Spin-off ATOP project by Ronald, March 19, 1999.

List of used constants :

- Global average of gravity at mean sea level: $g_0 = 9.80665 \mathrm{m\,s^{-2}}$
- Standard temperature: $T_0 = 273.15\mathrm{K}$
- Boltzmann's constant: $k = 1.3807 \cdot 10^{-23} \mathrm{J\,K^{-1} molecule^{-1}}$
- Standard pressure: $p_0 = 1.01325 \cdot 10^5 \mathrm{Pa}$
- Avogadro's number: $N_A = 6.0220 \cdot 10^{23}$
- Mean mass of air (with background concentration of water): $M_A = 28.94 \cdot 10^{-3} \mathrm{kg}$
- Specific gas constant for air : $R = \frac{kN_A}{M_A} = 287.3 \mathrm{J\,kg^{-1} K^{-1}}$

TOTAL COLUMN CALCULATION

Objective

Computation of the total column amount of a trace gas out of a vertical profile.

Algorithm description

The profile between level 0 and N can be integrated, using:

$$\mathtt{COLUMN} = 10 \cdot \frac{RT_0}{g_0 p_0} \cdot \sum_{i=1}^{N-1} 0.5(\mathtt{VMR}(i) + \mathtt{VMR}(i+1))(p_i - p_{i+1}) \tag{0.1}$$

where p is the pressure in hPa, `VMR` the volume mixing ration in ppm and `COLUMN` is the trace gas column amount in Dobson Units.

UNIT CONVERSION

Objective

The objective of this algorithm is to convert different units into each other. The considered units are: for trace gas column amounts: DU, $\mathrm{cm^{-2}}$; for pressure/height: Pa, hPa, m; for trace gas profiles: vmr (ppm), partial pressure (mPa), number density ($\mathrm{cm^{-3}}$).

Algorithm description

Conversion from pressure to geopotential height: To go from pressure p to geopotential height Z :

$$Z = \frac{R}{g_0} \int_{p\prime=p}^{p_s} T(p\prime) d \ln p\prime \ , \tag{0.2}$$

where R is the gas constant for air, g_0 is the global average of gravity at mean sea level, p_s is the pressure at $Z = 0$, and T is the temperature. The unit of the pressure has to be Pa. The resulting geopotential height is given in m. An estimate is needed for the surface pressure p_s, and a profile of the temperature as a function of the pressure $T(p\prime)$ between p_s and p. If the surface pressure p_s and n temperatures are given at pressures between p_s and p, approximate the above integral by:

$$Z = \frac{R}{g_0} \sum_{i=1}^{n} T(p_i)(\ln p_{i+1} - \ln p_{i-1})/2 \ , \tag{0.3}$$

where $p_{n+1} = p$.

Conversion from geopotential height to pressure : To go from geopotential height Z to pressure p :

$$p = p_s \exp{(-\frac{g_0}{R} \int_{h=0}^{Z} \frac{1}{T(h)} dh)} \ , \tag{0.4}$$

where R is the gas constant for air, g_0 is the global average of gravity at mean sea level, p_s is the pressure at $Z = 0$, and T is the temperature. The unit of the geopotential height has to be m. The resulting pressure is given in Pa. An estimate is needed for the surface pressure p_s, and a profile of the temperature as a function of the geopotential height $T(h)$ between 0 and Z. If the surface pressure p_s and n temperatures are given at geopotential heights between 0 and h, approximate the above integral by:

$$p = p_s \exp{(-\frac{g_0}{R} \sum_{i=1}^{n} \frac{1}{T(h_i)} (h_{i+1} - h_{i-1})/2)} \ , \tag{0.5}$$

where $h_{n+1} = h$ and $h_0 = 0$.

Conversion of trace gas column amounts:

- Conversion from DU to cm^{-2}:

  To go from a trace gas amount x_{DU} in DU to a trace gas amount $x_{\text{cm}^{-2}}$ in cm^{-2} :

  $$x_{\text{cm}^{-2}} = 10^{-9} \frac{p_0}{kT_0} x_{\text{DU}} \ , \tag{0.6}$$

  where k is Boltzmann's constant, T_0 is the standard temperature and p_0 is the standard pressure.

- Conversion from cm^{-2} to DU:

  To go from a trace gas amount $x_{\text{cm}^{-2}}$ in cm^{-2} to a trace gas amount x_{DU} in DU use the equation

  $$x_{\text{DU}} = 10^{9} \frac{kT_m}{p_0} x_{\text{cm}^{-2}} \ , \tag{0.7}$$

  where k is Boltzmann's constant, T_0 is the standard temperature and p_0 is the standard pressure.

Conversion of trace gas profiles:

- Conversion from vmr to partial pressure :

  To go from vmr in ppm to partial pressure p_{part} in mPa use the equation

  $$\text{vmr} = 10^3 \frac{p_{\text{part}}}{p} \tag{0.8}$$

  where p is the pressure in Pa at the specified point. When the pressure is not given, use the conversion from geopotential height to pressure to calculate the pressure at the specified point.

- Conversion from partial pressure to vmr :

  To go from the partial pressure p_{part} in mPa to vmr in ppm use the equation

  $$p_{\text{part}} = 10^{-3} \text{vmr} \cdot p \tag{0.9}$$

  where p is the pressure in Pa at this point. When the pressure is not given, use the conversion from geopotential height to pressure to calculate the pressure at the specified point.

- Conversion from partial pressure to number density :

  To go from partial pressure p_{part} in mPa to number density n in cm^{-3} use the equation

  $$n = 10^{-9} \frac{p_{\text{part}}}{kT} \tag{0.10}$$

  where k is Boltzmann's constant and T is the temperature in Kelvin at this point.

- Conversion from number density to partial pressure :

  To go from number density n in cm^{-3} to partial pressure p_{part} in mPa, use the equation

  $$p_{\text{part}} = 10^9 nkT \tag{0.11}$$

  where k is Boltzmann's constant and T is the temperature in Kelvin at this point.

- Conversion from vmr to number density :

  Use the conversion from number density to partial pressure and subsequently the conversion from partial pressure to number density.

- Conversion from number density to vmr :

  Use the conversion from number density to partial pressure and subsequently the conversion from partial pressure to number density.