Note on RTTOV v12 unit conversions for gases, clouds and aerosols

Jérôme VIDOT (Meteo France), James HOCKING (Met Office)

March 6, 2017

1 Introduction

This note describes the conversion of units applied within RTTOV v12 for gases, clouds and aerosols.

1.1 Gases

The optical depth regression coefficients are trained using atmospheric predictors calculated from gas concentrations in units of ppmv over dry air. All calculations within RTTOV which use the input gas profiles (e.g. the optical depth predictor calculations, the local path calculations, the relative humidity calculations for aerosol optical property interpolation, and the Rayleigh scattering calculations) expect gas concentrations in units of ppmv over dry air.

RTTOV v12 allows users to input gas profiles in units of ppmv over moist air, $\mathrm{kg\,kg^{-1}}$ over moist air or ppmv over dry air. This document derives the formulae used to convert the input profiles to units of ppmv over dry air. These formulae are also implemented in the test suite to allow input profile data in any one of the three unit options to be converted for input to RTTOV in one of the other units.

1.2 Clouds/Aerosols

The cloud and aerosol optical depth calculations are computed in terms of liquid/ice water content ($\mathrm{g\,m^{-3}}$) for clouds and number concentration ($\mathrm{cm^{-3}}$) for aerosols. RTTOV v12 provides the option for users to supply both cloud and aerosol profiles in $\mathrm{kg\,kg^{-1}}$ over moist air. This document describes the conversions applied for cloud and aerosol concentrations.

2 Constants and quantities

(a) Physical constants and their values in `rttov_const.F90`

N_A	$6.022\,140\,857 \times 10^{23}$	Avogadro's number (number of molecules in one mole)
k_B	$1.380\,648\,52 \times 10^{-23}\ \mathrm{J\,K^{-1}}$	Boltzmann constant
R	$8.314\,459\,8\ \mathrm{J\,mol^{-1}\,K^{-1}}$	Ideal gas constant ($=N_A k_B$; `rgc` in `rttov_const.F90`)

Mean molar masses

M_{dry}	$28.9644\ \mathrm{g\,mol^{-1}}$	(`mair` in `rttov_const.F90`)
M_{h2o}	$18.015\,28\ \mathrm{g\,mol^{-1}}$	(`mh2o` in `rttov_const.F90`)
M_{o3}	$47.9982\ \mathrm{g\,mol^{-1}}$	
M_{co2}	$44.0095\ \mathrm{g\,mol^{-1}}$	
M_{ch4}	$16.042\,46\ \mathrm{g\,mol^{-1}}$	
M_{n2o}	$44.0128\ \mathrm{g\,mol^{-1}}$	
M_{co}	$28.0101\ \mathrm{g\,mol^{-1}}$	
M_{so2}	$64.064\ \mathrm{g\,mol^{-1}}$	

(b) Gas law - volume V ($\mathrm{m^3}$) of ideal gas at temperature T (K)

P	hPa	Total gas pressure
P_{dry}	hPa	Partial pressure of dry air
n_{moist}	$\mathrm{mol\,m^{-3}}$	Mole density of moist air
n_{dry}	$\mathrm{mol\,m^{-3}}$	Mole density of dry air
ρ_{moist}	$\mathrm{kg\,m^{-3}}$	Density of moist air
ρ_{dry}	$\mathrm{kg\,m^{-3}}$	Density of dry air

For unit volume: $10^2\mathrm{P} = n_{air} N_A k_B T$

(c) Quantities for gas j

n_j	$\mathrm{mol\,m^{-3}}$	Mole density
M_j	$\mathrm{g\,mol^{-1}}$	Molar mass
ρ_j	$\mathrm{kg\,m^{-3}}$	Density ($=10^{-3} n_j M_j$)
P_j	hPa	Partial pressure
e	hPa	Partial pressure of water vapour
q_j	$\mathrm{kg\,kg^{-1}}$	Mass mixing ratio over moist air
r_j	$\mathrm{kg\,kg^{-1}}$	Mass mixing ratio over dry air
x_j^{moist}	$\mathrm{\mu mol\,mol^{-1}}$ or ppmv	Mole fraction over moist air
x_j^{dry}	$\mathrm{\mu mol\,mol^{-1}}$ or ppmv	Mole fraction over dry air

(d) Quantities for mixtures

Σ_j		Sum over all gases in dry air
$\Sigma_j n_j$	$\mathrm{mol\,m^{-3}}$	Mole density of dry air (n_{dry})
$\Sigma_j n_j + n_{h2o}$	$\mathrm{mol\,m^{-3}}$	Mole density of moist air (n_{moist})

(e) Cloud quantities

LWC	$\mathrm{g\,m^{-3}}$	Liquid water content
IWC	$\mathrm{g\,m^{-3}}$	Ice water content
q_{ice}	$\mathrm{kg\,kg^{-1}}$	Mass mixing ratio for ice cloud over moist air
q_{liq}	$\mathrm{kg\,kg^{-1}}$	Mass mixing ratio for liquid cloud over moist air

(f) aerosol quantities for type i

q_i	$\mathrm{kg\,kg^{-1}}$	Mass mixing ratio over moist air
N_i	$\mathrm{cm^{-3}}$	Number concentration
ρ_i	$\mathrm{kg\,m^{-3}}$	Density
$n_i(r)$		Particle size distribution
r	µm	Size
M_i^*	$\mathrm{g\,m^{-3}/(part.cm^{-3})}$	Conversion term between mass concentration and number concentration

3 The unit conversions for gases

The mean molar mass of moist air, M_{moist}, takes all gases into account including water vapour:

$$M_{moist} = \frac{\Sigma_j n_j M_j + n_{h2o} M_{h2o}}{\Sigma_j n_j + n_{h2o}} = 10^3 \frac{\rho_{moist}}{n_{moist}} \tag{1}$$

The equivalent formula for dry air is:

$$M_{dry} = \frac{\Sigma_j n_j M_j}{\Sigma_j n_j} = 10^3 \frac{\rho_{dry}}{n_{dry}} \tag{2}$$

The value of M_{dry} is considered constant in RTTOV (see section 2(a)) and is stored in the parameter `mair` in `rttov_const.F90`. The mass mixing ratio for gas j over moist air is:

$$q_j = \frac{n_j M_j}{\Sigma_j n_j M_j + n_{h2o} M_{h2o}} = \frac{n_j M_j}{n_{moist} M_{moist}} = \frac{\rho_j}{\rho_{moist}} \tag{3}$$

Similarly the mass mixing ratio for gas j over dry air is:

$$r_j = \frac{n_j M_j}{\Sigma_j n_j M_j} = \frac{n_j M_j}{n_{dry} M_{dry}} = \frac{\rho_j}{\rho_{dry}} \tag{4}$$

In particular we have:

$$q_{h2o} = \frac{n_{h2o} M_{h2o}}{\Sigma_j n_j M_j + n_{h2o} M_{h2o}} \tag{5}$$

and

$$r_{h2o} = \frac{n_{h2o} M_{h2o}}{\Sigma_j n_j M_j} \tag{6}$$

From this we obtain expressions to convert between kg kg^{-1} over moist air and kg kg^{-1} over dry air:

$$\boxed{q_j = \frac{r_j}{1 + r_{h2o}}} \tag{7}$$

and

$$\boxed{r_j = \frac{q_j}{1 - q_{h2o}}} \tag{8}$$

The mole fraction is the number of moles of a gas within one mole of the mixture (moist or dry air). This is the volume mixing ratio because, at the given temperature, a mole of each ideal constituent will take up exactly the same volume. This is therefore also the ratio of mole densities:

$$10^{-6} x_j^{moist} = \frac{n_j}{\Sigma_j n_j + n_{h2o}} = \frac{P_j/RT}{P/RT} = \frac{P_j}{P} \tag{9}$$

Similarly for dry air:

$$10^{-6} x_j^{dry} = \frac{n_j}{\Sigma_j n_j} = \frac{P_j/RT}{P_{dry}/RT} = \frac{P_j}{P - e} \tag{10}$$

Using equations (9) and (10) and substituting for e/P from equation (9) applied to water vapour we have:

$$x_j^{moist} = x_j^{dry} \left(\frac{P - e}{P} \right) = x_j^{dry} \left(1 - \frac{e}{P} \right) = x_j^{dry} \left(1 - 10^{-6} x_{h2o}^{moist} \right) \tag{11}$$

This provides the expression to convert from ppmv over moist air to ppmv over dry air:

$$\boxed{x_j^{dry} = \frac{x_j^{moist}}{1 - 10^{-6} x_{h2o}^{moist}}} \tag{12}$$

We can also write, using (4):

$$10^{-6} x_j^{dry} = \frac{n_j}{n_{dry}} = \frac{\rho_j / M_j}{\rho_{dry} / M_{dry}} = \left(\frac{\rho_j}{\rho_{dry}} \right) \left(\frac{M_{dry}}{M_j} \right) = r_j \left(\frac{M_{dry}}{M_j} \right) \tag{13}$$

Using equation (8) we obtain an expression to convert from kg kg^{-1} over moist air to ppmv over dry air:

$$\boxed{x_j^{dry} = 10^6 \left(\frac{q_j}{1 - q_{h2o}} \right) \left(\frac{M_{dry}}{M_j} \right)} \tag{14}$$

4 The unit conversion for clouds

The optical properties of ice and water clouds in RTTOV are parameterized from ice water content (IWC) and liquid water content (LWC) in $\mathrm{g\,m^{-3}}$, respectively. However, NWP models provide cloud information in units of mass mixing ratio (or specific cloud ice or liquid water content) in $\mathrm{kg\,kg^{-1}}$, i.e. ratio between the mass of ice/liquid water and the mass of moist air. If we consider that the air follows the perfect gas law, then the conversion for ice cloud is:

$$IWC = q_{ice} \frac{10^2 P}{R_{moist} T} \tag{15}$$

where q_{ice} is the mass mixing ratio for ice cloud, P is the atmospheric pressure in hPa, T is the atmospheric temperature in K and R_{moist} is the moist air gas constant (in $\mathrm{J\,g^{-1}\,K^{-1}}$) given by:

$$R_{moist} = R_{dry} \left(1 + \frac{1-\varepsilon}{\varepsilon} q_{h2o}\right) \tag{16}$$

where R_{dry} is the gas constant for dry air and q_{h2o} is the specific humidity (given as the ratio between the mass of water vapor and the mass of moist air). The equation (16) is demonstrated in [2] (Equation 2.31). The coefficient ε is given by:

$$\varepsilon = \frac{M_{h2o}}{M_{dry}} \tag{17}$$

The gas constant for dry air is given by:

$$R_{dry} = \frac{R}{M_{dry}} \tag{18}$$

The same equations are used for liquid clouds, by replacing IWC by LWC and q_{ice} by q_{liq} in Eq. (15)

5 The unit conversion for aerosols

The optical properties of aerosols in RTTOV are pre-calculated for one particle per $\mathrm{cm^{-3}}$. To calculate the total optical properties within each aerosol layer, the pre-calculated optical properties have to be multiplied by the aerosol number concentration. As for clouds, NWP models such as MACC provide aerosol information in unit of mass mixing ratio in $\mathrm{kg\,kg^{-1}}$ (ratio between the aerosol mass and the mass of moist air). For aerosols the unit conversion is more complex than for clouds since the RTTOV aerosol unit is in number concentration instead of mass concentration. Fortunately, for RTTOV aerosol types based on OPAC [1], the conversion term between mass concentration and number concentration, called M^* (in $\mathrm{g\,m^{-3}}$/part.cm^{-3}), is provided for each OPAC aerosol types (number 1 to 10 in RTTOV) in Table 1c of [1]. The conversion of the mass mixing ratio (q_i) of aerosol type i in number concentration (N_i) is given by:

$$N_i = q_i \frac{10^2 P}{R_{moist} T M_i^*} \tag{19}$$

where q_i is the mass mixing ratio for RTTOV aerosol type i, P is the atmospheric pressure in hPa, T is the atmospheric temperature in K and R_{moist} is given by equation (16). The terms M_i^* in $\mathrm{g\,m^{-3}}$/part.cm^{-3} are given in Table 1 for each RTTOV aerosol model. For other aerosol types not based on OPAC (number 11: volcanic ash or VOLA; number 12: new volcanic ash or VAPO; and number 13: Asian dust or ASDU), the conversion term M_i^* is calculated from the particle size distribution (PSD) $n_i(r)$ using the same assumptions than for OPAC. If we consider that the aerosol is spherical then:

$$M_i^* = \int_{r_{min}}^{r_{max}} \frac{4}{3} \pi r^3 \rho_i n_i(r) dr \tag{20}$$

where r_{min} and r_{max} are the minimum and maximum radius of the PSD and ρ_i is the particle density of type i. In [1], r_{max} is fixed to 7.5 µm. For volcanic ash aerosol model of RTTOV (named VOLA), the particle size distribution is a modified Gamma size distribution, given by:

$$n_i(r) = N_i a r^{\alpha} \exp\left[-\frac{\alpha}{\gamma}\left(\frac{r}{r_{mod,i}}\right)^{\gamma}\right] \tag{21}$$

Table 1: Values M_i^* of Eq. (19) for RTTOV aerosol types

Type	RTTOV Number	M_i^*
INSO	1	2.37×10^{-5}
WASO	2	1.34×10^{-9}
SOOT	3	5.99×10^{-11}
SSAM	4	8.02×10^{-7}
SSCM	5	2.24×10^{-4}
MINM	6	2.78×10^{-8}
MIAM	7	5.53×10^{-6}
MICM	8	3.24×10^{-4}
MITR	9	1.59×10^{-5}
SUSO	10	2.28×10^{-8}
VOLA	11	39.258
VAPO	12	13.431
ASDU	13	1.473×10^{-4}

where the different coefficients are a=5461, α=1, γ=0.5 and $r_{mod,i}$=0.0156 µm. For the integration of Eq. (20), we used $r_{min} = 0.005$ µm and r_{max}=20 µm ([3]). By considering that the calculation is relative to 1 particle per cm^{-3} (i.e., N_i=1), then the value of M^* is given in Table 1.

For the new volcanic ash aerosol model (named VAPO), a log-normal PSD is used, i.e.:

$$n_i(r) = \frac{N_i}{\sqrt{2\pi}r\log(\sigma_i)\ln(10)} exp\left[-\frac{1}{2}\left(\frac{\log(r)-\log(r_{mod,i})}{\log(\sigma_i)}\right)^2\right] \quad (22)$$

with $r_{mod,i}$=0.610 482 µm and σ_i=1.85. Again, by considering $r_{min} = 0.005$ µm, r_{max}=7.5 µm and that the calculation is relative to 1 particle per cm^{-3} (i.e., N_i=1), then the value of M^* is also given in Table 1.

For the Asian dust aerosol model (named ASDU), the particle size distribution is given by a linear combination of log-normal PSDs (Eq. (22)) for mineral nucleated (MINM), accumulated (MIAM) and coalesced (MICM) types and with relative weights of 0.862, 0.136 and 0.217×10^{-2}, respectively. The parameters of the log-normal PSDs are given in Table 2 of [3]. Again, by considering that the calculation is relative to 1 particle per cm^{-3} (i.e., N_i=1) and by integrating between 0.005 and 7.5 µm, the value of M^* is also given in Table 1.

References

[1] M. Hess, P. Koepke, and I. Schult. Optical properties of aerosols and clouds: The software package opac. *Bulletin of the American Meteorological Society*, 79(5):831–844, 1998.

[2] M. Z. Jacobson. *Fundamentals of atmospheric modelling.* Cambridge Eds., 2005.

[3] M. Matricardi. The inclusion of aerosols and clouds in rtiasi, the ecmwf fast radiative transfer model for the infrared atmospheric sounding interferometer. Technical Report 474, ECMWF, 2005.