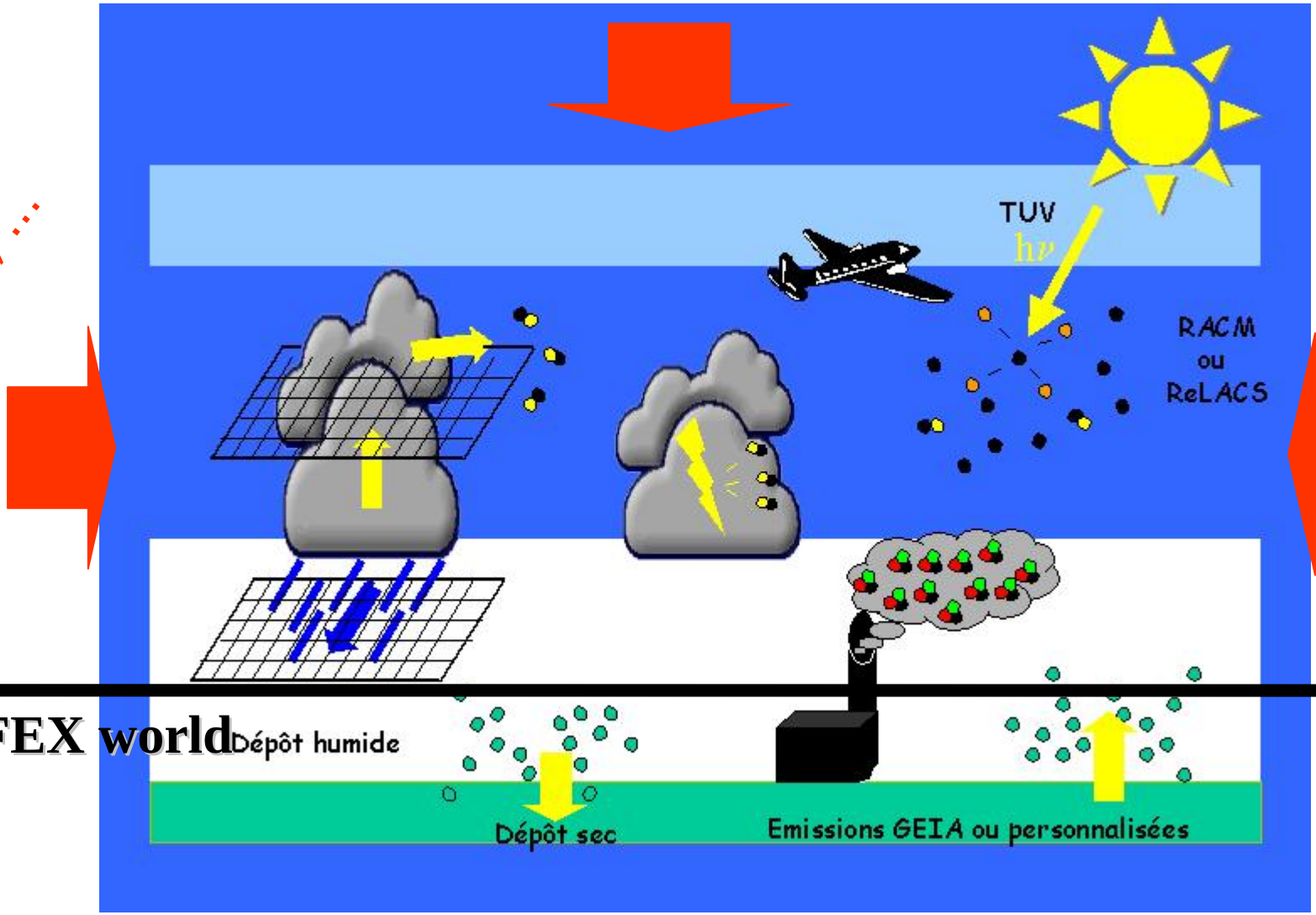
Modelling of atmospheric chemistry from local (dx=1 km) to synoptic scale (dx=50 km)

http://www.aero.obs-mip.fr/mesonh



SURFEX world

1. Surface (SURFEX) – Atmosphere (MESONH–AROME) exchanges

During run, at each timestep

Radiative fluxes
Sun position
Atm. Forcing
Rain, snow fall
Scalars concentrations
Scalars names

Albedo,
Emissivity,
radiative temp.
Momentum fluxes
Heat flux
Water vapor flux
CO2 flux
Chemical fluxes (net emission - deposition)

COUPLING SURF_ATM


SEA LAKE VEGETATIVE TOWN

Atmospheric model MESONH

Surface SURFEX

2. Initiatilisation of Surfex scalar variable

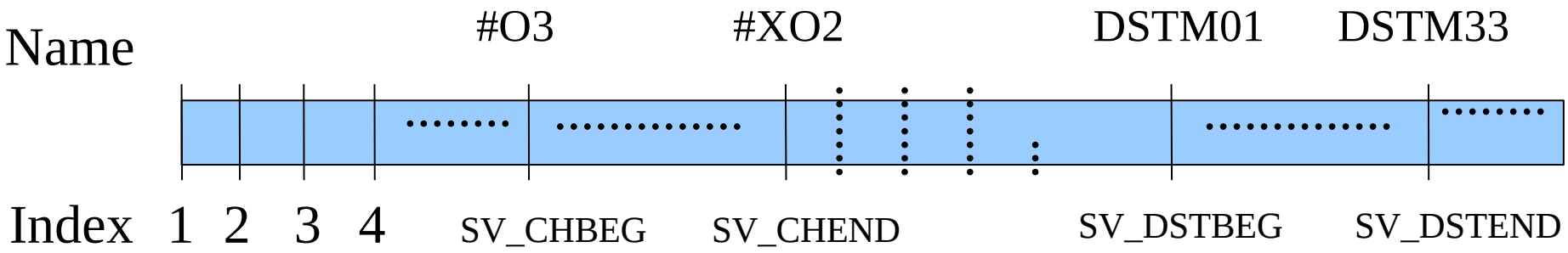
at the first time step

Surfex recognize the parameterisation uses in the atmospheric model using a name convention for scalar variable :

Name started by « # »: Gaseous chemical variable => surface gas chemistry
Name started by « @ » : Aerosol chemical variable => surface aerosol chemistry
Name started by « DST » : Dust aerosol variable => surface dust flux
Name started by « SLT » : Sea Salt aerosol variable => surface sea salt flux

Routines ch_init_names, dst_init_names and slt_init_names will recognize these conventions and initialize the begin and the ending indexes of each type of variable.

Scalar variable vector

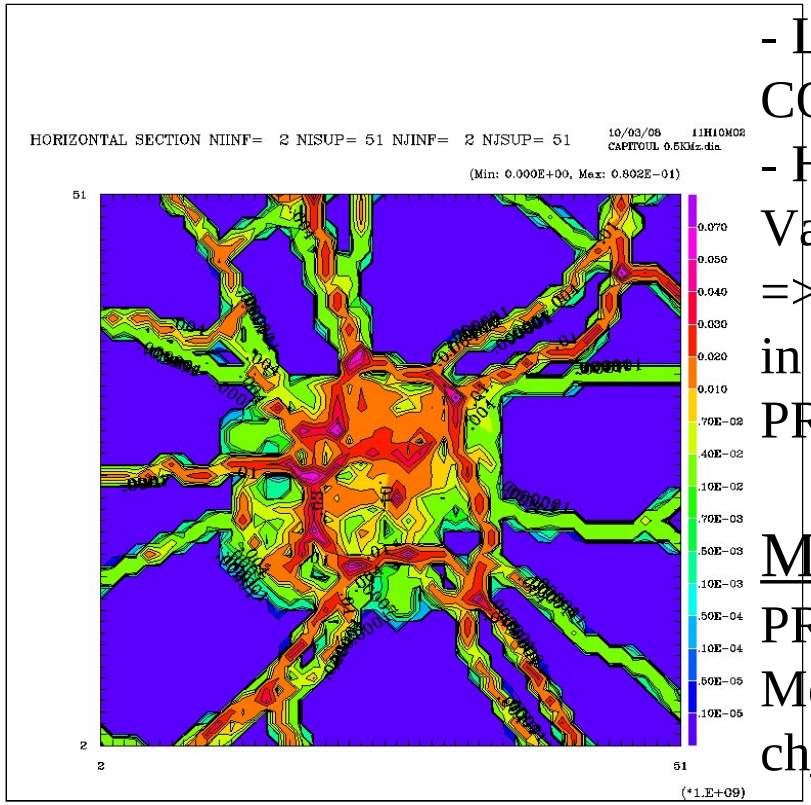


3. Off-line emission

Type : anthropogenic chemical emission.

Pollutants do not stictly depends on meteorological conditions: traffic, industries,...
So they need to be introduced using chemical emission database such as GENEMIS, EDGAR, GEMS, GEIA....

Ex: Toulouse NOx flux



- Large number of primary pollutant: NOx, CO, VOCs, NH3, SO2, aérosols, ..
- High spacial and temporal Variability

=> large number of fields have been interpolated in the simulation domain (done in the PREP_PGD step).

Main code:

PREP_PGD: pgd_chemistry.f90
MesoNH or AROME: ch_buidemissn.f90, ch_emission_fluxn.f90

3. Off-line emission

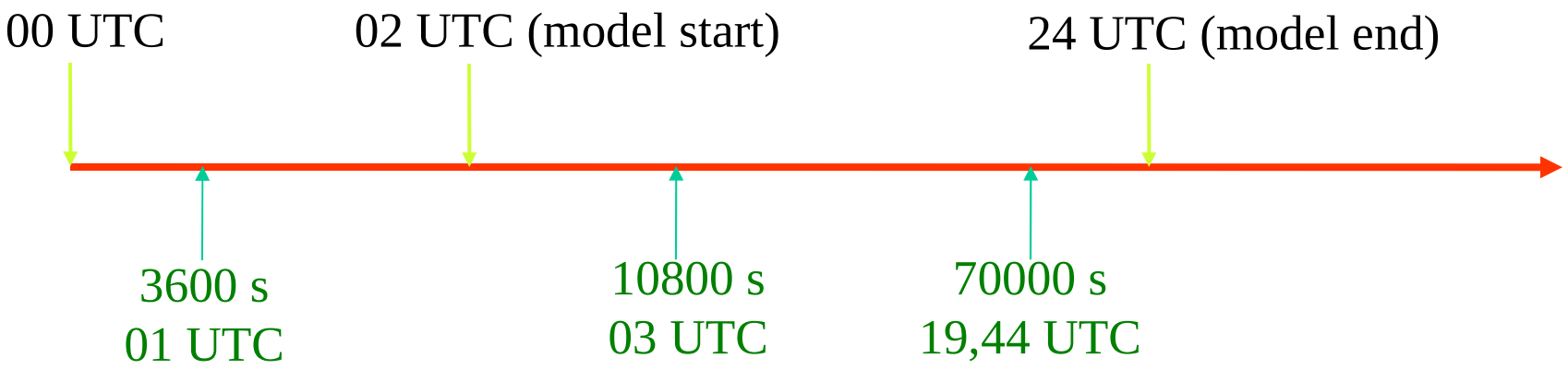
WHERE? in namelist PRE_PGD1.nam (surface field step) :

HOW?

&NAM_CH_EMIS_PGD
NEMIS_PGD_NBR = n , ! Total number of chemical emission fields
CEMIS_PGD_NAME(1) = 'SO2', ! Name of emitted chemical species
CEMIS_PGD_AREA(1) = 'LAN', ! Interpolation on LAND only…
NEMIS_PGD_TIME(1) = 3600, ! Time of the day in seconds
CEMIS_PGD_FILE(1) = 'name of the 1st file',
CEMIS_PGD_FILESTYPE = 'BINLLV', ! File format binary (lat,lon,value)
CEMIS_PGD_NAME(2) = 'SO2', ! Name of emitted chemical species
CEMIS_PGD_AREA(2) = 'SEA', ! Interpolation on SEA only…
NEMIS_PGD_TIME(2) = 7200, ! Time of the day in seconds
CEMIS_PGD_FILE(2) = 'name of the 2nd file',
CEMIS_PGD_FILESTYPE = 'ASCLLV' ! File format ascii (lat, lon, value)
…..
CEMIS_PGD_NAME(n) = 'NOX', ! Name of emitted chemical species
CEMIS_PGD_AREA(n) = 'ALL', ! Interpolation on all pgd domain…
NEMIS_PGD_TIME(n) = 86400, ! Time of the day in seconds
CEMIS_PGD_FILE(n) = 'name of the n file',
CEMIS_PGD_FILESTYPE = 'BINLLV' ! File format
.....
FILESGET_LIST=« emis.tar » ! tar file containing all the emission files (CEMIS_PGD_FILE)

3. Off-line emission

Example: You provide 3 emissions fields at 3600 s, 10800 s and 70000 s



The model will interpolate as follow:

02 UTC < RUN < 03 UTC: temporal interpolation between fields at 3600 s and 7200 s

03 UTC < RUN < 19.44 UTC : temporal interpolation between fields at 7200 s and 70000 s

19.44 UTC < RUN < 24 UTC : temporal interpolation between 70000 s and 3600 s
(return to the first values, if no time values are given after 70000s)

3. Off-line emission

How can I specify the link between emitted and prognostic chemicals ?

WHERE? By an ascii filename which the name is given by CCHEM_SURF_FILE of &NAM_CH_CONTROL in EXSEG1.nam

HOW?

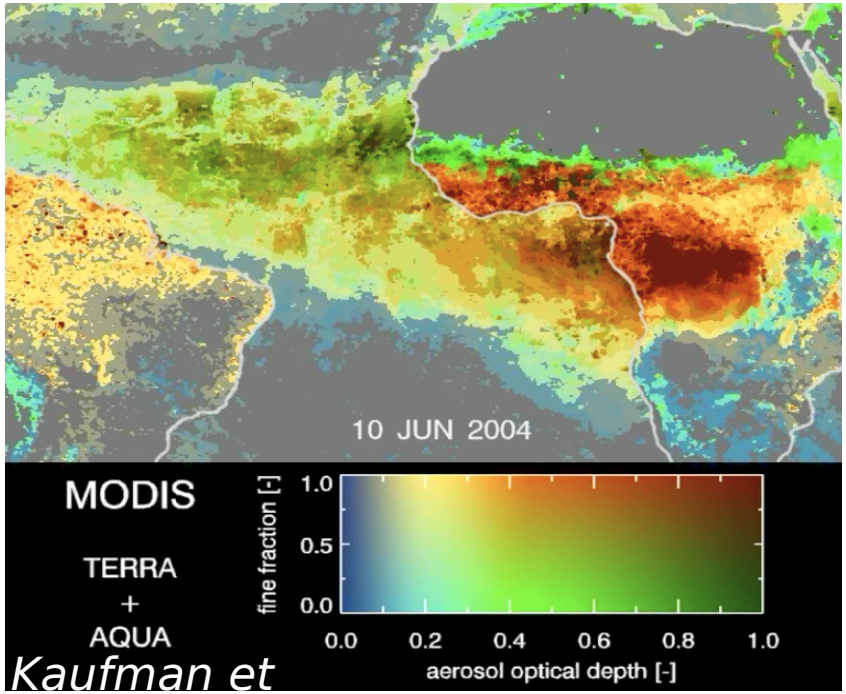
```
EMISUNIT              ! Keyword for off-line emission unit
GENEMIS emission      ! Comment
MIX                   ! Unit (here ppp m/s)

AGREGATION                        ! Keyword for off-line emission agregation
For ReLACS prognostic species     ! Comment
NO   0.8  NOX                     ! Flux of prognostic NO = 0.8 x prescribed flux of NOX
NO2 0.2 NOX                       ! Flux of the prognostic NO2 = 0.2 x prescribed flux of NOX
CO   CO                           ! Flux of prognostic CO = prescribed flux of CO
ALKA  1 HC3H03  1.3 HC8H30 ….
  ! Flux of prognostic ALKA = 1 x prescribed flux of HC3H03 + 1.3 x prescribed flux of HC8H30
END_AGREGATION
```

4. On-line emission

Type: emission that are dependant to meteorology and surface properties. Case of Dust and sea salt aerosols, Biogenics fluxes...
On-line Emission are parameterized are computed at each time step.

Example of dust observed by MODIS

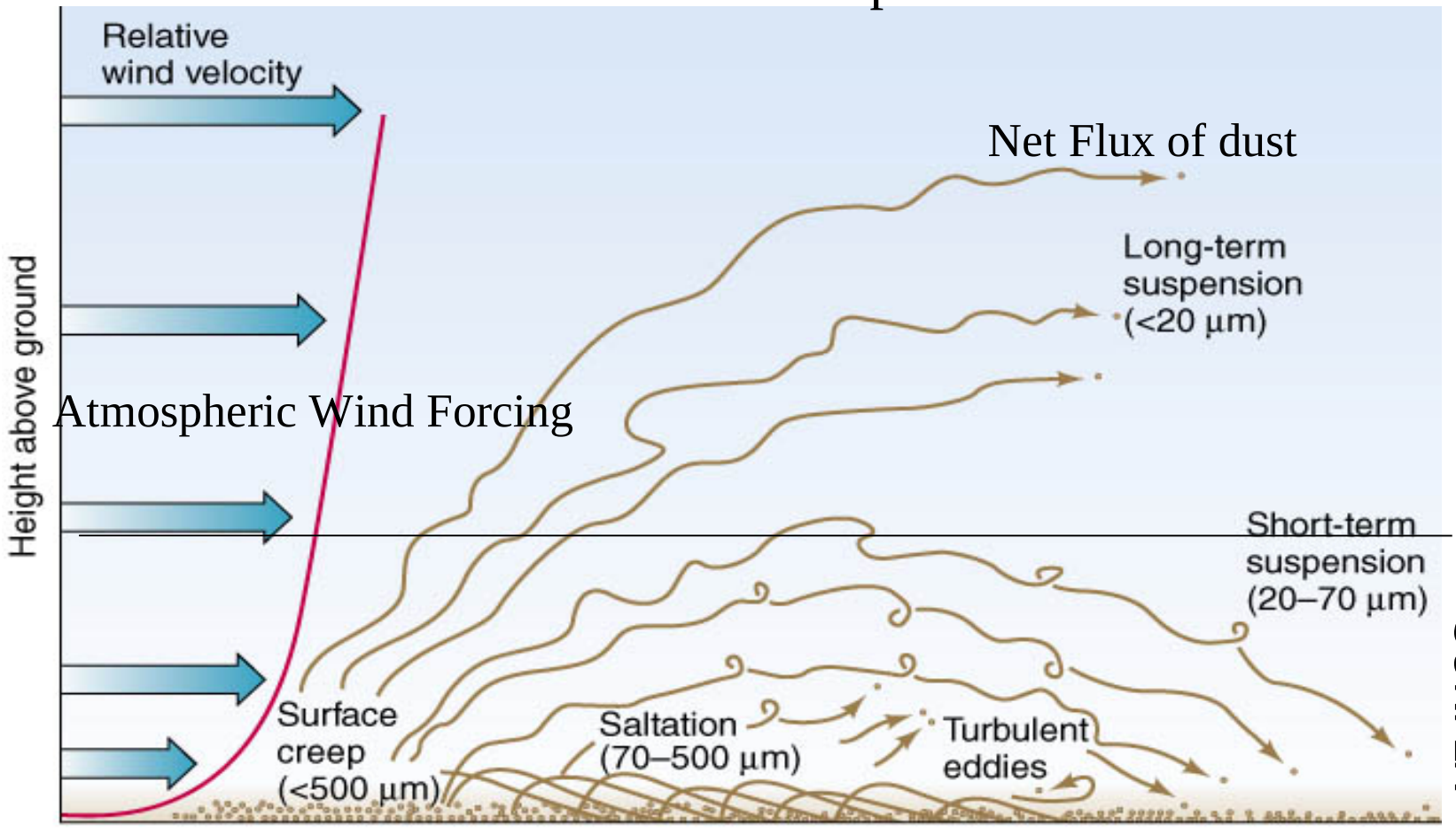


- Dust and Sea Salt paramerization are activated if Dust or Sea Salt names recognize the scalar variables names. But different parameterizations are introduced.

- For biogenics flux a flag exist (see follow)

4. On-line emission

Dust emission case process



Surface properties (soil humidity, soil type, rugosity, vegetation,;..)

Main codes: coupling_dstn.f90, mode_dstmbl.f90, mode_dstmblutl.f90, mode_dst_surf.f90, modd_dst.f90

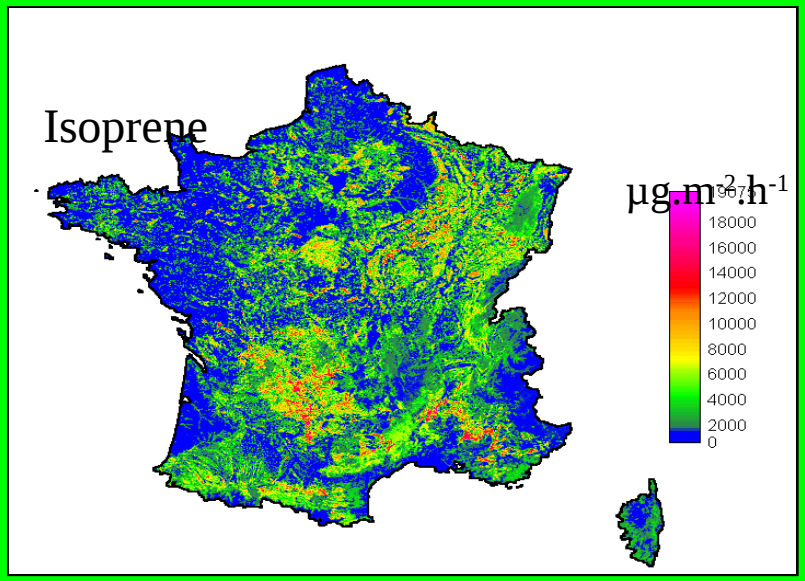
4. On-line emission

From Guenther et al. and Solmon et al, 2004

FLUX bio : F(t) = EP x ECF(t)

EP = Potentiel Emission (offline)

+ Corinne land cover
+ Statitics: Invantory from .French Forest. National.
+ Emission factor for ISOPRENE and MONOTERPENE



Main code: ch_bvocemn.f90

ISBA-Ags

Energy budget and evolution of surface parameters

Patch foret/ grassland / shrublands

T_s , D_s, ρ_a, $[CO_2]$ ...

PAR

Canopy homogeneous

radiation

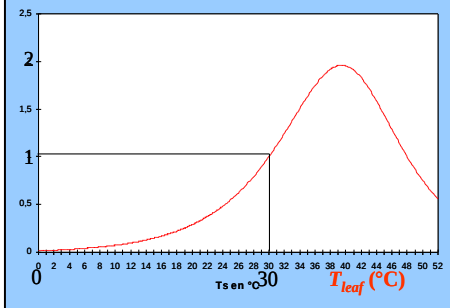
$T_{leaf} = T_s$

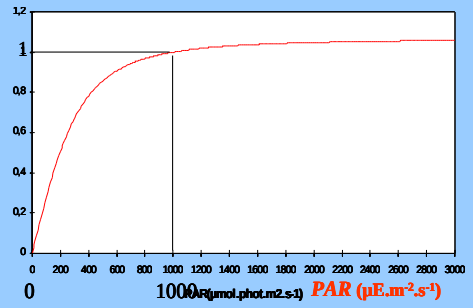
PAR

Correction factor.

$$ECF(t) = C_T\left(T_S(t)\right).\frac{1}{h}\int_0^h C_L\left(\mathrm{PAR}(z,t)\right)\times dz$$

Ex isoprène





4. On-line emission

On-line chemical emissions

Example: You provide potential emission factors for isoprene (ISOPOT) and monoterpene (MONOPOT) that will be used for the calculation of biogenic fluxes at each time step during the model run.

WHERE? in namelist PRE_PGD1.nam (surface field step) :

HOW?

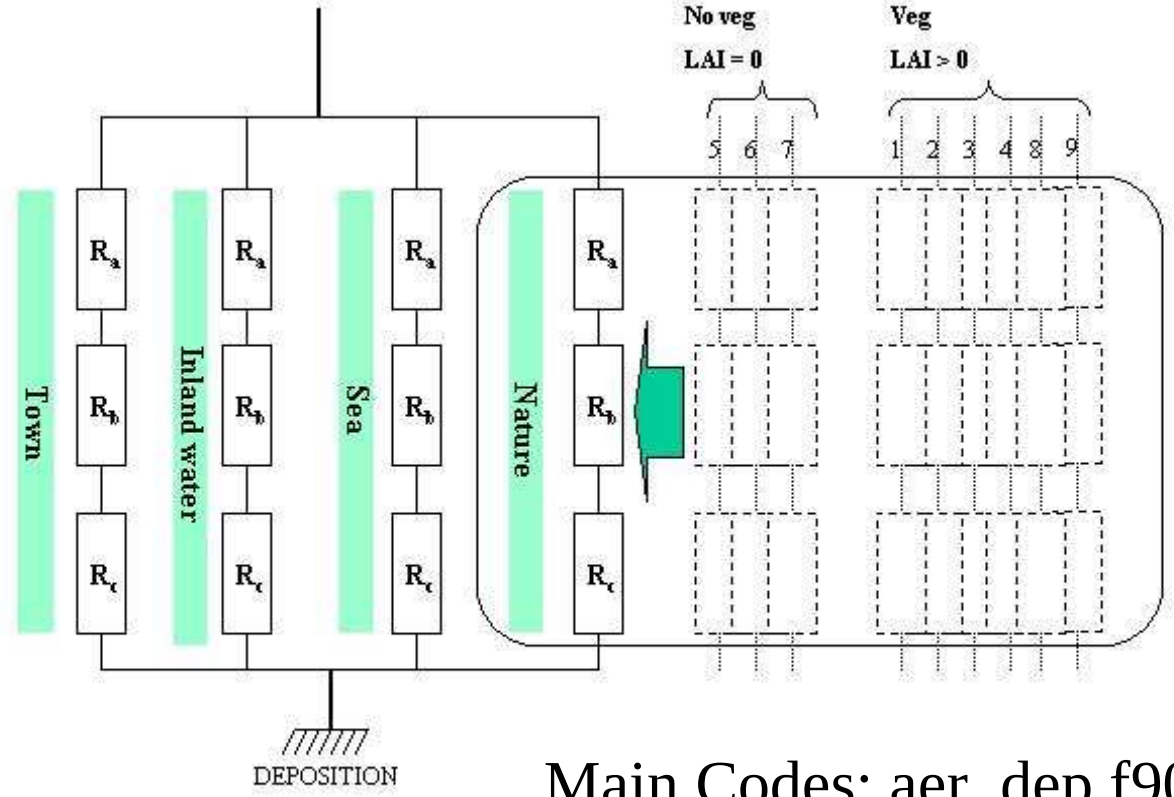
```
&NAM_CH_EMIS_PGD

…..
CEMIS_PGD_NAME(n-1) = ‘ISOPOT’, ! Name of parameters for use in flux calculations
CEMIS_PGD_AREA(n-1) = ‘LAN’, ! Interpolation on all pgd domain…
NEMIS_PGD_TIME(n-1) = -1,          ! Négative values => no time interpolation
CEMIS_PGD_FILE(n-1) = ‘isopot.txt’, ! Name of the file containing 2D map of parameters
CEMIS_PGD_FILESTYPE = ‘ASCLLV’ ,
CEMIS_PGD_NAME(n) = ‘MONOPOT’, ! Name of parameters for use in flux calculations
CEMIS_PGD_AREA(n) = ‘LAN’, ! Interpolation on all pgd domain…
NEMIS_PGD_TIME(n) = -1,
CEMIS_PGD_FILE(n) = ‘monopot.txt’,
CEMIS_PGD_FILESTYPE = ‘ASCLLV’

.....
FILESGET_LIST=« emis.tar isopot.txt monopot.txt»
```

4. Dry deposition

Deposition of aerosol and gas on the surface have been parameterized upon Wesely (1989) scheme.
Caracteritics of gas must be introduced in namelist such as, their solubility (Henry constant), their molecular mass, and their interaction with the biology.
See Seinfeld and Pandis, (2001) for more explanations.



Example of combinaison of dry deposition resistance for each surface type of surfex

Main Codes: aer_dep.f90, and ch_dep.f90

4. Dry deposition:
How can I specify parameters for dry deposition ?

WHERE? MNHC_INPUT.nam

HOW?

```
SURFVALU                    ! Keyword for prescribed surface value (flux = surfvalu x exchgvel)
value at the surface are set to zero expect DMS (unit are ppp) ! Comment
1                           ! number of prognostic species with prescribed surf value
(1X, A12,1X,F5.1)           ! Format
‘DMS        ‘   1E-12       ! Name of prognostic variable and associated surf value

EXCHGVEL                    ! Keyword for prescribed exchange velocity (flux = surfvalu x exchgvel)
Exchange velocity in m/s    ! Comment
1                           ! Number of prognostic variable with prescribed exchange velocity
(1X, A12,1X,F5.1)           ! Format
‘O3         ‘   0.004       ! Name of prognostic variable and corresponding exchange velocity

SURF_RES                    ! Keyword for surface resistance (for use with Wesely dep scheme)
Wesely surface resistance values (if none default values are used) ! Comment
1                           ! Number of surface resistance
(1X, A12,1X,F5.1)           ! Format
‘LANDEXT      ‘   150.      ! Keyword for surface resistance and corresponding value
```

4. Dry depostion:
How can I specify parameters for dry deposition – (continuing) ?

WHERE? MNHC_INPUT.nam

HOW?

```
MASS_MOL                          ! Keyword for molecular mass
Molecular mass (g/mol)            ! Comment
1                                 ! Number of prognostic species for which molecular mass is prescribed
(1X, A12,1X,F5.1)                 ! Format
'O3           ' 48.00             ! Name of prognostic variable and corresponding molecular mass

REA_FACT                          ! Keyword for reactivity factor
Reactivity factor with biology    ! Comment
1                                 ! Number of prognostic species
(1X, A12,1X,F5.1)                 ! Format
'O3           '  1.               ! Name of prognostic variable and corresponding reactivity factor

HENRY_SP                          ! Keyword for Henry's law constant
Henry specific constant           ! Comment
1                                 ! Number of prognostic species
(1X, A12,1X,E15.2,1X,F8.0)        ! Format
'O3           '  1.1E-2  '  -2300. ! Name of prognostic variable and corresponding values
```

5. Surface (SURFEX) chemical parameterization:
How do I specify options for dry deposition and emissions?

WHERE? EXSEG1.nam splits into SURF1.nam:

HOW?

&NAM_CH_SURFn LCH_SURF_EMIS = .TRUE ., Switch for off-line chemistry emissions
CCHEM_SURF_FILE = « MNHC_INPUT.nam »
Input file containing chemistry parameters (see after)

&NAM_CH_ISBAn CCH_DRY_DEP = « WES89 » , Wesely deposition scheme on biosphere
LCH_BIO_FLUX=.TRUE. Switch for on-line biogenic emission

&NAM_CH_WATFLUXn CCH_DRY_DEP = « WES89 » Wesely deposition scheme on lakes
&NAM_CH_SEAFLUXn CCH_DRY_DEP = « WES89 » Wesely deposition scheme on sea
&NAM_CH_TEBn CCH_DRY_DEP = « WES89 » Wesely deposition scheme on town

&NAM_SURF_DST CEMISPARAM = « AMMA »
Parameterization type for on-line emission of dust aerosols

&NAM_CHS_ORILAM LCH_AERO_FLUX=.TRUE., Switch for on-line aerosol emission - ORILAM
XEMISRADIUSI = 0.005, First mode: emission mean radius in micrometers
XEMISRADIUSJ= 0.1, 2nd mode: emission mean radius in micrometers
XEMISSIGI= 1.89, First mode: emission standard deviation
XEMISSIGJ=2.02, 2nd mode: emission standard deviation
LCO2PM=.TRUE
Switch for conversion of CO emission to BC/POM emission
(in case no off-line emissions are provided for BC and POM precursors) .