

1.2.4 Relative humidity

First are computed the partial pressure of vapor P_{vapor} and the saturation pressure of vapor $P_{\text{vapor}}^{\text{sat}}$:

$$P_{\text{vapor}} = \frac{q}{q + \frac{M_{\text{vapor}}}{M_{\text{air}}}(1-q)} P \quad (9)$$

$$P_{vapor}^{sat} = 611.2 \exp\left(\frac{17.67(T - 273.15)}{T - 29.65}\right) \quad (10)$$

from which is derived relative humidity:

$$h = \frac{P_{vapor}}{P_{vapor}^{sat}} \quad (11)$$

`ComputeRelativeHumidity`

1.2.5 Winds

Note: this section deals with a transformation specific to the chemistry-transport model Polair3D^{†1}.

The zonal and meridional winds U and V from the meteorological models are transformed so as to be input of the chemistry-transport model Polair3D:

$$\begin{cases} U_{Polair3D} = \frac{U}{\cos \varphi} \\ V_{Polair3D} = V \cos \varphi \end{cases} \quad (12)$$

where φ represents the latitude.

`TransformMeridionalWind, TransformZonalWind`

1.2.6 Module of Winds

The wind module is, of course, the Euclidean norm of the vector (U, V) :

$$\mathcal{W} = \sqrt{U^2 + V^2} \quad (13)$$

`ComputeModule`

1.2.7 Richardson number

The Richardson number Ri is computed as follows. We set:

$$DW_k = \sqrt{\left(\frac{\Delta U_k}{\Delta z_k}\right)^2 + \left(\frac{\Delta V_k}{\Delta z_k}\right)^2}$$

^{†1}<http://www.enpc.fr/cerea/polair3d/>

with $\Delta X_k = X_k - X_{k-1}$, and then

$$Ri_k = \frac{g \Delta\theta_k}{\max(DW_k^2, WT^2) \theta_{k-1} \Delta z_k} \quad (14)$$

where WT is the wind threshold, set to 0.001 by default.

`ComputeRichardson`

1.2.8 Planetary boundary layer height

The planetary boundary layer height, $PBLH$, is usually retrieved from the outputs of a meteorological model. Otherwise, two diagnoses are proposed. One returns the height at which the Richardson number reaches a critical value (usually set to 0.21). The other diagnosis follows [12]. Details are provided in section 2.2.2.

`ComputeBoundaryLayerHeight_Richardson,`
`ComputeBoundaryLayerHeight_TM`

1.3 Clouds

1.3.1 Critical relative humidity

The critical relative humidity is the threshold value above which there is formation of clouds.

There are several parameterizations in `AtmoData` for CRH , taking in account the dependence upon the altitude and the special case of the planetary boundary layer.

- **Parameterization with σ**

This is a well known parameterization, widely used (e.g. in CMAQ, [1]).

It approximates CRH with:

$$CRH_k = 1 - \lambda_0 \sigma_k (1 - \sigma_k) (1 + \lambda_1 (\sigma_k - 0.5)) \quad (15)$$

where σ_k is the ratio of pressure at level k on the surface pressure, and the λ_i are empirical coefficients. Their default values are $\lambda_0 = 2$ and $\lambda_1 = \sqrt{3}$.

A more general parameterization is derived from the previous one:

$$CRH_k = 1 - \lambda_0 \sigma_k^{a_0} (1 - \sigma_k)^{a_1} (1 + \lambda_1 (\sigma_k - 0.5)) \quad (16)$$

Default values: $\lambda_0 = 1.1$, $\lambda_1 = \sqrt{1.3}$, $a_0 = 0$, and $a_1 = 1.1$.

- **In the planetary boundary layer**

Within the planetary boundary layer, one may set the critical relative humidity to a constant (e.g., [1, pages 48-49]):

$$z_k < PBLH \implies CRH_k = CRH_{PBL} \quad (17)$$

where $PBLH$ is the PBL height, and $CRH_{PBL} = 0.98$ by default.

- **Pressure parameterization**

$$CRH_k = \begin{cases} CRH_0 & , P_{ref,0} < P_k \\ CRH_1 & , P_{ref,1} < P_k < P_{ref,0} \\ CRH_2 & , P_k < P_{ref,1} \end{cases} \quad (18)$$

By default, $P_{ref,0} = 70,000$ Pa, $P_{ref,1} = 40,000$ Pa, $CRH_0 = 0.75$, $CRH_1 = 0.95$, $CRH_2 = 0.95$.

ComputeCriticalRelativeHumidity,
ComputeCriticalRelativeHumidity_extended

1.3.2 Cloud Fraction

The cloud fraction CF is computed using CRH , by one of the following formulae (one may refer to [1, pages 48-49]):

$$CF_k = \begin{cases} 0.34 \left(\frac{h_k - CRH}{1 - CRH} \right) & , z_k < PBLH \\ \left(\frac{h_k - CRH}{1 - CRH} \right)^2 & , z_k > PBLH \end{cases} \quad (19)$$

In an alternative and simplified parameterization, one uses the second formula for all vertical levels.

ComputeCloudFraction

1.3.3 Cloudiness

The parameterization is similar to that of CMAQ model ([1]). One considers three layers and thus low, medium and high cloudinesses. The layer limits are determined by the two given pressures $P_{lim,0}$ and $P_{lim,1}$. In each layer, the clouds are contained within the levels k_{base} (included) and k_{top} (excluded), with $k_{base} < k_{top}$. k_{base} is the first layer (starting from the ground) where CF reaches 50% of its maximum value along the vertical column and

in the low, medium or high cloud-layer, and k_{top} is the first above k_{base} where CF is less than this threshold. Finally, the low, medium and high cloudinesses are computed with:

$$\mathcal{N} = \frac{\sum_{k_{base}}^{k_{top}-1} CF_k \Delta z_k}{\sum_{k_{base}}^{k_{top}-1} \Delta z_k} \quad (20)$$

ComputeCloudiness

1.3.4 Clouds basis height

The height CH of the basis of clouds is

1. at the first level k where the relative humidity exceeds the critical relative humidity, or
2. given by the base of the clouds as it appears when the cloudiness is computed (k_{base} in section 1.3.3).

ComputeCloudHeight

1.4 Attenuation

The attenuation \mathcal{A} measures the decrease in the photolysis rates of chemical reactions when solar radiation is partially absorbed by clouds. The photolysis rates should be multiplied by \mathcal{A} .

1.4.1 “RADM” parameterization

AtmoData implements the parameterization from [2, 5]. The photolysis rates J become:

$$J_{below} = \mathcal{A}_{below} J_{clear}$$

below the clouds, and

$$J_{above} = \mathcal{A}_{above} J_{clear}$$

above the clouds, to take in account the enhancement in photolysis rates due to the reflection of radiations. The attenuation coefficients are computed with:

$$\mathcal{A}_{below} = 1 - cfrac(1 - 1.6Tr \cos Z) \quad (21)$$

$$\mathcal{A}_{above} = 1 + cfrac(1 + (1 - Tr) \cos Z) \quad (22)$$

where $cfrac$ is the cloud coverage fraction (computed, with the sum of medium and high cloudinesses, as $\min(1, \mathcal{N}_{medium} + \mathcal{N}_{high})$), Z is the zenith angle, and Tr is the cloud transmissivity, calculated with:

$$Tr = \frac{5 - e^{-\tau}}{4 + 3(1 - f)\tau} \quad (23)$$

where f represents the scattering phase function assymetry factor, set to 0.86, and τ the cloud optical depth, following an empirical formula from [11]:

$$\log(\tau) = 0.2633 + 1.7095 \ln(\log LWP) \quad (24)$$

where LWP is the liquid water path, which is a function of the liquid water content: $LWP = LWC\Delta z$, and Δz is the cloud thickness.

The attenuation coefficients are computed from the top to the bottom. Until $\tau_k < 0.5$, Tr_k is set to 1 and \mathcal{A}_k is computed with the equation (21). Below the clouds and if $\tau_k > 0.5$, equations (23) and (22) are used. Inside clouds, the attenuation coefficients are linearly interpolated..

`ComputeAttenuation_LWC`

1.4.2 ESQUIF parameterization

This parameterization was developed during the ESQUIF campaign ([3]) with measurements of the photolysis rates for NO_2 :

$$\mathcal{A} = (1 - a \mathcal{N}_{high})(1 - b \mathcal{N}_{medium})e^{-cB} \quad (25)$$

with:

$$B = \frac{\int_{z=0}^{z<1500m} \min(0., h(z) - 0.7)}{\int_{z=0}^{z<1500m} 1 - 0.7}$$

and h is piecewise linear.

Note that the attenuation coefficients do not depend on the altitude.

`ComputeAttenuation_ESQUIF`

2 Vertical diffusion

The vertical diffusion coefficient K_z is computed in AtmoData using two parameterizations respectively introduced in [4] and [12] (the latter is especially designed for models with a low vertical resolution). Notice that K_z is provided at the interfaces of the vertical grid.

2.1 Louis' parameterization

For each vertical cells, the stability function F is first calculated:

$$F(Ri_k) = \begin{cases} (1 + 3BRi_k\sqrt{1 + DRi_k})^{-1} & , Ri_k \geq 0 \\ 1 - 3BRi_k \left(1 + \frac{3BC l_{k_{interf}}^2}{(z_{k_{interf}} + z_0)^2} \sqrt{\frac{|Ri_k|}{27}} \right)^{-1} & , Ri_k < 0 \end{cases} \quad (26)$$

where Ri is the Richardson number (refer to section 1.2.7), and $l_{k_{interf}}$ is the mixing length at level k_{interf} :

$$l_{k_{interf}} = \frac{\kappa z_{k_{interf}}}{1 + \frac{\kappa z_{k_{interf}}}{\lambda}} \quad (27)$$

κ is the Von Kármán constant set to 0.40, λ is the asymptotic mixing length, set to 100m. The default values of the other parameters are:

$$B = C = D = 5 \text{ and } z_0 = 1$$

In addition, a threshold value Ri_t ($Ri_k > Ri_t \implies Ri_k = Ri_t$) for the Richardson number is computed following [8, 9]:

$$Ri_t = a \left(\frac{\Delta z_k}{\Delta z_0} \right)^b \quad (28)$$

with $a = 0.115$, $b = 0.175$ and $\Delta z_0 = 0.01$, by default.

Finally

$$K_{z,k_{interf}} = l_{k_{interf}}^2 F(Ri_k) \left\| \frac{\partial(U_k, V_k)}{\partial z} \right\|_2 \quad (29)$$

where $\frac{\partial(U_k, V_k)}{\partial z}$ is approximated with first-order finite differences.

ComputeLouisKz

2.2 Troen's & Mahrt's parameterization

2.2.1 K_z

K_z is computed with the following formula

$$K_{z,k_{interf}} = u_* \kappa z_{k_{interf}} \Phi_{m,k_{interf}}^{-1} \left(1 - \frac{z_{k_{interf}}}{PBLH} \right)^p \quad (30)$$

u_* is the surface friction velocity and Φ_{mk} the nondimensional shear. In *stable* conditions, it is computed as

$$\Phi_{m,k_{interf}} = 1 + 4.7 \frac{z_{k_{interf}}}{LMO} \quad (31)$$

LMO being the Monin-Obukhov length. In *unstable* conditions:

- in the surface layer ($z < \varepsilon PBLH$, with $\varepsilon = 0.1$),

$$\Phi_{m,k_{interf}} = \left(1 - 7 \frac{z^{k_{interf}}}{LMO}\right)^{-1/3} \quad (32)$$

- above the surface layer, Φ_m is constant

$$\Phi_m = \frac{u_*}{w_s} \quad (33)$$

w_s is the velocity scale given by

$$w_s = (u_*^3 + 7\varepsilon\kappa w_*^3)^{1/3} \quad (34)$$

where w_* is the convective velocity scale:

$$w_* = \left(\frac{gQ_0}{T_{2m}}h\right)^{1/3} \quad (35)$$

T_{2m} being the temperature at 2 m above the ground and Q_0 the surface sensible heat flux.

The exponent p is set to 2, but its value can be modified to adjust the vertical profile of K_z (see the discussion in [12]).

ComputeTroenMahrtKz

2.2.2 PBLH

Troen & Mahrt propose to compute $PBLH$ so that it satisfies:

$$PBLH = Ri_c \frac{T_{surf} \mathcal{W}^2(PBLH)}{g(\theta(PBLH) - \theta_s)} \quad (36)$$

Ri_c is the critical Richardson number (set to 0.21 by default), θ is the potential temperature, θ_s is the potential temperature of the air near the surface. θ_s is estimated as the potential temperature θ_0 in the first layer plus a scaled virtual temperature excess θ_e :

$$\theta_s = \theta_0 + \theta_e$$

with

$$\theta_e = C \frac{Q_0}{w_s}$$

C is a coefficient, usually set to 6.5, and the velocity scale w_s is given by equations (34) and (35). In AtmoData, one searches for the lowest level k_s (starting from the first layer) where

$$\theta_{k_s} \geq \theta_s + Ri_c \frac{T_{surf} \mathcal{W}_{k_s}^2}{gz_{k_s}} \quad (37)$$

Then one performs the following interpolation:

$$PBLH = z_{k_s-1} + \frac{-\Delta_{k_s-1}}{\Delta_{k_s} - \Delta_{k_s-1}}(z_{k_s} - z_{k_s-1}) \quad (38)$$

with

$$\Delta_k = \theta_k - \left(\theta_s + Ri_c \frac{T_{srf} \mathcal{W}_k^2}{gz_k} \right)$$

An additional parameterization is based on the Richardson number. $PBLH$ is determined by the first level where the Richardson number Ri becomes greater than its critical value Ri_c . If

$$k_c = \min\{k | Ri_k > Ri_c\}$$

then

$$PBLH = z_{k_c-1} + \frac{Ri_c - Ri_{k_c-1}}{Ri_{k_c} - Ri_{k_c-1}}(z_{k_c} - z_{k_c-1})$$

ComputeBoundaryLayerHeight_Richardson,
ComputeBoundaryLayerHeight_TM

3 Deposition velocities

The deposition velocities are assumed to be in the form:

$$V_d = \frac{1}{R_a + R_b + R_c} \quad (39)$$

V_d is in $\text{m} \cdot \text{s}^{-1}$. R_a is the aerodynamic resistance, R_b is the quasi-laminar sublayer resistance, and R_c is the canopy resistance. In general the efforts are dedicated to the calculation of R_c .

3.1 R_a

The value of R_a can be either diagnosed according to wind and stability, or parameterized with the momentum flux or the heat flux (function of the Richardson number).

3.1.1 Diagnosis with the drag coefficient

The (rough) formula for R_a is

$$R_a = \frac{1}{C_D \max(0.1, \mathcal{W})} \quad (40)$$

W is the wind module and C_D is the drag coefficient of momentum. It is computed with

$$C_D = r_0 \psi \quad (41)$$

and

$$r_0 = \frac{\kappa^2}{\ln \frac{25}{Z_r}}$$

Z_r is the roughness height. ψ is the stability function:

$$\psi = \begin{cases} 1 - 9.4 \frac{Ri}{1 + r_1 \sqrt{-Ri}} & , \quad Ri < 0 \\ (1 + 4.7 Ri)^2 & , \quad Ri > 0 \end{cases} \quad (42)$$

with

$$r_1 = 9.4 \times 7.4 r_0 \sqrt{\frac{25}{Z_r}}$$

The Richardson number is taken at the surface.

ComputeRa_drag

3.1.2 Using the momentum flux

First, to estimate the momentum flux, we introduce:

$$f_m = \begin{cases} 1 - 2b_1 \frac{Ri}{1 + 3c\sqrt{-Ri}} & , \quad Ri < 0 \\ \left(1 + 2b_1 \frac{Ri}{\sqrt{1 + d_1 Ri}}\right)^{-1} & , \quad Ri > 0 \end{cases} \quad (43)$$

where $b_1 = d_1 = 5$. The value of c is more complicated:

$$c = b_1 c_1 A_u A_t \sqrt{1 - \frac{Z_t}{z_0 + Z_t} \left(\left(\frac{z_0 + Z_t}{Z_t} \right)^{1/3} - 1 \right)^{3/2}}$$

where $c_1 = 5$ and Z_t is the roughness length for heat assumed to be equal to $\frac{Z_r}{10}$.

$$A_u = \frac{\kappa}{\ln \left(\frac{z_0 + Z_r}{Z_r} \right)}$$

and A_t has the same expression where Z_r is replaced with Z_t .

Then

$$R_a = (A_u^2 f_m W)^{-1} \quad (44)$$

ComputeRa_momentum

3.1.3 Using the heat flux

The heat flux is

$$f_h = \begin{cases} 1 - 3b_1 \frac{R_i}{1 + 3c\sqrt{-R_i}} & , \quad Ri < 0 \\ \left(1 + 3b_1 \frac{R_i}{1 + d_1 Ri}\right)^{-1} & , \quad Ri > 0 \end{cases} \quad (45)$$

The coefficients b_1 , c and d_1 are the same as for the momentum flux.

Then

$$R_a = (A_u A_t f_h \mathcal{W})^{-1} \quad (46)$$

`ComputeRa_heat`

3.2 R_b

R_b can also be diagnosed as R_a , or is computed as function of the friction velocity.

3.2.1 Diagnosis with the drag coefficient

The formula is

$$R_b = \frac{2}{\kappa} \left(\frac{\nu \sqrt{M_i/18}}{D_e Pr} \right)^{2/3} \frac{1}{C_D \max(0.1, \mathcal{W})} \quad (47)$$

where ν is the kinematic viscosity of air, set to 0.15, M_i is the molar mass of the species for which R_b is calculated, D_e is the molecular diffusivity of water, set to 0.25, and Pr is the Prandtl number, set to 0.74.

`ComputeRb_drag`

3.2.2 Using the friction velocity

In this case

$$R_b = \frac{1}{\kappa u_*} \left(\frac{Sc(s)}{Pr} \right)^{2/3} \quad (48)$$

where $Sc(s)$ is the Schmidt number for species s , which is the ratio of the kinematic viscosity of air upon the molecular diffusivity D_s of the species.

$$Sc(s) = \frac{\nu}{D_s}$$

The formula 48 is multiplied by two in presence of *vegetation*.

`ComputeRb_friction`

3.3 R_c

Two parameterizations are proposed to compute R_c for a given species s . H_s is the Henry constant of this species, f_s its reactivity and D_s its molecular diffusivity.

3.3.1 Wesely's parameterization

Warning: in this section, temperatures are in degrees Celsius.

This parameterization is described in [14]. R_c is divided into four parallel resistances:

$$\frac{1}{R_c} = \frac{1}{R_{stom} + R_m} + \frac{1}{R_{lu}} + \frac{1}{R_{dc} + R_{cl}} + \frac{1}{R_{ac} + R_{gs}} \quad (49)$$

- R_{stom} is the stomatal resistance, computed with

$$R_{stom} = Ri \left(1 + \frac{200}{SR + 0.1} \right)^2 \frac{400}{T_{srf}(40 - T_{srf})} \frac{D_s}{D_e} \quad (50)$$

if $0^\circ\text{C} < T_{srf} < 40^\circ\text{C}$. Otherwise it is set to ∞ . T_{srf} is the surface temperature, and SR the solar radiation.

- R_m is the mesophyll resistance

$$R_m = \frac{1}{H_s/3000 + 100f_s} \quad (51)$$

- R_{lu} is the cuticle resistance

$$R_{lu} = \frac{R_{LUC}}{10^{-5}H_s + f_s} \quad (52)$$

where R_{LUC} is the leaf cuticle resistance for the current land cover (LUC means "land use coverage"). Note that typical values of R_{LUC} are provided in [14].

- R_{dc} is the buoyant convection (at sunlight) resistance

$$R_{dc} = \frac{100}{1 + \frac{1000}{SR + 10}} \quad (53)$$

- Finally R_{cl} , (the resistance of the exposed surfaces in the lowest structures above the ground) and R_{gs} (resistance to uptake at the ground) are computed as function of the values for O_3 and SO_2 (notably provided in [14]):

$$\frac{1}{R_{cl,gs}^s} = \frac{\alpha_s}{R_{cl,gs}^{\text{O}_3}} + \frac{\beta_s}{R_{cl,gs}^{\text{SO}_2}} \quad (54)$$

- R_{ac} (for transfers that depend only on the canopy height) is given in tables (in [14]).

ComputeWesely

3.3.2 Zhang's parameterization

Warning: in this section, temperatures are in degrees Celsius.

A detailed description of this parameterization may be found in [15]. The whole resistance is

$$\frac{1}{R_c} = \frac{1 - W_{st}}{R_{stom} + R_m} + \frac{1}{R_{cut}} + \frac{1}{R_{ac} + R_g} \quad (55)$$

- W_{st} is the fraction of stomatal blocking, which is added to the model in presence of dew or rain

$$\begin{cases} 0 & , \quad SR \leq 200 \text{ W.m}^{-2} \\ \frac{SR-200}{800} & , \quad 200 < SR \leq 600 \text{ W.m}^{-2} \\ 0.5 & , \quad 600 < SR \end{cases} \quad (56)$$

- R_{stom} is the stomatal resistance. His parameterization is quite complicated

$$R_{stom} = (G_s(PAR)f_{cr}(T)f_{cr}(\mathcal{D})f_{cr}(\psi) \text{frac}D_sD_e)^{-1} \quad (57)$$

First, G_s is the unstressed canopy stomatal conductance, depending on the photosynthetically active radiations (PAR). It may be computed as proposed in [16], through the formula

$$G_s(PAR) = \frac{F_{sun}}{r_{st}(PAR_{sun})} + \frac{F_{shade}}{r_{st}(PAR_{shade})} \quad (58)$$

F_{sun} and F_{shade} are the total sunlit and shaded leaf area indexes given by:

$$F_{sun} = \left(1 - e^{-\frac{LAI}{2 \cos Z}}\right) 2 \cos Z$$

$$F_{shade} = LAI - F_{sun}$$

Z is the zenith angle, and LAI the leaf area index (given in the tables). If $Z > 90^\circ$, F_{sun} and F_{shade} are set to 0.

r_{st} is the unstressed leaf stomatal resistance, given by equation 59, depending on PAR_{sun} and PAR_{shade} , the PAR received by sunlit and shaded leaves (equations 60 and 61):

$$r_{st} = r_{stmin} \left(1 + \frac{b_{rs}}{PAR}\right) \quad (59)$$

r_{stmin} depends on the LUC category, and b_{rs} is an empirical constant. Both are given in tables.

When $LAI < 2.5$ or $SR < 200 \text{ W.m}^{-2}$

$$\begin{aligned} PAR_{shade} &= R_{diff} e^{\frac{1}{2}LAI^{0.7}} \\ &\quad + 0.07R_{dir}(1.1 - 0.1LAI)e^{-\cos Z} \\ PAR_{sun} &= R_{dir} \frac{\cos\alpha}{\cos Z} + PAR_{shade} \end{aligned} \quad (60)$$

otherwise

$$\begin{aligned} PAR_{shade} &= R_{diff} e^{\frac{1}{2}LAI^{0.8}} \\ &\quad + 0.07R_{dir}(1.1 - 0.1LAI)e^{-\cos Z} \\ PAR_{sun} &= R_{dir}^{0.8} \frac{\cos\alpha}{\cos Z} + PAR_{shade} \end{aligned} \quad (61)$$

R_{diff} and R_{dir} are the downward visible radiation fluxes above the canopy from diffuse and direct-beam radiations, respectively. They are computed following [13]. α is the angle between the leaves and the sun, and has a mean value of 60° for a canopy assumed to have a spherical leaf angle distribution.

In equation 57, the f_{cr} factors are the conductance-reducing effects of temperature T , water-vapor-pressure deficit \mathcal{D} and water stress ψ , given by:

$$f_{cr}(T) = \frac{T - T_{min}}{T_{opt} - T_{min}} \left(\frac{T_{max} - T}{T_{max} - T_{opt}} \right)^{b_t} \quad (62)$$

with $b_t = \frac{T_{max} - T_{opt}}{T_{opt} - T_{min}}$. T_{min} , T_{max} and T_{opt} depend on the LUC category, and are provided in tables.

$$f_{cr}(\mathcal{D}) = 1 - b_{vpd}\mathcal{D} \quad (63)$$

with $\mathcal{D} = \frac{P_{vapor}^{sat} - P_{vapor}}{1000}$. b_{vpd} is the water-vapor-pressure-deficit constant, given in tables. P_{vapor}^{sat} and P_{vapor} , the saturation and ambient water vapor pressure, are computed with:

$$P_{vapor} = \frac{q_{srf} P_{srf}}{q_{srf} + 0.622(1 - q_{srf})}$$

$$P_{vapor}^{sat} = 610.78 e^{\frac{17.2694T_{srf}}{T_{srf} + 237.29}}$$

And

$$f_{cr}(\psi) = \frac{\psi - \psi_{c2}}{\psi_{c1} - \psi_{c2}} \quad (64)$$

with $\psi = -0.72 - 0.0013SR$ in presence of tall vegetation. Otherwise $\psi = 102(-0395 - 0.043T_{srf})$. If $\psi > \psi_{c1}$ (no water potential stress), $f_{cr}(\psi)$ is set to 1.

Note that if the temperature is out of the limits T_{min} and T_{max} (usually at night), R_{st} is set to ∞ .

- The mesophyll resistance R_m is given in the tables (as function of the species – refer to [16]).
- R_{ac} , the aerodynamic resistance in canopy is computed with

$$R_{ac} = \frac{R_{ac0}LAI^{1/4}}{u_*^2} \quad (65)$$

where the reference value R_{ac0} is to be found in tables, and depends on the LUC category.

- Finally the ground resistance R_g and the cuticular resistance R_{cut} are computed with equation 54.

Meanwhile, if $T_{srf} < -1^\circ\text{C}$, they are multiplied by an empirical coefficient: $e^{-0.2(1+T_{srf})}$.

ComputeZhang

4 Surface emissions

The surface emissions are divided in two parts: the anthropogenic emissions, that come from human activities (transport, industry, etc.), and the biogenic emissions, which are emitted by the vegetation.

4.1 Anthropogenic emissions

They are interpolated from EMEP^{†2} data to a grid with fixed steps along latitude and longitude. The EMEP emissions are adjusted so that, within a given EMEP cell, the ratios of urban emissions and forest emissions upon remaining emissions are equal to 1.6 and 1.2 respectively. They are also multiplied by monthly, daily (especially to adjust the saturday and sunday emissions) and hourly factors. The chemical species are handled as advocated in [7].

ReadEmep, EmepToPolair,
SpeciationAggregation, GridCorrespondences,
ComputeVerticalDistribution

^{†2}Co-operative Programme for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe –www.emep.int/

4.2 Biogenic emissions

They are computed for three species: isoprene, terpenes and NO. As proposed in [10], the biogenic emissions are computed as follows:

$$E_{s,i,j} = \sum_{c=1}^{N_c} \gamma_{s,i,j}(c) d(c) EF_s(c) LUC_{i,j}(c) \quad (66)$$

where N_c is the number of LUC classes, $d(c)$ is the foliar biomass density of the class c , $EF_s(c)$ is the emission factor of the species s for the class c , and $LUC_{i,j}(c)$ is the proportion (in $[0, 1]$) of the class c in the cell. $\gamma_{s,i,j}(c)$ is a correction factor depending on s , c , the temperature and the PAR in the cell (i, j) .

For isoprene, $\gamma = c_l * c_t$, with

$$c_l = \frac{\alpha c_{l1} PAR}{\sqrt{1 + \alpha^2 PAR^2}}$$

where $\alpha = 0.0027$ and $c_{l1} = 1.066$. And

$$c_t = \frac{e^{\frac{c_{t1}(T_{srf} - T_r)}{RT_r T_{srf}}}}{1 + e^{\frac{c_{t2}(T_{srf} - T_m)}{RT_r T_{srf}}}}$$

where $T_r = 303$ K, $T_m = 314$ K, $c_{t1} = 95,000$ and $c_{t2} = 230,000$. T_{srf} is the surface temperature and R the gas constant.

For terpenes, $\gamma = e^{0.09(T_{srf} - T_r)}$.

For NO $\gamma = e^{0.071 T_r^{NO}}$ where

$$T_r^{NO} = \begin{cases} 0.67(T_{srf} - 273.15) + 8.8 & , \quad EF_{NO,c} = 0.9 \\ 0.84(T_{srf} - 273.15) + 3.6 & , \quad \text{otherwise} \end{cases}$$

One can get the emission rates, too:

$$ER_{s,i,j} = \sum_{c=1}^{N_c} d(c) EF_s(c) LUC_{i,j}(c) \quad (67)$$

ComputeBiogenicEmissions, ComputeBiogenicRates

References

- [1] D. W. BYUN AND J. K. S. CHING, eds., *Science algorithms of the EPA models-3 community multiscale air quality (CMAQ) modeling system*, EPA, 1999.

- [2] J. CHANG, R. BROST, I. ISAKEN, S. MADRONICH, P. MIDDLETON, W. STOCKWELL, AND C. WALCEK, *A three-dimensional eulerian acid deposition model: physical concepts and formulation*, Journal of Geophysical Research, 92 (1987), pp. 14,681–14,700.
- [3] ESQUIF, *Étude et simulation de la qualité de l'air en île de France – rapport final*, June 2001.
- [4] J.-F. LOUIS, *A parametric model of vertical eddy fluxes in the atmosphere*, Boundary-Layer Meteorology, 17 (1979), pp. 187–202.
- [5] S. MADRONICH, *Photodissociation in the atmosphere: 1. actinic flux and the effects of ground reflections and clouds*, Journal of Geophysical Research, 92 (1987), pp. 9,740–9,752.
- [6] V. MALLET AND B. SPORTISSE, *Data processing and parameterizations in atmospheric chemistry and physics: the AtmoData library*, Submitted to Atmospheric Environment, (2005).
- [7] P. MIDDLETON, W. R. STOCKWELL, AND W. P. L. CARTER, *Aggregation and analysis of volatile organic compound emissions for regional modeling*, Atmospheric Environment, 24A (1990), pp. 1,107–1,133.
- [8] T. E. NORDENG, *Parameterization of physical processes in a three-dimensional numerical weather prediction model*, Tech. Rep. 65, Norwegian Meteorological Institute, 1986.
- [9] R. A. PIELKE, *Mesoscale meteorological modeling*, Academic Press, 2nd ed., 2002.
- [10] D. SIMPSON, W. WINIWARTER, G. BÖRJESSON, S. CINDERBY, A. FERREIRO, A. GUENTHER, C. N. HEWITT, R. JANSON, M. A. K. KHALIL, S. OWEN, T. E. PIERCE, H. PUXBAUM, M. SHEARER, U. SKIBA, R. STEINBRECHER, L. TARRASÓN, AND M. G. ÖQUIST, *Inventorying emissions from nature in Europe*, Journal of Geophysical Research, 104 (1999), pp. 8,113–8,152.
- [11] G. L. STEPHENS, *Radiation profiles in extended water clouds. II: parameterization schemes*, Journal of the Atmospheric Sciences, 35 (1978), pp. 2,123–2,132.
- [12] I. TROEN AND L. MAHRT, *A simple model of the atmospheric boundary layer; sensitivity to surface evaporation*, Boundary-Layer Meteorology, 37 (1986), pp. 129–148.
- [13] A. WEISS AND J. M. NORMAN, *Partitioning solar radiation into direct and diffuse, visible and near-infrared components*, Agricultural and Forest Meteorology, 34 (1985), pp. 205–213.

- [14] M. L. WESELY, *Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models*, Atmospheric Environment, 23 (1989), pp. 1,293–1,304.
- [15] L. ZHANG, J. R. BROOK, AND R. VET, *A revised parameterization for gaseous dry deposition in air-quality models*, Atmospheric Chemistry and Physics, 3 (2003), pp. 2,067–2,082.
- [16] L. ZHANG, M. D. MORAN, P. A. MAKAR, J. R. BROOK, AND S. GONG, *Modelling gaseous dry deposition in AURAMS: a unified regional air-quality modelling system*, Atmospheric Environment, 36 (2002), pp. 537–560.