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Aerosols
in the EMEP MSC-W model

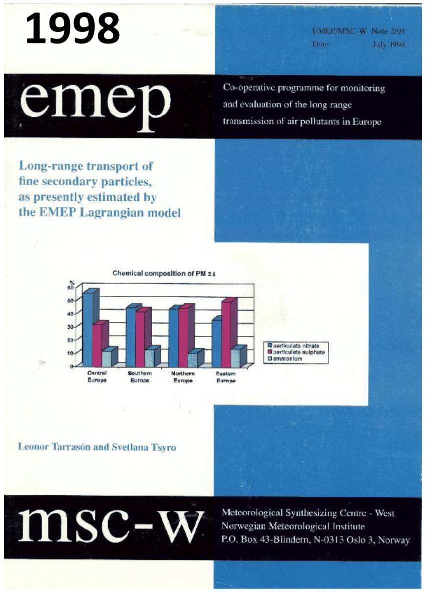
By Svetlana Tsyro

EMEP/MSC-W model training course,

24-26 April 2013

PM history in the EMEP

1998



EMEP/MSC-W Note 2/98
Date: July 1998

emep

Co-operative programme for monitoring
and evaluation of the long range
transmission of air pollutants in Europe

Long-range transport of
fine secondary particles,
as presently estimated by
the EMEP Lagrangian model

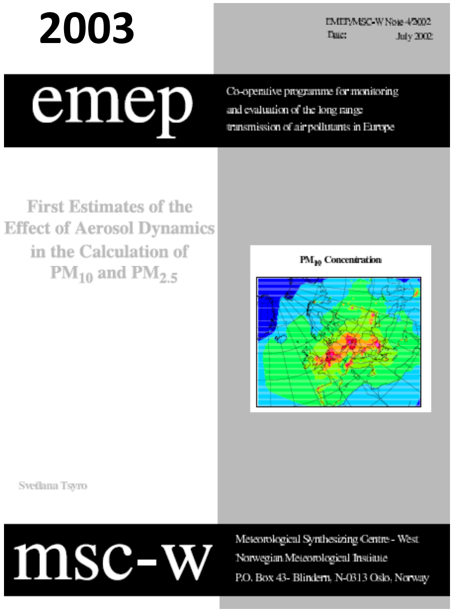
Leonor Tarrasón and Svetlana Tsyro

msc-w

Meteorological Synthesizing Centre - West
Norwegian Meteorological Institute
P.O. Box 43-Blindern, N-0313 Oslo 3, Norway

PM expert workshop (2000):
*** PPM10 & PM2.5 health effect**
*** Unclear which PM characteristics are responsible … mass, number, surface area…**

2003



EMEP/MSC-W Note 4/2002
Date: July 2002

emep

Co-operative programme for monitoring
and evaluation of the long range
transmission of air pollutants in Europe

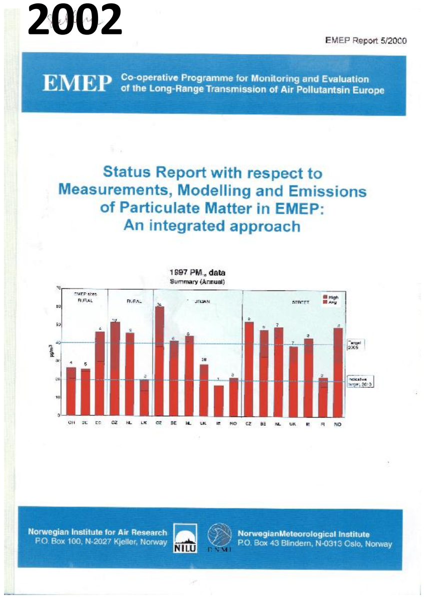
First Estimates of the
Effect of Aerosol Dynamics
in the Calculation of
PM_{10} and $PM_{2.5}$

Svetlana Tsyro

msc-w

Meteorological Synthesizing Centre - West
Norwegian Meteorological Institute
P.O. Box 43- Blindern, N-0313 Oslo, Norway

2002



EMEP Report 5/2000

EMEP Co-operative Programme for Monitoring and Evaluation
of the Long-Range Transmission of Air Pollutantsin Europe

Status Report with respect to
Measurements, Modelling and Emissions
of Particulate Matter in EMEP:
An integrated approach

Norwegian Institute for Air Research
P.O. Box 100, N-2027 Kjeller, Norway
NILU
DNMI
NorwegianMeteorological Institute
P.O. Box 43 Blindern, N-0313 Oslo, Norway

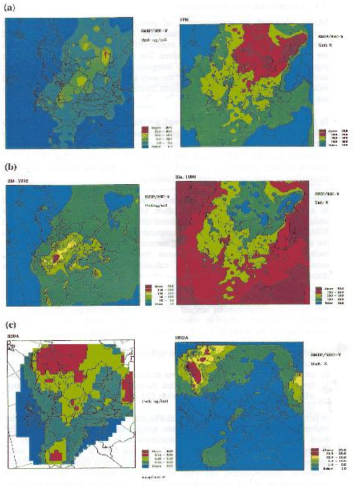


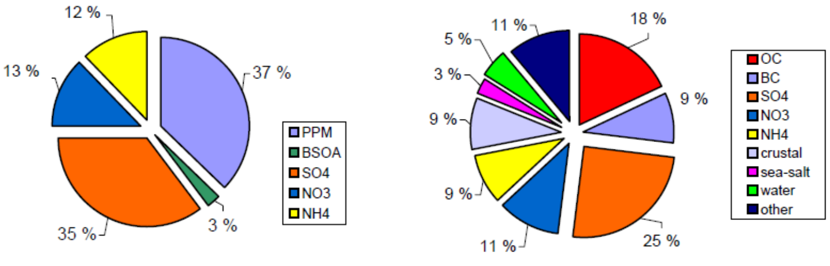
Figure 3.2: Annual mean concentrations and relative contributions to the total PM concentrations from: (a) primary PM_{10}, (b) secondary inorganic aerosols, and (c) biogenic secondary organic aerosols.

EMEP modelled PM_{10}

Measurements PM

Helsinki (rural)

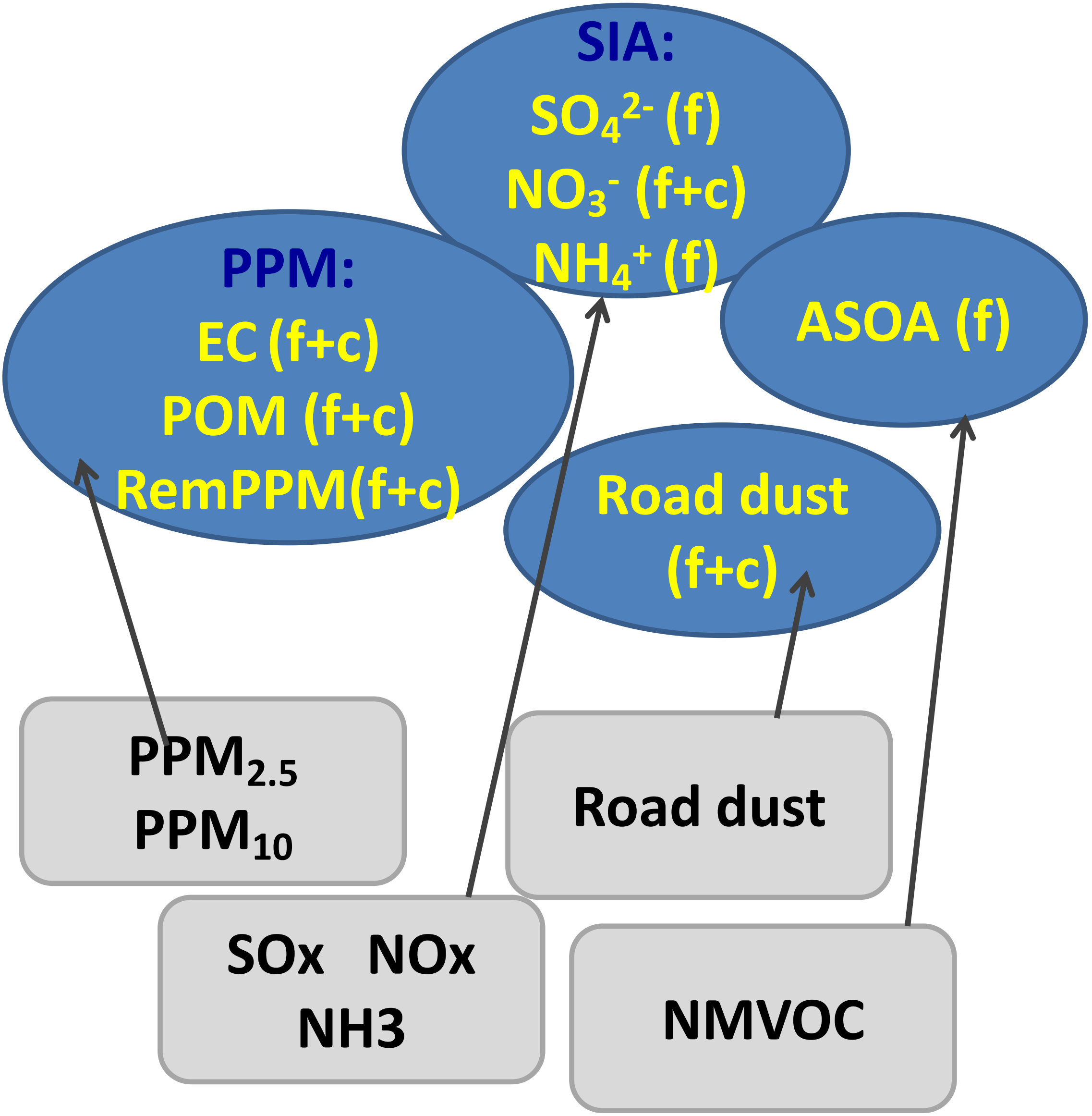
(Pakkanen et al., 1999)



1998 yearly aver. PM_{10} conc. = 3.5 $\mu g/m^3$

Apr-96/Jun-97 aver. $PM_{2.5}$ conc. = 7.8 µ

Aerosols and their sources….



SIA:
SO_4^{2-} (f)
NO_3^- (f+c)
NH_4^+ (f)

PPM:
EC (f+c)
POM (f+c)
RemPPM(f+c)

ASOA (f)

Road dust (f+c)

$PPM_{2.5}$
PPM_{10}

Road dust

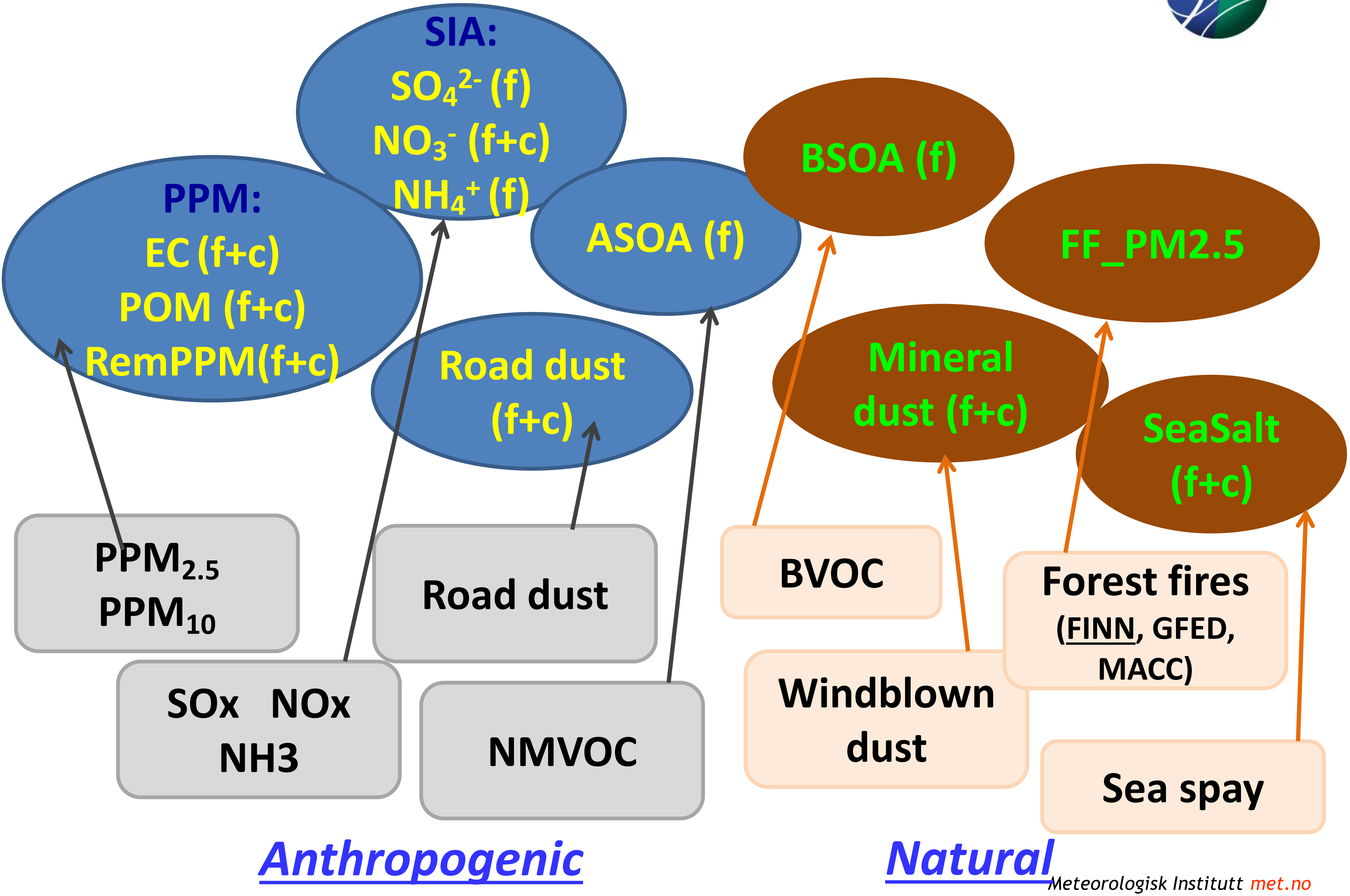
SOx NOx
NH3

NMVOC

Anthropogenic

SIA - Secondary Inorganic Aerosols
PPM – Primary Particulate Matter
EC – Elemental Carbon
POM – Primary Organic Matter (Aerosol)
ASOA/BSOA – Anthropogenic/Biogenic Secondary Aerosols

Aerosols and their sources….



SIA:
SO_4^{2-} (f)
NO_3^- (f+c)
NH_4^+ (f)

PPM:
EC (f+c)
POM (f+c)
RemPPM(f+c)

ASOA (f)

Road dust (f+c)

BSOA (f)

FF_PM2.5

Mineral dust (f+c)

SeaSalt (f+c)

$PPM_{2.5}$
PPM_{10}

Road dust

SOx NOx
NH3

NMVOC

BVOC

Forest fires
(FINN, GFED, MACC)

Windblown dust

Sea spay

Anthropogenic

Natural

Aerosol formation

Fine	Coarse	Formation	Modules
SO_4^{2-}	**-**	SO_2 gas/aqueous oxidation **(pH)**	**CM_Reactions2.inc**
NO_3^-	**NO_3^-**	Equilibrium (NH_4NO_3) HNO3 -> coarse NO3	**MARS_ml.f90** **CM_Reactions2.inc**
NH_4^+	**NH_4^+**	$(NH_4)_xSO_4$ + Equilibrium (NH_4NO_3)	**MARS_ml.F90**
EC	**EC**	PPM fraction (IIASA) EC ageing, Inert	**emissplit.specials.pm25** **emissplit.defaults.pmco** **ChemFunctions_ml.f90**
POM	**POM**	PPM fraction (IIASA); Inert	**emissplit.specials.pm25** **emissplit.defaults.pmco**
ASOA	**-**	VBS approach **- DAVE**	**My_SOA_ml.f90**
BSOA	**-**	VBS approach **- DAVE**	**My_SOA_ml.f90**
Sea salt	**Sea salt**	Source function (u10, Twater) Tsyro et al, ACP, 2011	**SeaSalt_ml.f90**
Anth. dust	**Anth. Dust**	Remaining PPM (IIASA) + Road dust	**Emissions_ml.f90**
Min. Dust	**Min. Dust**	Windblown (Martecorena et al. 1997) Saharan dust as bound. condition	**DustProd_ml.f90** **CTM-UiO (monthly 2000)**
PM water	**-**	Diagnostic **(SIA)**	**MARS_ml.f90**

Dry Deposition

Modules	Action	Details
DryDep_ml.f90	DryDep for each landuse (LU)	
Aero_Vds_ml.f90	DryDep velocities for a set of aerosol diameters and LUs	**real, .. dimension (NSIZE) :: &** **diam = (/ 0.33e-6, 3.0e-6,** **4.0e-6, 4.5e-6 ,22e-6 /)**
My_Aerosols_ml.f90	Number of diameters for Vd	**NSIZE=5**
Wesely_ml.f90	Mapping DryDep velocities (**PMfS, PMfN, PMc, SSc, DUc**) to diameters in Aero_Vds_ml	**.., dimension (CDDEP_PMfS: CDDEP_POLLd), parameter::** **& AERO_SIZE = (/ 1, 1, 2, 3, 4, 5/)**
CM_DryDep.f90	Mapping species & dry deposition velocities	

DryDep_ml.f90

$$V_\mathrm{d}(z) = \frac{v_\mathrm{s}}{1 - e^{-r(z)v_\mathrm{s}}} \qquad (70)$$

Venkratram & Pleaim (1999)

where v_s is settling velocity, $V_\mathrm{d}(z)$ is the deposition velocity at height z, and $r(z)$ is the sum of the aerodynamic resistance and inverse V_ds.

Vds - quasi-laminar layer resistance for differenf landuse types, stability dependent (Aero_Vds_ml.f90)

Dry Deposition

Aero_Vds_ml.f90

```
real, public, parameter, dimension(NSIZE) ::   &
        diam   = (/ 0.33e-6,  3.0e-6,  4.0e-6,  4.5e-6 ,   22e-6 /),
```

Wesely_ml.f90

```
integer, public, parameter :: NDRYDEP_AER = 6        ! aerosols

integer, public, parameter :: NDRYDEP_CALC = NDRYDEP_GASES + NDRYDEP_AER

integer, public, parameter :: CDDEP_PMfS= 12, CDDEP_PMfN= 13, CDDEP_PMc  = 14, &
                                        CDDEP_SSc = 15, CDDEP_DUc = 16, CDDEP_POLLd= 17

integer, dimension(CDDEP_PMfS : CDDEP_POLLd), public, parameter :: &
                                AERO_SIZE = (/ 1, 1, 2, 3, 4, 5/)   !! Corresponds «diam» in Aero_Vds
                                    !1=fine,2=coarse,3=coarse sea salt, 4=dust, 5 = pollen
```

CM_DryDep.f90

```
*) type(depmap), public,  dimension(NDRYDEP_ADV), parameter::          &
        DDepMap= (/  depmap( IXADV_SO4,            CDDEP_PMfS,   -1)       &
                   , depmap( IXADV_NO3_f,          CDDEP_PMfN,  -1)        &
                   , depmap( IXADV_NO3_c,          CDDEP_PMc,    -1)       &
                   , depmap( IXADV_SeaSalt_c,      CDDEP_SSc,     -1)      &
                   , depmap( IXADV_Dust_sah_c,  CDDEP_DUc,      -1)
```

Wet Deposition

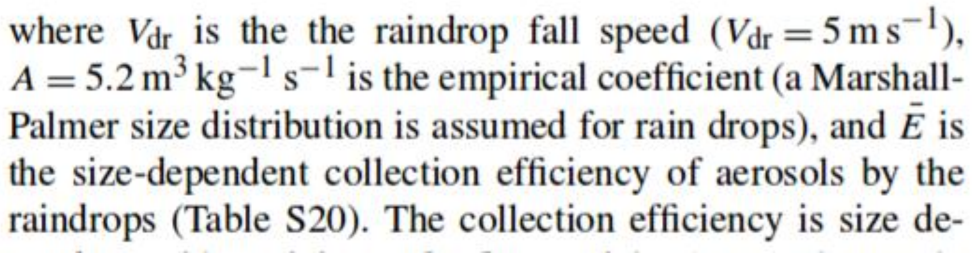
In cloud

$$S_{\mathrm{in}} = -\chi \frac{W_{\mathrm{in}} P}{h_s \rho_w}$$

W$_{\mathrm{in}}$ – scavenging ratio (reflects solubility)

Below cloud

$$S_{\mathrm{sub}}^{\mathrm{aer}} = -\chi \frac{A\ P}{V_{\mathrm{dr}}} \bar{E}$$



where V_{dr} is the the raindrop fall speed ($V_{\mathrm{dr}} = 5\,\mathrm{m\,s^{-1}}$), $A = 5.2\,\mathrm{m^3\,kg^{-1}\,s^{-1}}$ is the empirical coefficient (a Marshall-Palmer size distribution is assumed for rain drops), and $\bar{E}$ is the size-dependent collection efficiency of aerosols by the raindrops (Table S20). The collection efficiency is size de-

W$_{\mathrm{in}}$ E

Modules	Action	Details
Aqueous_n_WetDep_ml.f90	Sets: in-cloud, sub-cloud scavenging rates *(accounting for solubility, size)*	**WetDep(CWDEP_SO4) = WScav(1.0, EFF25)** **WetDep(CWDEP_ECfn) = WScav(0.05, EFF25)** **WetDep(CWDEP_SSf) = WScav(1.6, EFF25)** **WetDep(CWDEP_SSc) = WScav(1.6, EFFCO)** **WetDep(CWDEP_PMf) = WScav(1.0, EFF25)** **WetDep(CWDEP_PMc) = WScav(1.0, EFFCO)**

Wet Deposition

Modules	Action	Details
Aqueous_n_WetDep_ml.f90	Sets: in-cloud, sub-cloud scavenging rates *(accounting for solubility, size)*	**WetDep(CWDEP_SO4) = WScav(1.0, EFF25)** **WetDep(CWDEP_ECfn) = WScav(0.05, EFF25)** **WetDep(CWDEP_SSf) = WScav(1.6, EFF25)** **WetDep(CWDEP_SSc) = WScav(1.6, EFFCO)** **WetDep(CWDEP_PMf) = WScav(1.0, EFF25)** **WetDep(CWDEP_PMc) = WScav(1.0, EFFCO)**
include 'CM_WetDep.inc'	Mapping species & Wet scavenging rates	

```
type(depmap), public, dimension(NWETDEP_ADV), parameter   ::
        WDepMap=    (/ &
            depmap( IXADV_SO4,                  CWDEP_SO4, -1)  &
          , depmap( IXADV_NO3_f,                CWDEP_PMf, -1)  &
          , depmap( IXADV_NO3_c,                CWDEP_PMc, -1)  &
          , depmap( IXADV_POM_f_WOOD,           CWDEP_PMf, -1)  &
          , depmap( IXADV_EC_f_FFUEL_new,       CWDEP_ECfn, -1) &
          , depmap( IXADV_EC_f_FFUEL_age,       CWDEP_PMf, -1)  &
          , depmap( IXADV_EC_c_FFUEL,           CWDEP_PMc, -1)  &
          , depmap( IXADV_Dust_wb_f,            CWDEP_PMf, -1)  &
          , depmap( IXADV_Dust_wb_c,            CWDEP_PMc, -1)  &
```

«Tricky» stuff: PM

$PM_{2.5}$ = PM_Fine + fracPM25 * coarse_NO3

PM_{10} = $PM_{2.5}$ + sum of Coarse aerosols

CM_ChemGroups_ml.f90

```
  integer, public, target, save, dimension (15) ::        PMFINE_GROUP    =    &
(/SO4,NO3_F,NH4_F,PART_OM_F,EC_F_WOOD_NEW,EC_F_WOOD_AGE,EC_F_FFUEL_NEW,
EC_F_FFUEL_AGE,REMPPM25,FFIRE_BC,FFIRE_REMPPM25,SEASALT_F,DUST_ROAD_F,DUST
_WB_F,DUST_SAH_F /)
```

Also groups **PM10, SIA, PPM25, PPMco, SS, DUST…….**

..even more tricky stuff

Derived_ml.f90:

PM25_rh50 and **PM10_rh50** *- at Rh=50% and T= 20C for comparison with observations (Tsyro, ACP, 2004)*

PM25X_rh50 = PM_Fine + fracPM25 * coarse (NO3+EC+POM)

Some «advanced» stuff:

AOD and 3D extinction coefficients are included in the model, but those are still under development and testing ("False" as default) – to be updated soon

Using mass specific extinction efficiencies. Implicit accounting for aerosol effective radius for light extinction (cross-section weighted) and the effect of air humidity.

Encouragement for testing and development

- ✓ **Mineral dust** (windblown, agricultural)
- ✓ **Coarse NO_3** (on sea salt and dust),
  ….also **coarse SO4**
- ✓ **NO_3NO_4** – equilibrium models aren’t doing
  too good works for warm seasons
- ✓ **Dry Deposition** (for different landuse, stability…)
- ✓ **Wet Deposition**
- ✓ **Aerosol optics** – AOD, extinction
- ✓ **Size-resolved aerosol, aerosol dynamics**

That was about aerosols in the EMEP MSC-W model in a nutshell

Relevant publications:

D. Simpson, A. Benedictow, H. Berge, R. Bergström, L. D. Emberson, H. Fagerli, C. R. Flechard, G. D. Hayman, M. Gauss, J. E. Jonson, M. E. Jenkin, A. Nyíri, C. Richter, V. S. Semeena, S. Tsyro, J.-P. Tuovinen, Á. Valdebenito, and P. Wind (2012). The EMEP MSC-W chemical transport model – technical description. Atmos. Chem. Phys., 12, 7825-7865, 2012.

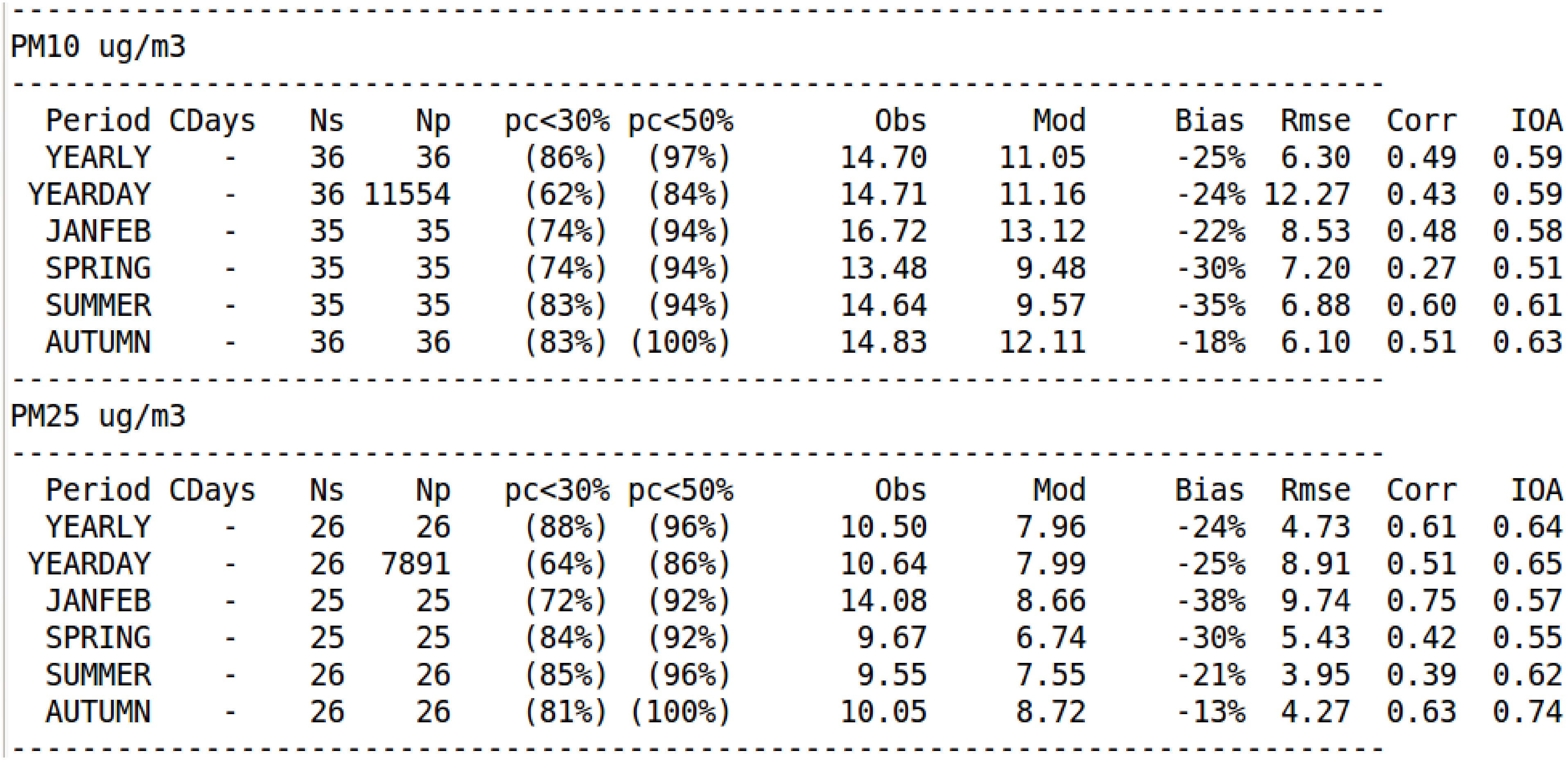
Tsyro, S, Aas, W., Soares, J., Sofiev, M., Berge, H., and G. Spindler (2011). Modelling of sea salt pollution over Europe: key uncertainties and comparison with observations. Atmos. Chem. Phys., 11, 10367-10388, 2011.

Tsyro, S. (2005). To what extent can aerosol water explain the discrepancy between model calculated and gravimetric PM10 and PM2.5?. Atmos. Chem.. Phys., 5, 602, 1-8, 2005.

W. Aas, S. Tsyro, E. Bieber, R. Bergström, D. Ceburnis, T. Ellermann, H. Fagerli, M. Frölich, R. Gehrig, U. Makkonen, E. Nemitz, R. Otjes, N. Perez, C. Perrino, A. S. H. Prévôt, J.-P. Putaud, D. Simpson, G. Spindler, M. Vana, and K. E. Yttri (2012). Lessons learnt from the first EMEP intensive measurement periods. Atmos. Chem. Phys., 12, 8073-8094, 2012.

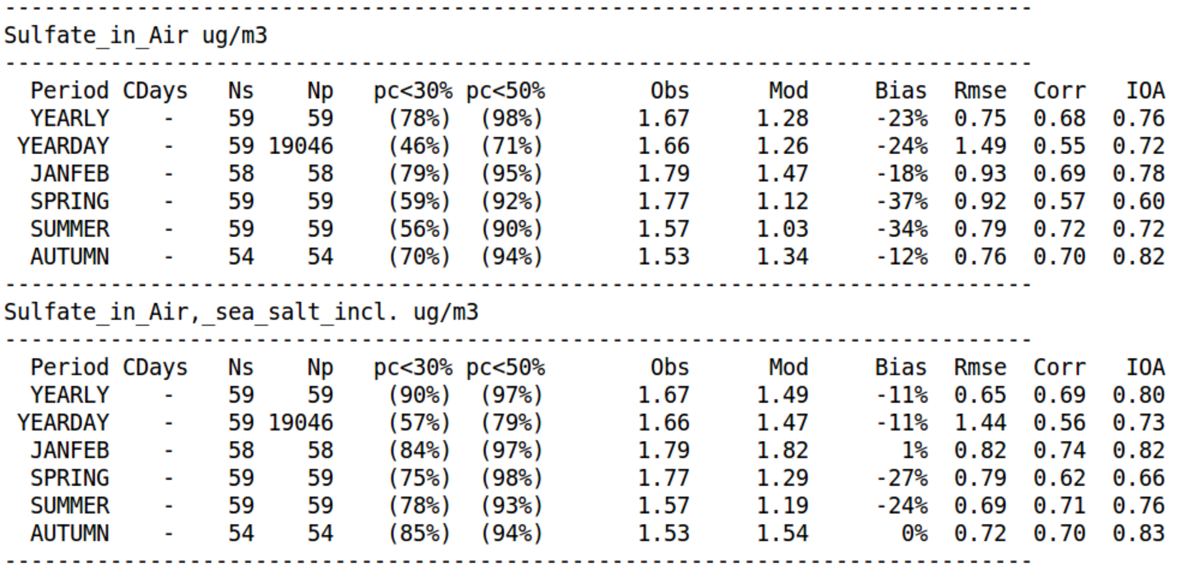
Lots interesting stuff in EMEP Report 4/YYYY (http://emep.int)

From recent model evaluation

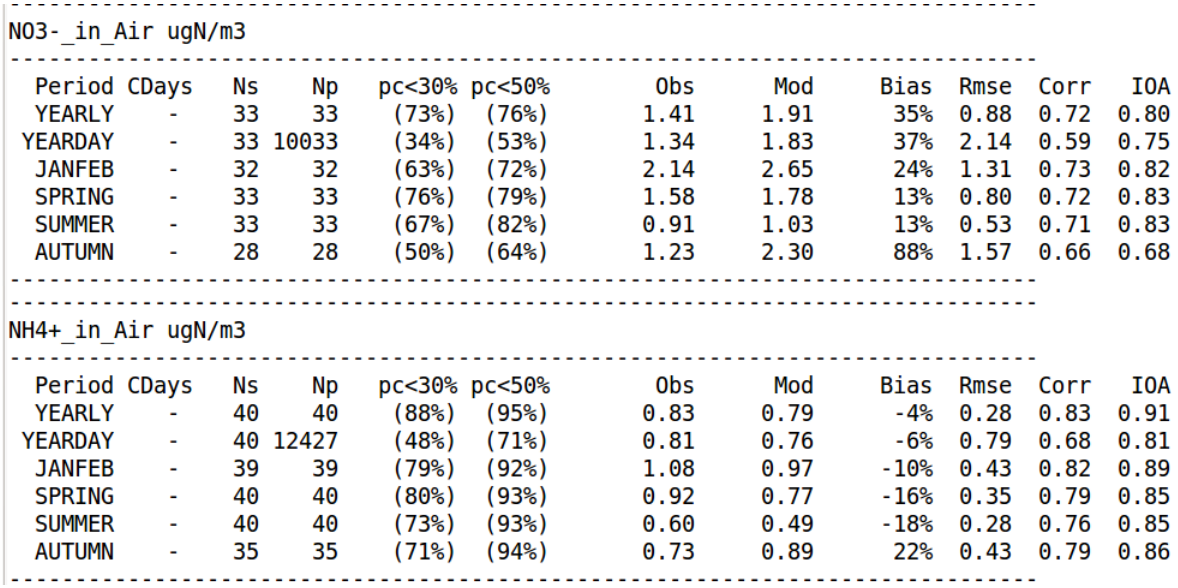


```
------------------------------------------------------------------------------
PM10 ug/m3
------------------------------------------------------------------------------
  Period CDays   Ns    Np   pc<30% pc<50%        Obs      Mod     Bias  Rmse  Corr   IOA
  YEARLY    -    36    36    (86%)  (97%)      14.70    11.05     -25%  6.30  0.49  0.59
 YEARDAY    -    36 11554    (62%)  (84%)      14.71    11.16     -24% 12.27  0.43  0.59
  JANFEB    -    35    35    (74%)  (94%)      16.72    13.12     -22%  8.53  0.48  0.58
  SPRING    -    35    35    (74%)  (94%)      13.48     9.48     -30%  7.20  0.27  0.51
  SUMMER    -    35    35    (83%)  (94%)      14.64     9.57     -35%  6.88  0.60  0.61
  AUTUMN    -    36    36    (83%) (100%)      14.83    12.11     -18%  6.10  0.51  0.63
------------------------------------------------------------------------------
PM25 ug/m3
------------------------------------------------------------------------------
  Period CDays   Ns    Np   pc<30% pc<50%        Obs      Mod     Bias  Rmse  Corr   IOA
  YEARLY    -    26    26    (88%)  (96%)      10.50     7.96     -24%  4.73  0.61  0.64
 YEARDAY    -    26  7891    (64%)  (86%)      10.64     7.99     -25%  8.91  0.51  0.65
  JANFEB    -    25    25    (72%)  (92%)      14.08     8.66     -38%  9.74  0.75  0.57
  SPRING    -    25    25    (84%)  (92%)       9.67     6.74     -30%  5.43  0.42  0.55
  SUMMER    -    26    26    (85%)  (96%)       9.55     7.55     -21%  3.95  0.39  0.62
  AUTUMN    -    26    26    (81%) (100%)      10.05     8.72     -13%  4.27  0.63  0.74
------------------------------------------------------------------------------
```

From recent model evaluation

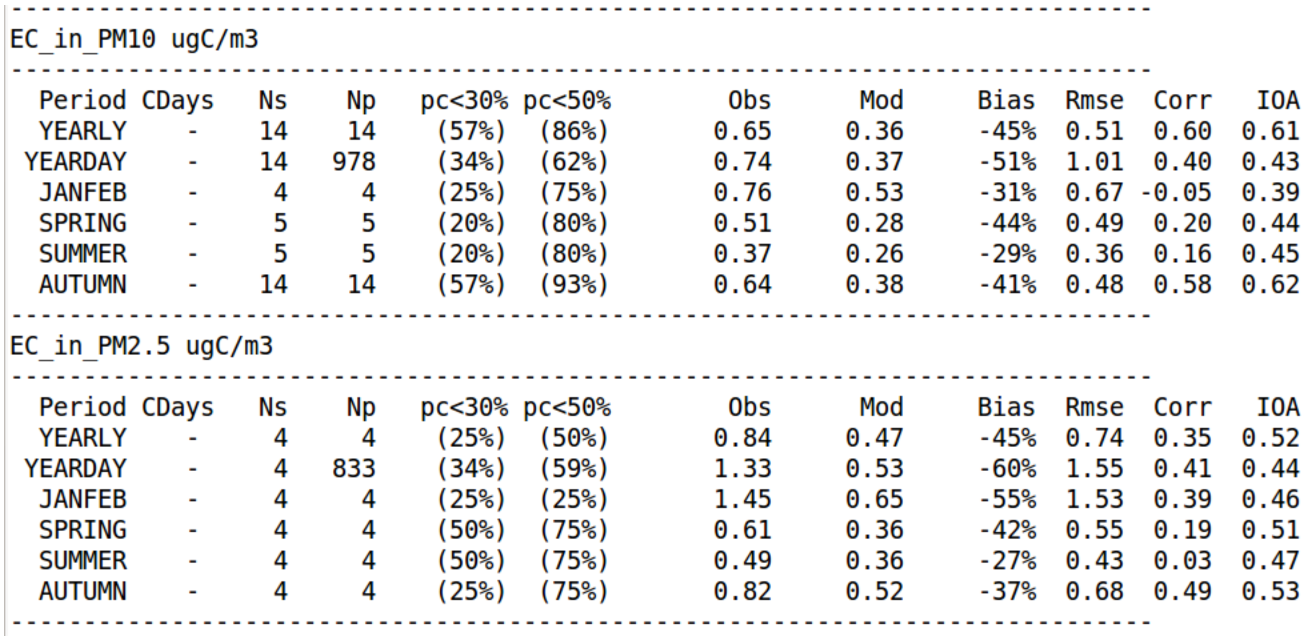


```
-----------------------------------------------------------------------
Sulfate_in_Air ug/m3
-----------------------------------------------------------------------
  Period CDays   Ns    Np   pc<30% pc<50%       Obs      Mod     Bias  Rmse  Corr   IOA
  YEARLY   -     59    59   (78%)  (98%)       1.67     1.28     -23%  0.75  0.68  0.76
 YEARDAY   -     59 19046   (46%)  (71%)       1.66     1.26     -24%  1.49  0.55  0.72
  JANFEB   -     58    58   (79%)  (95%)       1.79     1.47     -18%  0.93  0.69  0.78
  SPRING   -     59    59   (59%)  (92%)       1.77     1.12     -37%  0.92  0.57  0.60
  SUMMER   -     59    59   (56%)  (90%)       1.57     1.03     -34%  0.79  0.72  0.72
  AUTUMN   -     54    54   (70%)  (94%)       1.53     1.34     -12%  0.76  0.70  0.82
-----------------------------------------------------------------------
Sulfate_in_Air,_sea_salt_incl. ug/m3
-----------------------------------------------------------------------
  Period CDays   Ns    Np   pc<30% pc<50%       Obs      Mod     Bias  Rmse  Corr   IOA
  YEARLY   -     59    59   (90%)  (97%)       1.67     1.49     -11%  0.65  0.69  0.80
 YEARDAY   -     59 19046   (57%)  (79%)       1.66     1.47     -11%  1.44  0.56  0.73
  JANFEB   -     58    58   (84%)  (97%)       1.79     1.82       1%  0.82  0.74  0.82
  SPRING   -     59    59   (75%)  (98%)       1.77     1.29     -27%  0.79  0.62  0.66
  SUMMER   -     59    59   (78%)  (93%)       1.57     1.19     -24%  0.69  0.71  0.76
  AUTUMN   -     54    54   (85%)  (94%)       1.53     1.54       0%  0.72  0.70  0.83
-----------------------------------------------------------------------
```

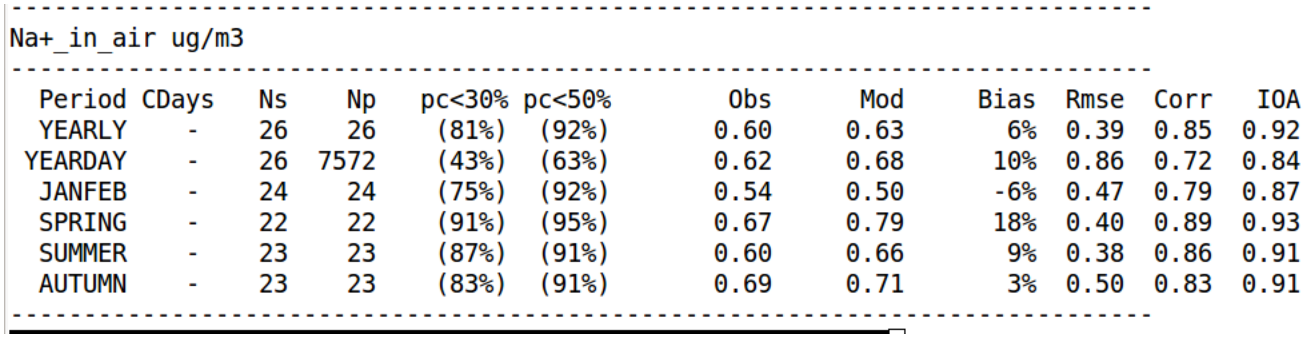


```
-----------------------------------------------------------------------
NO3-_in_Air ugN/m3
-----------------------------------------------------------------------
  Period CDays   Ns    Np   pc<30% pc<50%       Obs      Mod     Bias  Rmse  Corr   IOA
  YEARLY   -     33    33   (73%)  (76%)       1.41     1.91      35%  0.88  0.72  0.80
 YEARDAY   -     33 10033   (34%)  (53%)       1.34     1.83      37%  2.14  0.59  0.75
  JANFEB   -     32    32   (63%)  (72%)       2.14     2.65      24%  1.31  0.73  0.82
  SPRING   -     33    33   (76%)  (79%)       1.58     1.78      13%  0.80  0.72  0.83
  SUMMER   -     33    33   (67%)  (82%)       0.91     1.03      13%  0.53  0.71  0.83
  AUTUMN   -     28    28   (50%)  (64%)       1.23     2.30      88%  1.57  0.66  0.68
-----------------------------------------------------------------------
-----------------------------------------------------------------------
NH4+_in_Air ugN/m3
-----------------------------------------------------------------------
  Period CDays   Ns    Np   pc<30% pc<50%       Obs      Mod     Bias  Rmse  Corr   IOA
  YEARLY   -     40    40   (88%)  (95%)       0.83     0.79      -4%  0.28  0.83  0.91
 YEARDAY   -     40 12427   (48%)  (71%)       0.81     0.76      -6%  0.79  0.68  0.81
  JANFEB   -     39    39   (79%)  (92%)       1.08     0.97     -10%  0.43  0.82  0.89
  SPRING   -     40    40   (80%)  (93%)       0.92     0.77     -16%  0.35  0.79  0.85
  SUMMER   -     40    40   (73%)  (93%)       0.60     0.49     -18%  0.28  0.76  0.85
  AUTUMN   -     35    35   (71%)  (94%)       0.73     0.89      22%  0.43  0.79  0.86
-----------------------------------------------------------------------
```

From recent model evaluation



```
-------------------------------------------------------------------------------
EC_in_PM10 ugC/m3
-------------------------------------------------------------------------------
  Period CDays    Ns     Np   pc<30% pc<50%        Obs      Mod      Bias  Rmse  Corr   IOA
  YEARLY    -     14     14    (57%)  (86%)       0.65     0.36      -45%  0.51  0.60  0.61
 YEARDAY    -     14    978    (34%)  (62%)       0.74     0.37      -51%  1.01  0.40  0.43
  JANFEB    -      4      4    (25%)  (75%)       0.76     0.53      -31%  0.67 -0.05  0.39
  SPRING    -      5      5    (20%)  (80%)       0.51     0.28      -44%  0.49  0.20  0.44
  SUMMER    -      5      5    (20%)  (80%)       0.37     0.26      -29%  0.36  0.16  0.45
  AUTUMN    -     14     14    (57%)  (93%)       0.64     0.38      -41%  0.48  0.58  0.62
-------------------------------------------------------------------------------
EC_in_PM2.5 ugC/m3
-------------------------------------------------------------------------------
  Period CDays    Ns     Np   pc<30% pc<50%        Obs      Mod      Bias  Rmse  Corr   IOA
  YEARLY    -      4      4    (25%)  (50%)       0.84     0.47      -45%  0.74  0.35  0.52
 YEARDAY    -      4    833    (34%)  (59%)       1.33     0.53      -60%  1.55  0.41  0.44
  JANFEB    -      4      4    (25%)  (25%)       1.45     0.65      -55%  1.53  0.39  0.46
  SPRING    -      4      4    (50%)  (75%)       0.61     0.36      -42%  0.55  0.19  0.51
  SUMMER    -      4      4    (50%)  (75%)       0.49     0.36      -27%  0.43  0.03  0.47
  AUTUMN    -      4      4    (25%)  (75%)       0.82     0.52      -37%  0.68  0.49  0.53
-------------------------------------------------------------------------------
```



```
-------------------------------------------------------------------------------
Na+_in_air ug/m3
-------------------------------------------------------------------------------
  Period CDays    Ns     Np   pc<30% pc<50%        Obs      Mod      Bias  Rmse  Corr   IOA
  YEARLY    -     26     26    (81%)  (92%)       0.60     0.63        6%  0.39  0.85  0.92
 YEARDAY    -     26   7572    (43%)  (63%)       0.62     0.68       10%  0.86  0.72  0.84
  JANFEB    -     24     24    (75%)  (92%)       0.54     0.50       -6%  0.47  0.79  0.87
  SPRING    -     22     22    (91%)  (95%)       0.67     0.79       18%  0.40  0.89  0.93
  SUMMER    -     23     23    (87%)  (91%)       0.60     0.66        9%  0.38  0.86  0.91
  AUTUMN    -     23     23    (83%)  (91%)       0.69     0.71        3%  0.50  0.83  0.91
-------------------------------------------------------------------------------
```