

Documentation on the Boundary Conditions provided by MET Norway to EDIII

Trend exercise

The boundary conditions (BCs) supplied for the EDIII study are a simplified version of those used in the standard EMEP MSC-W model. The values are loosely based upon climatological data (except from those for natural particles). The most important gaseous BC compounds are certainly O₃, CO and CH₄, and these values are believed to be well founded. BCs for other gaseous and particulate compounds are much more uncertain. In principle results from global 3-D models could have been used, but this would introduce very complex and likely equally uncertain BCs into the EDII exercise. The values documented below aim rather to be simple and transparent.

The BCs are provided as monthly mean 3D fields of the following species:

- Gases: O₃, PAN, CO, CH₄
- Aerosols (fine < 2.5 μm, coarse 2.5 – 10 μm):
 - fine SO₄ (“SO₄”)
 - fine NO₃ (“NO₃_F”)
 - coarse NO₃ (“NO₃_C”)
 - fine NH₄ (“NH₄”)
 - sea salt fine (“SEASALT_F”)
 - coarse (“SEASALT_C”)
 - mineral dust fine (“DUST_WB_F”)
 - mineral dust coarse (“DUST_WB_C”)

UNITS: volume mixing ratios. Note: dust molecular weight = 200 g/mol

GRID: Identical to the ERA/WRF meteorological data grid
Horizontal - rotated spherical
Vertical - 31 layers

IMPLEMENTATION:

No temporal interpolation between the months

BCs BRIEF DESCRIPTION:

The parameters used to prescribe the seasonal cycle are provided in Table 1 (cf Eqn 74 in Simpson et al., 2012).

The vertical distribution of most species are characterized with the scale-heights Hz (e-fold decrease of the surface concentrations) and other parameters as specified in Table 1 (cf Eqns (75), *ibid*). The main simplification from Simpson et al 2012 is that the latitudinal variations (Table S22, *ibid*) were omitted. These variations were based upon old literature, and recent work has shown that these variations have little impact on model results.

Table 1 Adapted from Table S21 (Supplement, Simpson et al., 2012)

Component	χ_{mean} ppb	d_{max} days	$\Delta\chi$ ppb	Hz km	$\chi_{\text{min}}^{\text{v}}$ ppb	Annual Trend
CO	125.0	75.0	35.0	25.0	70.0	no
PAN	0.20	120	0.15	∞	0.20	yes
SO4	0.15	180	0.00	∞	0.05	yes
NO3 fine	0.07	15	0.03	1.6	0.025	yes
NO3 coarse	0.07	15	0.00	1.6	0.025	yes
NH4	0.15	180	0.00	1.6	0.05	yes
Sea salt fine	0.2	15	0.05	1.6	0.01	no
Sea salt coarse	1.5	15	0.25	1.6	0.01	no

χ_{mean} - the annual mean surface concentration, $\Delta\chi$ - the amplitude of the cycle, d_{max} - the day number of χ maximum; Hz - the scale-heights of vertical distribution. For trends, see below.

For Ozone, BCs have zonal, monthly and vertical variation and annual trend (see below)

For Sea salt, BCs over land are set to 0.001 * BCs over sea

Mineral Dust – monthly 3D fields from EMEP global run for 2012

Constant BCs (no 3-D or monthly variations) are set for:

CH4 - 1870 ppb

H2 - 600 ppb

REFERENCES / NOTES

Ozone

For BCs, we make use of Logan's climatological data (Logan, JGR, 1999).

These climatological values are modified each month to ensure that they match concentrations observed in clean westerly Atlantic air masses as measured at Mace Head on the coast of Ireland. This 'Mace Head correction' is calculated using IE31 O3 data and trajectory sectors (based on ECMWF met) for respective years, as described in Simpson et al., 2012.

PAN

Trends are based on NOx emission trend in North America (see SIA below)

CH4

The following values are set: 1780 ppb in 1990, 1820 ppb in 2000, and 1870 ppb in 2010. For other year, interpolation is applied. Values from Simpson et al. (2012), Table 6.2 for 1990, and from CDIAC (Mace Head) data for 2000. 2010 also from Mace Head

SIA

For SO4 and NO3, the trends for 1980-2003 are derived from the trend in EPA emissions for North America of SO2 and NOx.

For NH4, the trends are derived as $2/3 * SO4 + 1/3 * NOx$

Support for SO2 can be found in Hicks, Artz, Meyer and Hosker (2002) in Figure 7 (Eastern US) which show 'close' correspondence between national emissions and concentration trend.

The trend-factors look like this:

	SO2	NOx	NH4
SIAfac (1990,	0.890,	0.943,	0.920)
SIAfac (2000,	0.631,	0.835,	1.046)
SIAfac (2010,	0.292,	0.543,	0.925)

The reference value for SO2 and SO4 is 0.15 ppb in 1980 (for both), loosely based upon a number of studies (Table S21 in Simpson et al. 2012 gives references). For example, Warneck (1999, Fig. 10.6) showed SO2 concentrations being around 0.1-0.5 ug/m3 (STP, ca. 0.04-0.2 ppb) over marine areas. Observations at Valentia Observatory on the west coast of Ireland show ca. 1 ug/m3 for both SO2 and SO4 around 1980 (although certainly influenced by polluted sources). In earlier EMEP studies a scale height of 1.6 km was used for SO2 and SO4, but model studies suggest that SO4 should show little vertical variation with height.

Warneck, Chemistry of the Natural Atmosphere, 2nd edition, 1999; Academic Press. (Fig 10-6)

References for NO3 fine & coarse and NH4:

BCs are based on ACE-2 measurements. Lots of conflicting measurements exist, from NH4/SO4=2 to NH4/SO4=0.5 Thus, a 'mean' value of NH4/SO4=1 is therefore selected. Otherwise NH4 is assumed to

act as SO₄.

Fine NO₃ is assumed to act as SO₄, but with 1/2 concentrations and seasonal var.

Coarse NO₃ is assumed to act like sea salt in the vertical, with decreasing concentrations with height, and has approximately same concentration levels as fine NO₃.

Reference for Sea Salt

A constant value over ocean has been selected, loosely based on EMEP global runs and on Na⁺ verification with EMEP observations.