Geophysical model and atmospheric layering

M. Höpfner

Abstract: The quantities and variables which determine the atmospheric state in KOPRA are given. It is described how the hydrostatic equilibrium is calculated and how horizontal gradients are taken into account. Finally, the different possibilities and criteria for the atmospheric layering determining the radiative transfer discretization are presented.

1 Introduction

The radiative transfer modeling in KOPRA is based on a layer-by-layer approach, i.e. during the ray-tracing partial gas columns and Curtis-Godson means (of temperature, pressure, non-LTE/LTE population ratios) are determined for each path segment. A path segment is a part of the line-of-sight inside one layer, i.e. between two successive equi-altitude surfaces (=levels). While more levels increase the accuracy of a radiative transfer calculation the run-time depends in first order linearly on their number. Hence, a trade-off between run-time and accuracy adapted to each experiment has to be done during the discretization of the problem (the so-called 'layering').

This approach implies two important steps: (1) the calculation of atmospheric state quantities (temperature, pressure, vmr, non-LTE/LTE population ratios) at arbitrary locations in the atmosphere and (2) the layering itself. These two subjects will be described separately in the following sections.

2 Geophysical model

How does KOPRA get to know the value of an atmospheric state quantity for a location (latitude, longitude, altitude) in the atmosphere? The answer is: it is calling one of the functions **give_p, give_T, give_vmr,give_Tvib**[1] with the geolocation as arguments. Hence, inside these functions the transformation (in the simplest case interpolation) from discrete profile values (or parameters) to continuous profiles is computed. The reason why we speak generally of transformations and not only of interpolations is the distinction between input profiles and retrieval parameters (see paragraph 4 in Part XIII: 'Derivatives and interface to the retrieval'). In the following we describe the interpolation procedures for input profiles with values of atmospheric quantities at fixed altitude levels. (The transformation rules for retrieval parameters are to be defined by the user.)

2.1 Input profiles

All input profiles belong to one geolocation: **inprof(1)%lon, inprof(1)%lat**. They are stored in the following variables (e.g. for altitude levels i):

altitude	**inprof(i)%alt**
pressure	**inprof(i)%p**
temperature	**inprof(i)%T**
vmr for each species j	**inprof(i)%vmr(j)**
vibrational temperature for each state j of one isotope species k	**inprof(i)%Tvib(j,k)**
continuum absorption coefficient for each microwindow j	**inprof(i)%aerabs(j)**
continuum scattering coefficient for each microwindow j	**inprof(i)%aersca(j)**

Information about horizontal gradients for each altitude level (only for p, T, non-LTE/LTE population ratios, vmr) is stored in:

(gradient profiles along latitude circles, positive to east):

inprof(i)%latgrad%p
inprof(i)%latgrad%T
inprof(i)%latgrad%Tvib(k,j)
inprof(i)%latgrad%vmr(j)

(gradient profiles along longitude circles, positive to south):

inprof(i)%longrad%p
inprof(i)%longrad%T
inprof(i)%longrad%Tvib(j,k)
inprof(i)%longrad%vmr(j)

These variables are set up in the subroutines:

input_pTprof@input_m	**input_vmrprof@input_m**
input_pTgradprof@input_m	**input_vmrgradprof@input_m**
input_contprof@input_m	**input_Tvibprof@input_m**
input_Tvibgradprof@input_m	

Herein the profiles are read from the files (one extra file for each subroutine; the

[1] though new versions of KOPRA handle non-LTE/LTE population ratios instead of vibrational temperatures the name give_Tvib and variables with Tvib are not changed internally

file names are defined in *kopra.inp*; standard names are: *pt.prf, vmr.prf, ptgra.prf, vmrgra.prf, cont.prf, Tvib.prf, Tvibgra.prf* in directory *kopra/input/profiles/*). In these files the profiles can be on arbitrary altitude grids (one grid per file). They are interpolated/extrapolated linearly (only the pressure and pressure-gradient logarithmic) to the input level altitudes (**inprof(i)%alt**) defined in *kopra.inp*. Furthermore, for single isotopomeres of species the vmr and vmr-gradient profiles are multiplied by the isotopic abundance profile in subroutine **isomult@input_m**. (The isotopic abundances are stored in variable **mol()%iso()%abunprof()** which is initialized in **input_isoprof@input_m** by reading from file; standard name: *kopra/input/profiles/isoabu.prf*.)
After this initialization of the **inprof()%**-variables the user can select if the p/T/altitude profiles should be recalculated taking into account hydrostatic equilibrium (**make_hydroequi@input_m, press@varsub_m, alti@varsub_m, g@varsub_m**). To put pressures into hydrostatic equilibrium the following procedure is used:
First, the actual layer (between level i and $i+1$) is subdivided into n sub-layers of 0.1 km thickness. In a loop over the sub-levels $j=1$ to n the pressure is determined iteratively ($j=1$ corresponds to level i and $j=n+1$ to level $i+1$):

$$p_{j+1} = p_j \exp\left(-\frac{M_{air}(z_j)}{y(p_j,T_j)R} g\left(\varphi, z_j\right) \frac{z_{j+1}-z_j}{\left(T_{j+1}+T_j\right)/2}\right) \tag{1}$$

with z_j, z_{j+1} the sub-level altitudes [km], T_j, T_{j+1} the sub-level temperatures [K] which are interpolated linearly in altitude between the level temperatures T_i and T_{i+1}, p_j, p_{j+1} the level pressures [hPa], φ the geographical latitude, and R the gas-constant. The gravitational acceleration g is:

$$g(\varphi, z) = \left[g_0(\varphi) + \omega^2 R_c \cos^2\varphi\right] \left[\frac{R_e}{R_e+z}\right]^2 - \omega^2 \left[R_c + z\right] \cos^2\varphi \tag{2}$$

with $R_e(\varphi)$ the local distance to the earth's center, $R_c(\varphi)$ the distance to the y-axis of the ellipse along the ellipse's normal, ω the earth's angular velocity, and the empirical formula for the gravitational acceleration at ground:

$$g_0(\varphi) = 9.80616 \cdot (1 - 0.0026373 \cdot \cos 2\varphi + 0.0000059 \cdot \cos^2 2\varphi) \tag{3}$$

$$R_c(\varphi) = \frac{a}{\sqrt{1-\left(1-\frac{b^2}{a^2}\right)\sin^2\varphi}} \tag{4}$$

$$R_e(\varphi) = R_c(\varphi)\sqrt{1-\left(1-\frac{b^4}{a^4}\right)\sin^2\varphi}. \tag{5}$$

M_{air} is the molecular mass of air which is composed of the molecular masses and volume mixing ratios of H_2O, CO_2, N_2, O_2, O, and Ar:

$$\begin{aligned} M_{air}(z) \quad = \quad & M_{H_2O} VMR_{H_2O}(z) + M_{CO_2} VMR_{CO_2}(z) + M_{N_2} VMR_{N_2} + \\ & M_{O_2} VMR_{O_2} + M_O VMR_O + M_{Ar} VMR_{Ar}. \end{aligned} \tag{6}$$

The compressibility factor y is given by [1]:

$$
\begin{aligned}
y \;=\; & 1-\frac{p}{T}\left(a_0+a_1T+a_2T^2+(b_0+b_1T)\,VMR_{H_2O}+(c_0+c_1T)\,VMR^2_{H_2O}\right)+\\
& \left(\frac{p}{T}\right)^2\left(d+eVMR^2_{H_2O}\right). \qquad (7)
\end{aligned}
$$

Where

$$
\begin{aligned}
a0 &= 1.58123\times10^{-6}KPa^{-1}\\
a1 &= -2.9331\times10^{-8}Pa^{-1}\\
a2 &= 1.1043\times10^{-10}K^{-1}Pa^{-1}\\
b0 &= 5.707\times10^{-6}KPa^{-1}\\
b1 &= -2.051\times10^{-8}Pa^{-1}\\
c0 &= 1.9898\times10^{-4}KPa^{-1}\\
c1 &= -2.376\times10^{-6}Pa^{-1}\\
d &= 1.83\times10^{-11}K^2Pa^{-2}\\
e &= -0.765\times10^{-8}K^2Pa^{-2}.
\end{aligned}
$$

2.2 Use of input profiles in give-functions

In the give-functions the input-profiles are interpolated to a position (indicated by latitude: lat, longitude: lon, and altitude: z) in the atmosphere.
The interpolation in altitude between two levels is performed linearly in temperature, non-LTE/LTE population ratio and volume mixing ratio and logarithmic in pressure.
The horizontal interpolation is computed in the following way:
at the position of the profile (lat_0, lon_0), also the local gradient profiles in south-direction and the gradients orthogonal to the south-direction are given in units of the atmospheric quantity per km. Then the local tangent plane at the point of the profile is constructed. The geolocation of the position to which the interpolation should be done (lat,lon) is projected (central projection outgoing from the earth's center) into this plane. In the tangent plane the interpolation of the profile to (lat,lon) at one distinct altitude z is done by:

$$
\begin{aligned}
y(lat,lon,z)=y(lat_0,lon_0,z) \;&+\; dx(lat,lon)\cdot grad_x(lat_0,lon_0,z) \qquad (8)\\
&+\; dy(lat,lon)\cdot grad_y(lat_0,lon_0,z)
\end{aligned}
$$

With grad_x and grad_y the gradient profiles interpolated to the altitude z, y(lat_0,lon_0,z) the profile value at z, and the (orthogonal) distances dx and dy:

$$
\begin{aligned}
dx &= \frac{R_e\arccos(z')}{\sqrt{x'^2+y'^2}}x' \qquad (9)\\
dy &= \frac{R_e\arccos(z')}{\sqrt{x'^2+y'^2}}y'
\end{aligned}
$$

With the earth's radius R_e and the Cartesian co-ordinates x', y', z' of the position (lat,lon) relative to a co-ordinate system centered at the earth's center and z-axis through (lat_0,lon_0). This system is constructed outgoing from an earth centered system with z-axis through north pole and x-axis through (0°,0°): first rotate around z-axis so that the x-axis is now at (0°,lon_0) and then rotated around new y-axis until z-axis is at (lat_0,lon_0):

$$\begin{aligned} x' &= \cos(lat)\cdot\cos(lon-lon_0)\cdot\sin(lat_0)-\sin(lat)\cdot\cos(lat_0) \\ y' &= \cos(lat)\cdot\sin(lon-lon_0) \\ z' &= \cos(lat)\cdot\cos(lon-lon_0)\cdot\cos(lat_0)+\sin(lat)\cdot\sin(lat_0) \end{aligned} \tag{10}$$

3 Layering

As stated before the layering of the atmosphere is very important for the performance (regarding quality of the results and computing time) of the code. The starting point for the layering are the so-called base-levels which are fixed. Their **n%baselev** altitudes are stored in variable **accu%basealt()** which is initialized in **input_main@input_m**. Depending on the switch **sw%baselev** :
0) the input-profile levels (**inprof()%alt**) from *kopra.inp ($7.32)* are used exclusively, or
1) the input-profile levels (**inprof()%alt**) are used and additional levels are introduced in subroutine **make_modelgrid@modlev_m**, or
2) new base-levels are read from *kopra.inp ($7.32)*, or
3) new base-levels are read from *kopra.inp ($7.32)* and additional levels are introduced in subroutine **make_modelgrid@modlev_m**, or
4) the levels are set up automatically in **make_modelgrid@modlev_m**.

For cases 1), 3), and 4) starting from the base-levels KOPRA introduces additional layers depending on three criteria:
1. pressure variation between two levels,
2. temperature variation between two levels, and
3. a finer layering near tangent points.

The layering is performed by calling subroutine **make_modelgrid@modlev_m**. In detail the following procedure is adopted:

- in **grid_t_hw@ modlev_m** according to absolute temperature variation (maximum **accu%Tvar1, accu%Tvar2**) and relative pressure variation (maximum **accu%wvar**) additional levels are introduced in the middle between two successive levels in a recursive procedure. For levels below **accu%zTvar** km **accu%Tvar1** and above **accu%zTvar** km the maximum T-variation **accu%Tvar2** is used.
- in **grid_tang@modlev_m** up to **accu%upto** km above all tangent altitudes additional levels with maximum spacing of **accu%dif** km are inserted.
- in **min_distance@modlev_m** all levels which are no base-levels and which are less than **accu%dmin** km apart are deleted.
- the resulting **n%modlev** model level altitudes are stored in variable **modprof()%alt**.

Bibliography

[1] P. E. Ciddor, "Refractive index of air: new equations for the visible and near infrared", *Appl. Opt.* **35(9), 1996.**