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Adding Species to model and output

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Adding Species

Species are listed in `CM_ChemSpecs_ml.f90`

Advected (IAXDV) , Short lived (IXSHL) and total.

Ex: SO2

, IXADV_SO2 = 52 & in advected

, SO2 = 68 & in total

Listed in species array (type Chemical)

species(SO2) =

Chemical("SO2", 64.00, 0, 0, 0, 1, 0.0, 0.000, 0.0)

Name

molw

nmhc

carbons

nitrogens

sulphurs

ExtC

CiStar

DeltaH



Reactions

Handled in **Solver_ml.f90**

CM_Reactions1.inc

The chemistry is iterated several times, more iterations closer to the ground than in the higher layers, example SO₂

!-SO₂

P = &

rcemis(SO₂,k)

L = &

2e-12*AQRCK(ICLOHSO₂,K)* xnew(OH) &

+ AQRCK(ICLRC1,K)* xnew(H₂O₂) &

+ AQRCK(ICLRC2,K)* xnew(O₃) &

+ AQRCK(ICLRC3,K)

xnew(SO₂)= (xold(SO₂) + dt2 * P) / (1.0 + dt2*L)



Reactions

Handled in **Solver_ml.f90**

CM_Reactions2.inc

Simpler reactions, or species with no chemical reactions that only need one iteration per chemical time step, example SeaSalt_f (emissions are handled in the module **SeaSalt_ml.f90**)

!-> SEASALT_F

P = &

rcemis(SEASALT_F,k)

! L = 0.0

xnew(SEASALT_F)= xold(SEASALT_F) + dt2 * P



Wet deposition

CM_WetDep.inc

```
, depmap( IXADV_SO2, CWDEP_SO2, -1) &  
, depmap( IXADV_SeaSalt_f, CWDEP_SSf, -1) &
```

Can assume specie to fall with an already established CWDEP, ex. CWDEP_PMf, or define your own in **Aqueous_n_WetDep_ml.f90**,

```
WetDep(CWDEP_SO2) = WScav( w_sca w_sub 0.3, 0.15)  
WetDep(CWDEP_SSf) = WScav( 1.6, EFF25)
```



Dry Deposition

CM_DryDep.inc

, depmap(IXADV_SO2, CDDEP_SO2, -1) &

, depmap(IXADV_SeaSalt_f, CDDEP_PMfS, -1) &

Can assume specie to fall with an already established CDDEP, ex. CDDEP_PMf

If you want to define you own CDDEP, this can be done in **Wesely_ml.f90** and **My_Aerosol_ml.f90**



Add Output

- `_fullrun.nc` The result of the whole run
- `_month.nc` Monthly results for the months in the run
- `_day.nc` Daily results for the days in the run

Output for these files are handled by the modules
My_Derived_ml and **Derived_ml**

- `_hour.nc` Hourly output
- `sites/sondes_2010.csv` Output from site and sondes

Output for these files are handled by the modules
My_Outputs_ml and **Output_hourly**

Both **My_Derived_ml** and **My_Output_ml** defines the output you want, and **Derived_ml** and **Output_hourly** sets up the species and groups for the output requested.



My_Derived_ml.f90

For surface concentrations in OutputConcs array

Ex: SURF_ug_PM10

Unit of

output

```
,typ_s5i("PM10 ", "ug ", D2,"AIR_CONCS", GROUP, D)&
```

D2: Surface concentrations

D3: All vertical layers and surface .

D: Output in _day.nc, _month.nc and fullrun.nc

M: Output in _month.nc and fullrun.nc

Column output are set with the two arrays:

COLUMN_MOLEC_CM2 and COLUMN_LEVELS. The units are molec/m², but can be changed in **Derived_ml.f90**

Ex: NO2 column over all 20 layers

COLUMN_COMPONENT_NLAYERS → COLUMN_NO2_k20



Dry and wet deposition are set by the arrays DDEP_WANTED and WDEP_WANTED. (Remember also the landtype for dry deposition)

```
typ_s3("SOX", GROUP, "mgS"), &
```

name

GROUP/SPEC

unit

See more in the UserGuide!

For other output ex meteorological variables, see the array D2_extra in **My_Derived_ml** and other examples in **Derived_ml** by using AddNewDeriv.



Hourly Output

My_Outputs_ml.f90

Output for **sites** and **sondes** are set in SITE_ADV, SITE_XTRA_MISC, SITE_XTRA_D2D. By default everything is set as output!

Hourly output in _hourly.nc is set by setting **nhourly_out** to the number of fields you want and **hr_out** to the field. See examples for other species.

There are preset a lot of output for different modes of the model. The mode for opensource is default. Look at examples.