NAME III Document
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Unit Conversion

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1 Introduction

This document describes how output for certain NAME fields can be requested in units that differ from those of the corresponding source species.

Up to version 6.0 of NAME the unit of an output field requirement was automatically set to the unit of the corresponding source species. We added functionality for requesting output in units that differ from the unit of the source species. In the simplest case this can be a conversion within a given unit "type", for example, the output can be in kilogram (`kg`) if the source species has a unit of gram (`g`) etc. This is described in section 2.1. If the source is specified in mass units, the air concentration can be output in volumetric units, i.e. it is possible to request the volumetric mixing ratio in units of parts-per-million (`ppm`) or parts-per-billion (`ppb`), see section 2.2. In section 2.3 we describe how vertically integrated air concentrations can be converted to Dobson units in the output file.

2 Unit conversions

2.1 Mass- and activity units

For the following quantities the unit of the source species can differ from the unit of the output requirement, as long as the unit type is identical, i.e. mass units can be converted to other mass units, activity units to other activity units etc.

- Air concentration
- Dry deposition rate
- Wet deposition rate
- Total deposition rate

For each of these field requirements an additional column with header `Material Unit` is required in the input file. For each unit, a conversion factor ρ relative to a standard

symbol	name	ρ
`t`	tonne	10^6
`kg`	kilogram	10^3
`g`	gram	1
`mg`	milligram	10^{-3}
`mcg`	microgram	10^{-6}
`lb`	pound	453.59237
`oz`	ounce	28.349523125

Table 1: Mass units and conversion factors. The reference unit is 1 gram (`g`).

symbol	name	ρ
`Bq`	Becquerel	1
`mBq`	milliBecquerel	10^{-3}
`mcBq`	microBecquerel	10^{-6}
`Ci`	Curie	3.7×10^{10}

Table 2: Activity units and conversion factors. The reference unit is 1 Becquerel (`Bq`).

unit is defined, the conversion is then carried out by multiplying the field values (stored internally in source species units) by the relative conversion factor of the species and output field requirement[1]:

$$F(iX, iY, iZ, \ldots) \quad \mapsto \quad \frac{\rho[\text{species}]}{\rho[\text{fieldrequirement}]} F(iX, iY, iZ, \ldots) \tag{1}$$

Currently the units and conversion factors in Tabs. 1 and 2 are defined in the code.

It is also possible to use units that are not defined in the code, as long as these agree between the source species and the output requirement. For example, the source could be specified in units of `Area of Risk` as long as the same unit is used for all output requirements of the above type that depend on this species.

Possible extensions

- Allow definition of new units in the input file.
- Conversion between mass and activity units for radioactive species.
- Conversion for other quantities (`Mass`, `sigmaZ`, `Chemistry field`)
- Conversion of length and time units, e.g. output deposition rate in kg/(m^{2}day)
- Only allow mass units in decay chains.
- Allow conversion of dosage units (currently: effective cloud gamma dose in Sv/s, specific doses such as lung, thyroid etc. in Gy/s)

[1] In probability calculations, the threshold values, given in units of the output field requirement, are internally converted to the unit of the species.

2.2 Volumetric units

To request the mixing ratio of a certain species relative to dry air a new output quantity `Mixing Ratio` was defined. Allowed units are `ppm` (parts-per-million) and `ppb` (parts-per-billion). The mixing ratio (MR) of species i is then given by one of the following two relations:

$$MR_i[\text{ppm}] = \frac{M_{\text{dry}}}{\rho_{\text{dry}}[\text{kg m}^{-3}] \cdot M_i} \times C_i[\text{mg m}^{-3}] \tag{2}$$

$$= \frac{R[\text{J mol}^{-1}\text{ K}^{-1}] \cdot T[\text{K}]}{p_{\text{dry}}[\text{Pa}] \cdot M_i[\text{g mol}^{-1}]} \times C_i[\mu\text{g m}^{-3}] \tag{3}$$

In these equations we have

- C_i: air concentration of species i
- $M_{\text{dry}} = 28.966\text{g mol}^{-1}$: molar mass of dry air
- ρ_{dry}: density of dry air
- M_i: molar mass of species i
- $R = 8.314\text{J mol}^{-1}\text{K}^{-1}$: ideal gas constant
- T: air temperature
- p_{dry}: partial pressure of dry air

In the NAME code we use relation (2) as it only requires one flow field. All quantities are defined at the centre of a gridbox and both a horizontal and a vertical grid have to be defined for mixing ratio calculculations.

Possible extensions

- Define boundary conditions in `ppm/ppb`.
- Using the flow fields at the centre of a gridbox is ok for fine grids but might use a better method for coarse grids (if we know the density ρ at two different heights in the gridbox, we can use the barometric formula to calculate a better average density in the gridbox).
- Mixing ratio is given relative to dry air, adjust for moisture in air (corrections probably very small).

2.3 Dobson units

Vertically integrated air concentrations $C^{(\text{int.})}$ can be converted to Dobson units. One Dobson unit corresponds to a layer of ozone that would be 10μm thick if brought to standard temperature and pressure. It is also common to use this unit for other species.

$$C_i^{(\text{int.})}[\text{DU}] \quad = \quad \frac{R[\text{J K}^{-1}\ \text{mol}^{-1}] \cdot T^{(\text{std.})}[\text{K}]}{10^{-5} \cdot p^{(\text{std.})}[\text{Pa}] \cdot M_i[\text{g mol}^{-1}]} \times C_i^{(\text{int.})}[\text{g m}^{-2}] \tag{4}$$

Standard pressure and temperature are defined as

$$T^{(\text{std.})} = 273\text{K}, \qquad\qquad p^{(\text{std.})} = 1.013 \cdot 10^5\text{Pa}. \tag{5}$$

The ideal gas constant used in the code is

$$R = 8.3145\text{J mol}^{-1}\text{K}^{-1}. \tag{6}$$

Note that conversion to Dobson units is only possible for vertically integrated fields, i.e. the z grid has to be left unspecified and boundary layer averages are not allowed.