

Chapter 3

The Radiative Transfer Model SARTre

The [Approximate] **S**pherical **A**tmospheric **R**adiative **T**ransfer model SARTre has been developed to provide a consistent tool for modeling radiative transfer of both solar and terrestrial radiation. In particular, emission as well as scattering of radiation can be taken into account as sources of light over the spectral range from ultraviolet to microwaves. SARTre is designed for monochromatic, high spectral resolution forward modeling of arbitrary observing geometries in spherical shell atmospheres. Emphasis has been placed on the ability of modeling limb radiances. As far as possible, modules of other, well-tested RT packages have been implemented. That includes modules from MIRART for the line-by-line calculation of molecular absorption cross sections as well as the DISORT package, used for the calculation of the incident radiation field when taking multiple scattering into account.

The basic concepts of SARTre for the calculation of intensity measurements are presented in section 3.1. Beside explaining the technique for solving the radiative transfer equation, it includes a description of the source terms taken into account. Sections 3.2 and 3.3 deal with the handling of the optical properties of molecular and particulate matter, respectively. A brief summary of the DISORT package is given in section 3.4. Issues of observational geometry are addressed in section 3.5. The structrogram of Fig. 3.1 shows the flow of data in the SARTre model and illustrates the relations between the individual modules of the program.

3.1 Basic Principles

Unlike plane-parallel radiative transfer models, that derive the radiation field of the complete atmosphere by solving a coupled system of integro-differential equations describing the transfer of radiation (Eq. (2.6)), most spherical models, and SARTre in particular, apply the Source Function Integration Technique. By using the integral form of the radiative transfer equation Eq. (2.7), contributions from radiation sources are “collected” along the observer’s line of sight and transmitted to the instrument following the Lambert-Bouguer-Beer law Eq. (2.3).

This technique yields great advantage, when source terms are only dependent on atmospheric conditions along the line of sight, which is usually valid for thermal emission. Scattering sources on the other hand depend on the incident radiation and, thus, on conditions in the vicinal or whole atmosphere. Issues on handling scattering source terms when solving the integral radiative

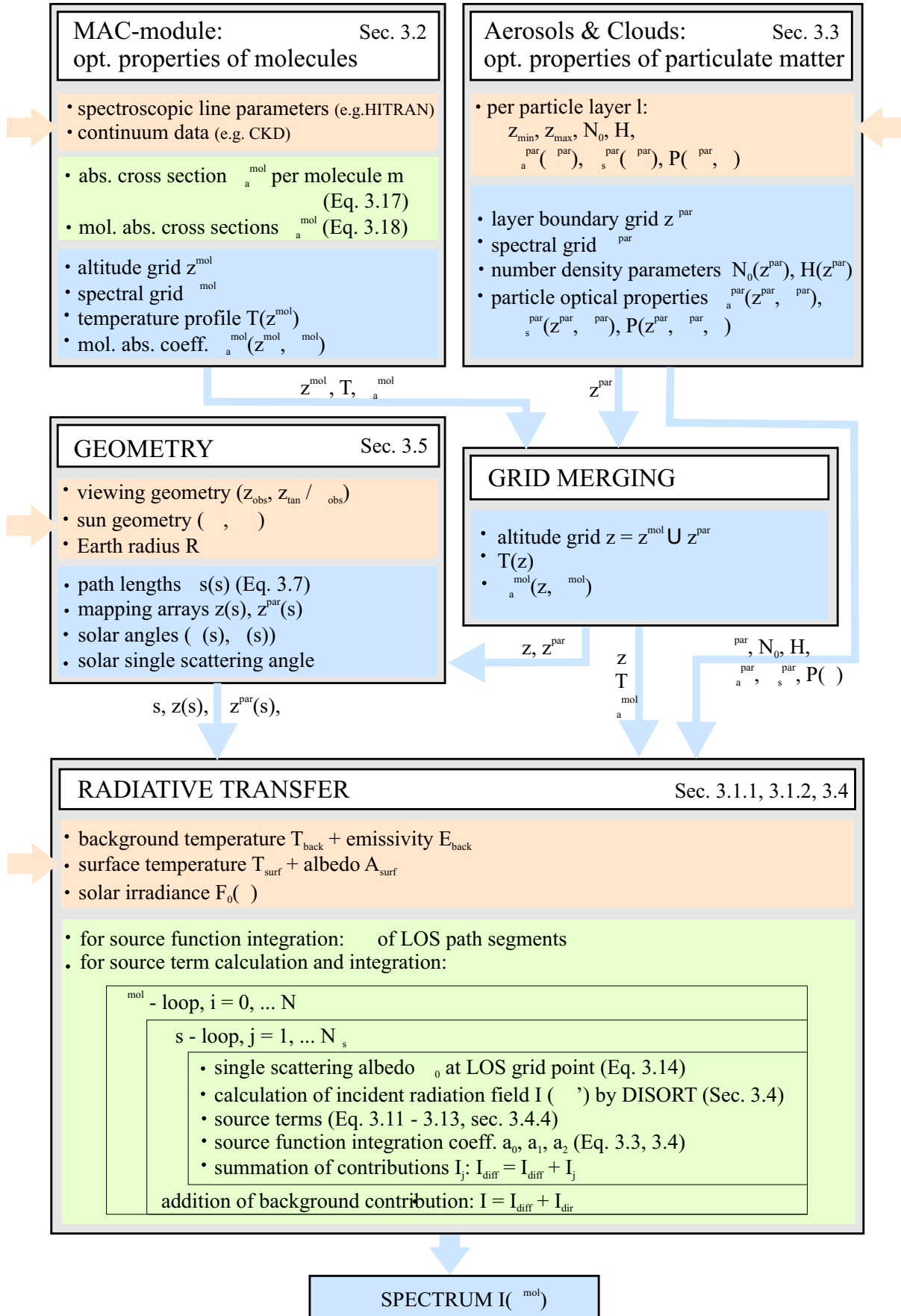


Figure 3.1: Structure of the SARTRE model

transfer equation (RTE) are addressed in subsection 3.1.2. However, obtaining global solutions of radiation fields for spherical atmospheres is a complex and costly task. Although some effort has been made (Walter and Landgraf, 2005), models that provide a closed-ended¹ universal solution in analogy to that of plane-parallel models do not exist yet.

3.1.1 Source Function Integration Technique

As pointed out previously, applying the Source Function Integration Technique basically means to calculate the intensity of radiation, incident to an instrument from a certain direction, by solving the integral form of the RTE:

$$I = I_{\text{dir}} e^{-\tau} + \int_0^{\tau} J(\tau') e^{-\tau'} d\tau', \quad (3.1)$$

where I_{dir} denotes direct attenuated radiation. Beside the direct solar beam in case of occultation measurements, I_{dir} can be used to describe background emission of the cold space for uplooking and limb geometries or surface emission for downlooking cases. J contains the sources of radiation and τ is the optical depth of the medium, measured from the observer along the line of sight (LOS). Splitting the LOS into N path segments, Eq. (3.1) can be rewritten as

$$I = I_{\text{dir}} e^{-\sum_{n=1}^N \Delta\tau_n} + \sum_{n=1}^N \left(e^{-\sum_{m=1}^{n-1} \Delta\tau_m} \int_0^{\Delta\tau_n} J_n e^{-\Delta\tau'} d\Delta\tau' \right), \quad (3.2)$$

with $\Delta\tau_n$ being the path optical depth of segment n of the LOS. Assuming linear interpolation of the source terms J_n within each path segment, the source integral can be solved analytically. The contribution from the individual path segments then can be expressed in terms of source terms evaluated at discrete path grid points and coefficients depending on the path segments optical depth:

$$\begin{aligned} \int_0^{\Delta\tau_n} J_n e^{-\Delta\tau'} d\Delta\tau' &= \int_0^{\Delta\tau_n} \left(\frac{\Delta\tau_n - \Delta\tau'}{\Delta\tau_n} J_n(0) + \frac{\Delta\tau'}{\Delta\tau_n} J_n(\Delta\tau_n) \right) e^{-\Delta\tau'} d\Delta\tau' \\ &= \frac{\Delta\tau_n - 1 + e^{-\Delta\tau_n}}{\Delta\tau_n} J_n(0) + \frac{1 - e^{-\Delta\tau_n} - \Delta\tau_n e^{-\Delta\tau_n}}{\Delta\tau_n} J_n(\Delta\tau_n) \\ &= a_{1,n} J_n(0) + a_{2,n} J_n(\Delta\tau_n). \end{aligned} \quad (3.3)$$

When further defining

$$a_{0,n} = e^{-\sum_{m=1}^{n-1} \Delta\tau_m} \quad (3.4)$$

then Eq. (3.2) can finally be written as

$$I = I_{\text{dir}} a_{0,N} + \sum_{n=1}^N a_{0,n} (a_{1,n} J_n(0) + a_{2,n} J_n(\Delta\tau_n)). \quad (3.5)$$

¹Closed-ended refers to an analytic or numeric solution of a system of coupled equations in contrast to iterative or statistical solutions as provided by successive order of scattering and Monte Carlo methods, respectively.

Basically, this linear-in- τ -parameterization of the source function is equivalent to a Gauss-Laguerre quadrature with linear interpolation assumption of the non-exponential integrand. Concerning accuracy of the quadrature, the line of sight has to be split into appropriate path segments over which linearity can be assumed. Eq. (3.5) is evaluated at discrete spectral points, i.e. monochromatic RT is modeled. Beside geometric parameters, e.g. path lengths and angles, all variables are spectrally dependent. However, subscripts denoting spectral dependency have been omitted for better readability within this chapter.

According to Eq. (2.4) $\Delta\tau$ describes the extinction, integrated along a path segment, which – neglecting Rayleigh scattering – is caused by molecular absorption on the one hand and scattering as well as absorption by particles on the other. With optical properties of gaseous matter and particles handled separately in SARTre, for $\Delta\tau$ applies

$$\Delta\tau = \Delta\tau^{\text{mol}} + \Delta\tau^{\text{par}}, \quad (3.6)$$

where $\Delta\tau^{\text{mol}}$ is the optical depth of the gaseous matter and $\Delta\tau^{\text{par}}$ denotes the particle optical depth. However, particle and molecular extinction are commonly given with respect to altitude z .

In a spherical atmosphere, altitude and length of a path segment Δs of an arbitrary LOS relate to each other by

$$\Delta s = \left| \sqrt{(R+z+\Delta z)^2 - (R+z_{\text{tan}})^2} - \sqrt{(R+z)^2 - (R+z_{\text{tan}})^2} \right|, \quad (3.7)$$

where R is the radius of the Earth or planet, z the altitude and Δz the change in altitude along the path segment of the LOS with tangent altitude z_{tan} (for non-limb cases, $z_{\text{tan}} < 0$). Differentiating Eq. (3.7) concerning Δz and substituting dz in Eq. (2.4) by ds leads to the so-called Chapman function (Kylling et al., 1995), which may generally not be evaluated analytically. The commonly used approximation (e.g. Dahlback and Stamnes, 1991) of $\Delta\tau_s = \Delta\tau_z \cdot \Delta s / \Delta z$, with $\Delta\tau_s$ and $\Delta\tau_z$ denoting the optical depth in path length Δs and layer thickness Δz , respectively, did not seem appropriate to derive the optical depth $\Delta\tau$ of a path segment with proper accuracy. In particular, this approximation is critical for path segments close to the tangent point of limb LOS.

Hence, a second order polynomial

$$\beta_e(\Delta s) = a \cdot \Delta s^2 + b \cdot \Delta s + c \quad (3.8)$$

is assumed to describe $\beta_e(s)$. Coefficients a , b and c are derived for individual path segments from extinction coefficients at the two altitude levels adjacent to the layer crossed by the LOS path segment and a third point at mean layer altitude. Extinction coefficients at the mean altitude are interpolated or calculated from scaling height dependency for gaseous matter and particles, respectively (see sections 3.2 and 3.3). For path segment optical depth $\Delta\tau$ follows from Eq. (2.4) and Eq. (3.8)

$$\Delta\tau(\Delta s) = \frac{a}{3} \cdot \Delta s^3 + \frac{b}{2} \cdot \Delta s^2 + c \cdot \Delta s \quad (3.9)$$

3.1.2 The Sources

As pointed out before, SARTre is capable of modeling solar and terrestrial radiative transfer. That means, both scattering of radiation from a beam source outside the atmosphere and emission as internal or imbedded source (Thomas and Stamnes, 1999, pg. 198) may be taken into

account. Furthermore, multiple scattered radiation can be included, regardless whether it is of solar or terrestrial origin. Thus, source term J from Eq. (3.1) is defined by

$$J = J_B + J_{SS} + J_{MS} \quad (3.10)$$

$$\text{with } J_B = (1 - \omega_0) B(T) \quad (3.11)$$

$$J_{SS} = \omega_0 \frac{1}{4\pi} P(\Theta_\odot) F_\odot \mathcal{T}_\odot \quad \text{and} \quad (3.12)$$

$$J_{MS} = \omega_0 \frac{1}{4\pi} \int_0^{4\pi} P(\Theta) I(\Omega') d\Omega', \quad (3.13)$$

where J_B describes thermal emission, J_{SS} the single scattering of solar radiation and J_{MS} multiple scattered radiation, respectively. For downlooking cases, J_{SS} further includes the contribution from solar radiation, transmitted from top-of-atmosphere (TOA) and reflected by the surface into the LOS. However, SARTre may also be used for separate modeling of either solar or terrestrial radiative transfer with or without multiple scattering.

According to the concept of source function integration explained in the previous subsection, source terms are evaluated at discrete grid points along the LOS. In a spherical shell atmosphere, single scattering albedo ω_0 , Planck emission term $B(T)$ and phase functions $P(\Theta_\odot)$ and $P(\Theta)$ depend on the altitude of the grid point. Thus, they are calculated only once per altitude level. The transmission \mathcal{T}_\odot of the solar beam from TOA to the LOS grid points as well as the incident radiation field $I(\Omega')$, required for the calculation of J_{MS} , have to be evaluated according to the individual grid point position along the LOS. F_\odot is the solar irradiance, which may be given via a look-up table from outside of SARTre (e.g. extracted from MODTRAN) or calculated by Planck's law for an arbitrary, input defined temperature.

The single scattering albedo ω_0 describes the scattering albedo of the ‘‘mixed’’ atmospheric medium at a discrete grid point of the LOS, i.e. is calculated from molecular and particle optical properties by

$$\omega_0 = \frac{\beta_s^{\text{par}}}{\beta_s^{\text{par}} + \beta_a^{\text{par}} + \beta_a^{\text{mol}}}, \quad (3.14)$$

where β_s and β_a are scattering and absorption coefficients with superscripts ‘mol’ and ‘par’ denoting properties of molecular and particulate matter, respectively. Although Rayleigh scattering might be taken into account equivalent to particle scattering (see section 3.3), it is basically not considered automatically. Thus, $\beta_s^{\text{mol}} \equiv 0$ applies in SARTre. The transmission of the solar beam \mathcal{T}_\odot is calculated according to Eq. (2.5), with τ_\odot derived by the same routines as used for optical depth calculation along the LOS, just replacing the instrumental LOS by the solar beam path.

Due to the definition of particle properties on the basis of atmospheric layers (for details see subsection 3.1.3), parameters related to particle properties within a layer (i.e. ω_0 , $P(\Theta_\odot)$, and $P(\Theta)$) get assigned two values per level based grid point, according to the different particle properties of the two adjacent layers. That means, source terms $J_n(\Delta\tau_n)$ and $J_{n+1}(0)$, evaluated from particle parameters valid for path segments n and $n+1$ through adjacent layers, may differ, although they basically correspond to the same grid point along the LOS.

With the spectral grid defined by the line-by-line routines (see section 3.2), properties of particles (aerosols and clouds) have to be interpolated from their much coarser spectral grid to

the monochromatic grid for RT calculation in SARTre. Currently, spectral interpolations are in principle done linearly, such that

$$\beta(\nu_{\text{mol}}) = \frac{\nu_{\text{par}}^{\text{r}} - \nu_{\text{mol}}}{\nu_{\text{par}}^{\text{r}} - \nu_{\text{par}}^{\text{l}}} \beta(\nu_{\text{par}}^{\text{l}}) + \frac{\nu_{\text{mol}} - \nu_{\text{par}}^{\text{l}}}{\nu_{\text{par}}^{\text{r}} - \nu_{\text{par}}^{\text{l}}} \beta(\nu_{\text{par}}^{\text{r}}) \quad \text{and} \quad (3.15)$$

$$\begin{aligned} \beta_{\text{s}}(\nu_{\text{mol}}) P(\Theta, \nu_{\text{mol}}) &= \frac{\nu_{\text{par}}^{\text{r}} - \nu_{\text{mol}}}{\nu_{\text{par}}^{\text{r}} - \nu_{\text{par}}^{\text{l}}} \beta_{\text{s}}(\nu_{\text{par}}^{\text{l}}) P(\Theta, \nu_{\text{par}}^{\text{l}}) \\ &+ \frac{\nu_{\text{mol}} - \nu_{\text{par}}^{\text{l}}}{\nu_{\text{par}}^{\text{r}} - \nu_{\text{par}}^{\text{l}}} \beta_{\text{s}}(\nu_{\text{par}}^{\text{r}}) P(\Theta, \nu_{\text{par}}^{\text{r}}), \end{aligned} \quad (3.16)$$

where β represents the absorption, scattering or extinction coefficients β_{a} , β_{s} , and β_{e} , respectively. For the grid points of the fine spectral grid at wavenumber ν_{mol} applies $\nu_{\text{par}}^{\text{l}} \leq \nu_{\text{mol}} \leq \nu_{\text{par}}^{\text{r}}$.

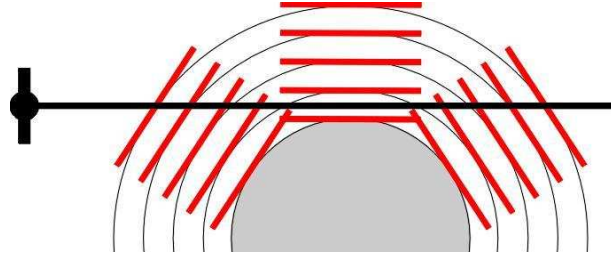


Figure 3.2: *Local planarity assumption in a spherical atmosphere. The incident radiation field at grid points along the LOS is derived in a local plane-parallel atmosphere, indicated in red.*

Out of the source terms that can be taken into account by SARTre, J_{B} and J_{SS} are calculated with full respect to the sphericity of the Earth-atmosphere system. Multiple scattering source term J_{MS} requires the knowledge of the incident radiation field $I(\Omega')$. Assuming a local planarity of the Earth and atmosphere, as indicated by Fig. 3.2, $I(\Omega')$ is derived within a plan-parallel atmosphere, using the DISORT radiative transfer package (Stamnes et al., 1988).

The resulting radiation field from DISORT is provided to SARTre in terms of azimuthally decomposed intensity fields $I^m(\theta')$ expanded in a Fourier cosine series, where m denotes the order of expansion and θ' is the zenith angle. The integral of the incident radiation field convoluted with the phase function $P(\Theta)$, with scattering angle Θ being dependent on incident and scattering direction Ω' and Ω , respectively, is solved on the basis of intensity and phase function expanded into Legendre terms (see subsection 3.4.3). Except for deriving $I(\Omega')$ from a plane-parallel model, source term J_{MS} is handled in a spherical atmosphere. I.e. contributions from multiple scattering are calculated for local parameter values assigned to the individual grid points along the LOS through a spherical atmosphere, e.g. direction Ω of the LOS and sun position.

3.1.3 Describing Atmospheric Conditions – The Philosophy of Levels and Layers

Basically, two ways of describing atmospheric conditions in RT modeling do exist. Assuming a one dimensional atmosphere, parameters are either defined at levels, given in terms of e.g. altitude or pressure, or on the basis of commonly homogeneous layers. Regarding “natural” behavior as well as computational means, there exist good reasons for both ways of definition.

First, in nature some parameters and quantities, e.g. temperature and pressure, do vary continuously in space in general and in altitude in particular, while others form layers (or clusters) with rather distinct boundaries. For instance, aerosols and clouds are often described to occur in relatively homogeneous layers with in comparison to that fast changing properties towards the layer boundaries.

Second, continuous level based data allows for the application of sophisticated quadrature methods without the need for explicit assumption about the behavior of the quantities in between the levels. Furthermore, obtaining derivatives basically requires a continuous definition of the parameters as well. On the other hand, integration over homogeneous layers is straight forward, and homogeneous layering permits the mathematical formulation of RT by a system of coupled equations, each describing radiative processes in a homogeneous layer.

In summary, depending on the focus of the model, both concepts are advantageous for certain tasks and can be found applied in RT models. For example, DISORT, MOMO (Fell and Fischer, 2001), and KOPRA (Stiller, 2000) solve the radiative transfer equation(s) on the basis of homogeneous layers, while MIRART (Schreier and Böttger, 2003) and SHSG (Evans, 1993) apply the level approach.

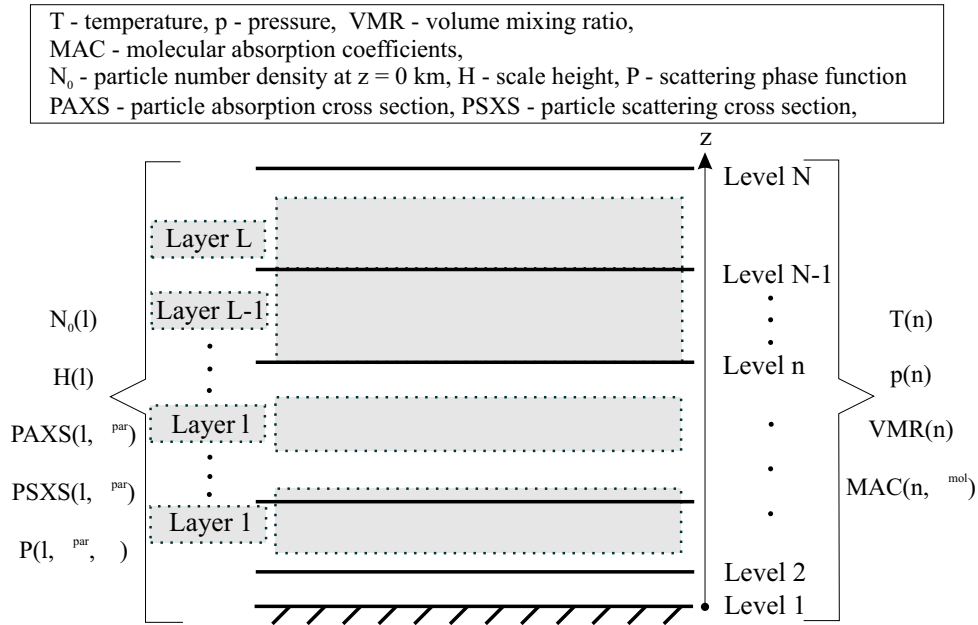


Figure 3.3: In SARTre, particle properties are described on layer basis (left). Atmospheric properties required for LbL-calculations are defined on discrete levels (right). Layers are not allowed to overlap, but do not need to adjoin each other or meet level altitudes.

With its heritage from the level based MIRART model, the definition of temperature, pressure and volume mixing ratios of (trace) gases on atmospheric levels has been kept within SARTre. But, according to the philosophy of DISORT as well as of WCRP's standard atmosphere definition (World Climate Research Program, 1986), aerosol and cloud properties are defined on the basis of atmospheric layers (see Fig. 3.3). Homogeneity within a layer thereby refers to microphysical (size distribution, shape) and optical properties (absorption and scattering cross sections, scattering phase function). It does not refer to particle number density, which is permitted to vary exponentially described by scale height (for more details see section 3.3).

To derive a consistent altitude grid in RT computation, both grids are merged within SARTre by inserting the layer boundary altitudes into the level grid and interpolating level based quantities to the inserted altitude levels. Interpolation is done linearly for temperature, but exponentially for pressure and volume mixing ratios. To reduce the amount of memory used, aerosol and cloud data is continued to be managed on initial layers and only transformed to another grid when required for the radiative transfer calculations.

3.2 Calculating Properties of Molecular Atmospheric Constituents

As a spectral high resolution RT model SARTre derives absorption properties of atmospheric (trace) gas constituents on the basis of line-by-line (LbL) calculations of the absorption cross sections of the individual molecules. The complete set of routines used for the computation of LbL cross sections and molecular absorption coefficients is taken from the MIRART package as a complete module, below called the MAC-module. This module is furthermore responsible for the initial definition of altitude and spectral grids. The input, required by the the MAC-module includes information about

- the molecules, which shall be considered
- the line shape to be applied for each molecule
- the spectroscopic database to use
- atmospheric profiles of temperature, pressure, and volume mixing ratio of each molecule
- continua to take into account.

The output provided to other SARTre modules contains

- monochromatic molecular absorption coefficients $\beta_m \text{athrma}^{\text{mol}}(z_{\text{mol}}, \nu_{\text{mol}})$
- altitude grid z_{mol}
- spectral grid ν_{mol}
- temperature profile $T(z_{\text{mol}})$.

A description of the LbL calculation concept is given in the following subsection. In subsection 3.2.2 the derivation of molecular absorption coefficients is explained briefly.

3.2.1 Line-by-Line Calculation of Molecular Absorption Cross Sections

According to Eq. (2.15), the absorption cross section of a molecule m due to line l at position ν_0^l is given by

$$\sigma_a^{m,l}(\nu) = S^{m,l}(T) F(\nu - \nu_0^l, T, p). \quad (3.17)$$

Spectroscopic line parameters like line strength at standard temperature $S(T_0)$ and line position ν_0 of all lines in a defined spectral interval are read from a spectroscopic line catalog, for each molecule individually. Further line parameters are required for the temperature conversion of

$S(T_0)$ to $S(T)$ according to Eq. (2.16). Temperature conversion of the partition function $Q(T)$ thereby follows the scheme used in the ATMOS software (Norton and Rinsland, 1991) with separate conversions of the rotational and vibrational partition functions. Spectroscopic line databases, which can be accessed by the SARTre MAC-module, are HITRAN (Rothman et al., 2005), JPL (Pickett et al., 1998), HiTemp (Rothman et al., 1995), SAO (Chance et al., 1994), and GEISA (Jacquinet-Husson et al., 1999).

Concerning line shape function F , Lorentz and Voigt line shape (Eqs. (2.17) and (2.21)) as well as Van Vleck–Huber line shape (van Vleck and Huber, 1977) are implemented. For the calculation of the Voigt line shape function, the MAC-module is able to use diverse optimized approaches (Schreier, 1992), e.g. inspired by Humlicek (1982); Hui et al. (1978); Kuntz (1997).

Since temperature T and pressure p depend on altitude, all calculations have to be done per altitude level. The wavenumber grid is chosen individually for each altitude level and molecule. A joint wavenumber grid is not established until the calculation of absorption coefficients.

3.2.2 Deriving Molecular Absorption Coefficients

With the absorption cross sections given at individual spectral grids for each molecule and altitude, a joint wavenumber grid has to be provided for summing up the contributions from all molecules to molecular absorption coefficients. The final wavenumber grid is determined by the finest of the individual grids. Interpolation from the coarser to the output spectral grid can be done by first to third order polynomials.

Spectral absorption coefficients are derived by summing up absorption cross sections σ_a^m of all the molecules m weighted by the corresponding number density n_m , derived from the volume mixing ratio and air density:

$$\beta_a^{\text{mol}}(\nu) = \sum_m (n_m \sigma_a^m(\nu) + \beta_{\text{ac}}^m(\nu)). \quad (3.18)$$

Additionally continuum absorption β_{ac}^m might be considered for individual molecules. Currently, Clough-Kneizy-Davies (CKD) continuum data from Clough et al. (1989) has been used with SARTre.

As mentioned before, the output of the MAC-module includes the absorption coefficients in terms of altitude and wavenumber, but no cross section data. Hence, the transformation of the molecular absorption data to further altitude levels, e.g. when merging with the particle altitude grid or deriving parameters at mean altitudes for $\Delta\tau$ calculation (see subsection 3.1.1), is done by logarithmic interpolation of absorption coefficients.

3.3 Particle Properties

Currently, for RT modeling with SARTre properties of particle layers are generally taken from external sources, e.g. from OPAC (Hess et al., 1998) and the ice particle database of Yang et al. (2005). Spectrally resolved scattering and absorption cross sections and scattering phase function with respect to scattering angle are provided to SARTre by data files. These optical properties are assumed to be constant over the whole layer in horizontal and vertical direction.

Following the aerosol model concept of World Climate Research Program (1986), a particle layer is furthermore defined by its minimum and maximum altitude z_{min} and z_{max} , respectively,

(virtual) particle number density N_0 at altitude $z = 0$ km and scale height H . Particle number density $N(z)$ is given by

$$N(z) = N_0 e^{-z/H}, \quad (3.19)$$

and absorption and scattering coefficients are derived by

$$\begin{aligned} \beta_{a/s}^{\text{par}}(z) &= \sigma_{a/s}^{\text{par}} \cdot N(z) \\ &= \sigma_{a/s}^{\text{par}} \cdot N_0 e^{-z/H}. \end{aligned} \quad (3.20)$$

No mixing of particulate matter inside SARTre is possible, i.e. overlapping of particle layers is not permitted, but optical properties of polydispersions have to be calculated externally. That means, when using databases containing single scattering properties of individual particles, particle regimes have to be mixed and size distribution parameterization has to be applied outside of SARTre.

At the current state, spectral grids of input optical property data are restricted to be the same for all particle layers. All particle layer optical property data is stored and transferred to subsequent routines on the spectral and the layer grid, which is derived directly from input data. Any transformation to the finer spectral and altitude grid, on which the RT equation Eq. (3.5) is solved, is only done at the mere moment when required. Spectral transformation is carried out by interpolation according to Eqs. (3.15) and (3.16), whereas the calculation of parameters on other altitudes follows Eq. (3.20)².

3.4 Deriving the Multiple Scattering Contribution from DISORT

As discussed above, the incident radiation field $I(\boldsymbol{\Omega}')$ required for the characterization of the multiple scattering source term J_{MS} is derived under the assumption of local planarity of the Earth-atmosphere system. For the calculation of $I(\boldsymbol{\Omega}')$ the pseudo-spherical version PSDISORT of the radiative transfer solver DISORT is used. Pseudo-spherical refers to the computation of the direct solar beam attenuation along the path through a spherical shell atmosphere. Nevertheless, the coupled system of integro-differential RT equations is formulated and solved for an atmosphere consisting of plane-parallel layers.

This section gives a brief summary of the discrete ordinate method and its implementation by DISORT. Furthermore, it deals with the preparation of the input parameters required by DISORT and with the handling of the output radiation field $I^m(\theta')$ in processing J_{MS} .

3.4.1 The DISORT Package

DISORT, the **DIS**crete **OR**dinate approximation to the **R**aditive **T**ransfer Equation, refers to the method as well as the computational code to solve the RT problem. Being a well known, freely available RT package, that has been proved to be reliable and stable (Stamnes et al., 1988; Kylling et al., 1995), DISORT has been selected as solving module used within SARTre for the derivation of the incident radiation field required to evaluate source term J_{MS} .

²Considering homogeneous layers, scattering phase function, normalized to unity or 4π , is independent of particle number density. Thus, the phase function is constant within each particle layer and requires no altitude transformation.

DISORT solves the radiative transfer problem for a plane-parallel one-dimensional atmosphere, being a single slab of constant refractive index. However, vertical inhomogeneity is considered by dividing the slab into homogeneous layers, i.e. layers that can be adequately characterized by constant single scattering albedo ω_0 and scattering phase function $P(\Theta)$. Furthermore, the RT solution by DISORT is based on the concept of azimuthal decomposition of phase function, intensity and sources by expanding these quantities into a Fourier cosine series. That allows to solve the integro-differential RT equation given by Eqs. (2.6) and (2.11) separately for each order of expansion, which reduces the computational efforts and memory requirements significantly. However, the phase function has already to be provided to DISORT in expansion coefficients and azimuthally decomposed intensities are used to characterize the incident radiation field, further processed within SARTre. Hence, azimuthal decomposition as done in SARTre is explained in subsections 3.4.3 and 3.4.4.

For solving the integro-differential RT equations for individual orders of expansion, they are converted to ordinary differential equations by replacing the scattering integrals by quadrature sums and formulating Eq. (2.6) for discrete upward and downward directions $+\mu_i$ and $-\mu_i$:

$$\begin{aligned} \pm\mu_i \frac{dI^m(\tau, \pm\mu_i)}{d\tau} &= I^m(\tau, \pm\mu_i) \\ &\quad - \frac{\omega_0}{4\pi} \sum_{j=1}^N w_j \left[p_m(\pm\mu_i, +\mu_j) I^m(\tau, +\mu_j) + p_m(\pm\mu_i, -\mu_j) I^m(\tau, -\mu_j) \right] \\ &\quad - S^m(\tau, \pm\mu_i), \end{aligned} \quad (3.21)$$

with $\mu = \cos \theta$ and θ denoting zenith angle. I^m , S^m and p_m are expansion terms of order m of the intensity, radiation field independent source terms ($S = J_B + J_{SS}$) and phase function, respectively, and ω_0 denotes the single scattering albedo. N is the number of discrete directions considered over a hemisphere with $N_{\text{str}} = 2N$ being the total number of quadrature terms or “streams”. Quadrature ordinates μ_j and weights w_j are chosen according to the Double-Gauss quadrature method.

The N_{str} equations given by Eq. (3.21) can be rewritten in matrix form:

$$\frac{d}{d\tau} \begin{bmatrix} \mathbf{I}^+ \\ \mathbf{I}^- \end{bmatrix} = \begin{bmatrix} -\tilde{\alpha} & -\tilde{\beta} \\ \tilde{\beta} & \tilde{\alpha} \end{bmatrix} \begin{bmatrix} \mathbf{I}^+ \\ \mathbf{I}^- \end{bmatrix} - \begin{bmatrix} \mathbf{S}^+ \\ \mathbf{S}^- \end{bmatrix}, \quad (3.22)$$

where \mathbf{I}^\pm and \mathbf{S}^\pm are vectors of intensity and source terms in upward and downward direction, respectively, whereas $\tilde{\alpha}$ and $\tilde{\beta}$ contain optical property characterization and quadrature weights. A solution to the homogeneous version of Eq. (3.22) is gained by assuming an eigenvalue problem with

$$\mathbf{I}^\pm = \mathbf{g}^\pm e^{-k\tau}. \quad (3.23)$$

From solving the algebraic eigenvalue problem for each layer l separately, the eigenvalues k and corresponding eigenvectors \mathbf{g} are determined. $I_l(\tau, \pm\mu_i)$ then is given by

$$I_l(\tau, \pm\mu_i) = \sum_{j=1}^N \left(C_{jl} g_{jl}(\pm\mu_i) e^{-k_{jl}\tau} + C_{-jl} g_{-jl}(\pm\mu_i) e^{k_{jl}\tau} \right) + U_l(\tau, \pm\mu_i), \quad (3.24)$$

with $U_l(\tau, \mu_i)$ denoting the particular solution to Eq. (3.22) of layer l . The coefficients $C_{\pm jl}$ are determined from applying boundary conditions on top and bottom of the atmosphere and

continuity condition at the layer interfaces. From Eq. (3.24) that leads to a coupled system of $(N_{\text{str}} \times L)$ equations, where L denotes the number of layers of the atmosphere. Boundary conditions are given by diffuse radiation incident on top of atmosphere and radiation emitted and reflected by the surface. Continuity conditions can be formulated as

$$I_l(\tau_l, \pm\mu_i) = I_{l+1}(\tau_l, \pm\mu_i) \quad (3.25)$$

for $l = 1 \dots L - 1$, with l as well as τ counted from top to bottom of the atmosphere. A description of deriving the particular solutions $U_l(\tau, \pm\mu_i)$ of Eq. (3.22) can be found in Stamnes and Swanson (1981).

In summary, the discrete ordinate method solves the RT problem by

- dividing the atmosphere into homogeneous layers
- azimuthal decomposition of the integro-differential RT equation by expanding intensity, sources and phase function into a Fourier cosine series
- replacing integrals by quadrature sums
- solving the homogeneous version of the RT equation separately for each layer on the basis of an eigenvalue problem
- deriving the complete solution by applying boundary and continuity conditions.

For the derivation of the radiation field by DISORT L systems of $(N_{\text{str}} \times N_{\text{str}})$ equations each have to be solved for the homogeneous solutions and one system of $N_{\text{str}} \times L$ equations for the complete solution. Hence, the computational effort is proportional to L and N_{str}^2 .

3.4.2 Preparation of DISORT Input

In DISORT, the atmosphere is described by a number of homogeneous layers of vertical optical thickness $\Delta\tau_z$, characterized by single scattering albedo ω_0^{DIS} and scattering phase function $P(\Theta)$, where Θ denotes the scattering angle. Therein, phase function is represented in azimuthally decomposed form by the coefficients or moments χ_m of its Legendre polynomial expansion (explained in subsection 3.4.3).

When considering thermal emission, level based temperature profiles have to be provided. In contrast to path optical thickness parameterization by Eq. (3.9), layer optical thickness is calculated by analytic integration of the explicitly given or assumed exponential change of particle and molecular scattering/absorption coefficients, respectively, within a layer. Due to the level based definition of molecular absorption coefficients within SARTre, single scattering albedo is not necessarily constant within a layer. For DISORT a representative average single scattering albedo of the layer is calculated by

$$\begin{aligned} \omega_0^{\text{DIS}} &= \frac{\Delta\tau_s^{\text{par}}}{\Delta\tau^{\text{mol}} + \Delta\tau^{\text{par}}} \quad (3.26) \\ &= \frac{\int_{z_{\text{min}}}^{z_{\text{max}}} N(z) \sigma_s^{\text{par}} dz}{\int_{z_{\text{min}}}^{z_{\text{max}}} N(z) (\sigma_s^{\text{par}} + \sigma_a^{\text{par}}) dz + \int_{z_{\text{min}}}^{z_{\text{max}}} \beta_a^{\text{mol}} dz}, \end{aligned}$$

where $\Delta\tau_s^{\text{par}}$ denotes the optical depth due to particle scattering, $\Delta\tau^{\text{mol}}$ and $\Delta\tau^{\text{par}}$ are the total molecular and particle optical depth of the layer, respectively.

The pseudo-spherical PSDISORT furthermore requires information about geometrical layer thickness for adjustment of solar beam path lengths through the spherical atmosphere. Although DISORT can basically deal with δ -scaling of RT, this option has not been used with SARTre yet when dealing with highly peaked scattering phase functions.

Parameters describing boundary conditions (temperature and albedo of the Lambertian surface, background temperature and emissivity, solar irradiance) are passed from SARTre input without any changes. Sun geometry is defined by local zenith angle and local relative azimuth to the LOS, which are calculated by SARTre's geometry module for each grid point along the line of sight. Observer angles are set to default values, since the DISORT output used by SARTre is the intensity field expanded in Legendre terms. Intensity in observer direction itself is of no interest.

The number of streams N_{str} , or discrete zenith directions, in the RT calculation as well as the number of Legendre terms N_m to be considered are SARTre input parameters, passed to DISORT. However, to assure accurate azimuthal decomposition, controlled by an adjustable error threshold parameter within SARTre, the number of Legendre terms can optionally be adjusted automatically to an appropriate value (see following subsection for details). Due to restrictions of the discrete ordinate method, $N_{\text{str}} \geq N_m$ has to be met. Thus, adjusting N_m might effect N_{str} .

3.4.3 Legendre Expansion of Scattering Phase Function

In modeling plane-parallel RT, azimuthal decomposition of the RT equation has been found an approved method for e.g. significant reduction of computation time and memory (Fell, 1997) in combination with high accuracy of the solution. Azimuthal decomposition of scattering phase function, intensities and source terms is done by appropriate series expansion. Doing so, RT equations can be solved separately for each order of expansion. Applying azimuthal decomposition requires the scattering phase function to be given in dependence of scattering angle, instead of a bidirectional function. Although that means, only spherical or randomly oriented particles can be considered accurately, the use of DISORT demands for Legendre expansion.

While for intensities and source terms Fourier expansion is commonly used (see following subsection), decomposition of the scattering phase function is based on expansion in terms of Legendre polynomials:

$$P(\cos \Theta) = \sum_{m=0}^{2M-1} (2m+1) \chi_m \mathcal{P}_m(\cos \Theta), \quad (3.27)$$

with $2M - 1 = N_m - 1$, Θ being the scattering angle and \mathcal{P}_m denoting the m th order Legendre polynomial. For expansion coefficients χ_m follows

$$\chi_m = \frac{1}{2} \int_{-1}^1 P(\cos \Theta) \mathcal{P}_m(\cos \Theta) d \cos \Theta \quad (3.28)$$

$$= \frac{1}{2} \sum_{n=1}^{2N} w_n \cdot P(\cos \Theta_n) \mathcal{P}_m(\cos \Theta_n), \quad (3.29)$$

In SARTre, quadrature weights w_n and ordinates $\cos \Theta_n$ are chosen according to Double-Gauss method of quadrature as proposed by Thomas and Stamnes (1999) with $2N = N_{\text{str}}$. The χ_m are evaluated on the input spectral and altitude grids of the particle layers (see section 3.3). Since scattering phase function is constant over the whole particle layer by definition, no transformation to other altitude grids needs to be carried out. Spectral interpolation is done linearly for phase functions weighted by scattering coefficients.

To check whether scattering phase function is appropriately represented by N_m Legendre terms, the Parseval relation (Bronstein et al., 2001)

$$\int_{-1}^1 P(\cos \Theta)^2 d \cos \Theta = \sum_{m=0}^{2M-1} 2(2m+1) \chi_m^2 \quad (3.30)$$

is tested to be valid within some error threshold ϵ , e.g. 0.01%, defined by SARTre input. When phase function is found to be not represented accurately by N_m Legendre terms, N_m can optionally be increased, until the error limit is met or N_m exceeds the maximum number of terms that is possible to be considered. However, high number of Legendre terms may cause oscillations around the “true” phase function. Hence, automatic increase of N_m might fail reaching convergence in phase function representation and should be critically reviewed by the user.

For reliable and stable RT modeling, energy conservation is as important as correct representation of the scattering phase function, avoiding loss or gain of energy through subsequent scattering processes. Basically, energy conservation is assured, when the zeroth order Legendre coefficient χ_0 is equal to one. In SARTre’s Legendre expansion routine, the set of χ_m derived from Eq. (3.29) is rescaled by χ_0^{-1} , to meet energy conservation demands. Additionally, in DISORT itself χ_0 is plainly set to unity by default.

3.4.4 Evaluation of the Multiple Scattering Source Term J_{MS}

To derive the multiple scattering source term J_{MS} , SARTre uses the azimuthally decomposed radiation field $I^m(\theta)$ from DISORT. The scattering integral

$$\int_{4\pi} P(\Theta) I(\Omega') d\Omega' \quad (3.31)$$

is evaluated from Fourier expansion series of $I(\Omega')$ with

$$I(\theta, \phi) = \sum_{m=0}^{2M-1} I^m(\theta) \cos m\phi, \quad (3.32)$$

where θ and ϕ denote zenith and azimuthal angle, respectively, and from $P(\Theta)$, expanded in terms of Legendre polynomials as given by Eq. (3.27). The $\sin(m\phi)$ Fourier expansion terms in Eq. (3.32) are neglected due to symmetry of the radiation field with respect to solar beam azimuthal direction ($\phi_{\odot} \equiv 0^\circ$).

Scattering angle dependence in Eq. (3.27) is reformulated into a dependence on incident and scattering directions by

$$\cos \Theta = \sin \theta \sin \theta' \cos \Delta\phi + \cos \theta \cos \theta', \quad (3.33)$$

where θ' and θ denote incident and scattering zenith angle, respectively, and $\Delta\phi = \phi - \phi'$ is the relative azimuth between incident and scattering direction. Applying the addition theorem for spherical harmonics results in

$$\begin{aligned} P(\boldsymbol{\Omega}, \boldsymbol{\Omega}') &= \sum_{m=0}^{2M-1} \cos m\Delta\phi (2 - \delta_{m,0}) \sum_{l=m}^{2M-1} (2l+1) \chi_l \tilde{\mathcal{P}}_l^m(\cos\theta) \tilde{\mathcal{P}}_l^m(\cos\theta') \\ &= \sum_{m=0}^{2M-1} \cos m\Delta\phi p_m(\theta, \theta'). \end{aligned} \quad (3.34)$$

Therein, δ is the Kronecker- δ and $\tilde{\mathcal{P}}_l^m$ are normalized associated Legendre polynomials. $\boldsymbol{\Omega}'$ and $\boldsymbol{\Omega}$ denote incident and scattering direction. By Eq. (3.34), scattering phase function is given azimuthally decomposed, corresponding to intensity decomposition, given by Eq. (3.32). Inserting Eqs. (3.32) and (3.34) into Eq. (3.31) yields

$$\begin{aligned} \int_{4\pi} P(\boldsymbol{\Omega}, \boldsymbol{\Omega}') I(\boldsymbol{\Omega}') d\boldsymbol{\Omega}' &= \int_{\phi'=0}^{2\pi} \int_{\theta'=0}^{\pi} \sum_{m=0}^{2M-1} p_m(\theta, \theta') \cos m(\phi - \phi') \cdot \sum_{m'=0}^{2M-1} I^{m'}(\theta') \cos m'\phi' \cdot \sin\theta' d\theta' d\phi' \\ &= \sum_{m=0}^{2M-1} \cos m\phi \pi(1 + \delta_{m,0}) \int_{\theta'=0}^{\pi} p_m(\theta, \theta') I^{m'}(\theta') \sin\theta' d\theta'. \end{aligned} \quad (3.35)$$

Replacing $p_m(\theta, \theta')$ by its equivalent from Eq. (3.34), substituting $\cos\theta = \mu$, and applying a Gaussian quadrature, the scattering integral is given by

$$\int_{4\pi} P(\boldsymbol{\Omega}, \boldsymbol{\Omega}') I(\boldsymbol{\Omega}') d\boldsymbol{\Omega}' = 2\pi \sum_{m=0}^{2M-1} \cos m\phi \sum_{l=1}^{2N} w_l I^m(\mu'_l) \sum_{n=m}^{2M-1} (2n+1) \chi_n \tilde{\mathcal{P}}_n^m(\mu) \tilde{\mathcal{P}}_n^m(\mu'_l), \quad (3.36)$$

where w_l denotes the quadrature weights at discrete ordinates μ'_l . Using Double-Gauss method, in SARTre the multiple scattering source term J_{MS} is derived from evaluating Eq. (3.36) for the same number of ordinates or streams N_{str} used in the DISORT solution, i.e. no interpolation of the intensity field is necessary.

3.5 Observational Geometry in Spherical Atmospheres

Source function integration by SARTre is proceeded starting from the observer along the line of sight. Relating the path of the LOS to the altitude grid, and thus e.g. to gridded optical properties, is straight forward for up- and downlooking cases. The LOS of limb observations practically “turns” around, crossing the atmospheric layers between observer and tangent altitude twice, while layers below the tangent point remain “unseen”. In SARTre, this ambiguity in altitude-LOS relation is solved by creating an array, describing the sequence of altitude levels along the LOS. Corresponding arrays give the sequence of particle layers and how they are linked to altitude levels crossed by the LOS.

In a one dimensional (1D) atmosphere, the whole spherical shell has identical properties, regardless of horizontal position. For limb observations that means, the line of sight crosses layers of homogeneous properties twice. That might meet reality for aerosol layers, but the

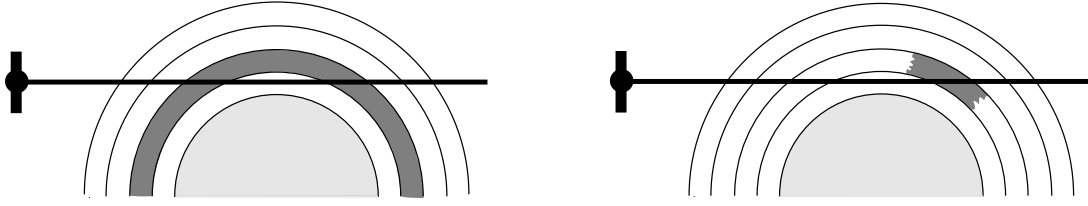


Figure 3.4: *Cloud layer in a “true” 1D atmosphere (left) and cloud in an “extended” 1D atmosphere (right), limited to the LOS’ opposite side of the tangent point.*

horizontal extent of clouds is often too small for the clouds to be met twice by the LOS. Due to the very long path lengths of limb LOS through layers close to the tangent point, the distance between crossing points becomes easily larger than 100 km.

Hence, for terrestrial RT modeling at least, SARTre provides the option to limit particle layers to the observer side of the tangent point or the far side of the LOS (see Fig. 3.4). This extension from a 1D atmosphere is realized by skipping the above explained mapping of particle layers to the path of the LOS. The cloud position option is not available yet with solar RT, where solar transmission from top of atmosphere to the scattering point has to be known. To determine whether the solar beam meets a cloud of reduced extent requires a more detailed definition of the cloud extent as well as the implementation of a ray tracing algorithm. Furthermore, to consistently address such geometry with standard DISORT is not possible.

While most of the parameters required for modeling RT in a spherical shell atmosphere only vary with altitude, some vary with (horizontal) position along the LOS. These primarily include quantities, which are characterized in a local coordinate system like the zenith angle of the LOS direction as well as sun position (see Fig. 3.5). Hence, they have to be calculated for the individual grid points of the line of sight. Local zenith angle of the LOS, required for the evaluation of the multiple scattering source term, is given by

$$\sin \theta_i = (R + z_{\text{tan}})/(R + z_i) \quad (3.37)$$

for downlooking cases and the limb path between observer and tangent point. R is the radius of the Earth, z_i denotes the altitude of grid point i of the LOS and z_{tan} is the tangent altitude assigned to the LOS, which is negative for non-limb cases. For uplooking cases and limb path segments of the observer opposite side of the tangent point, the local zenith of the LOS is calculated by

$$\sin(\pi - \theta_i) = (R + z_{\text{tan}})/(R + z_i). \quad (3.38)$$

For solar radiative transfer, in SARTre sun position is defined by sun zenith angle $\theta_{\odot}^{\text{obs}}$ and relative azimuth between sun direction and LOS at the observer $\Delta\phi_{\odot}^{\text{obs}}$ with

$$\Delta\phi_{\odot}^{\text{obs}} = \phi_{\text{obs}} - \phi_{\odot}^{\text{obs}}. \quad (3.39)$$

Setting $\phi_{\odot}^{\text{obs}} = 0$, i.e. sun azimuthal direction defines the reference azimuth, $\Delta\phi_{\odot}^{\text{obs}} = \phi_{\text{obs}}$. Resulting from the frame of reference rotating below the “object” LOS, corresponding local angles at LOS grid point i are derived from

$$\cos \theta_{\odot}^i = -\sin \theta_{\odot}^{\text{obs}} \cos \Delta\phi_{\odot}^{\text{obs}} \sin(\theta_{\text{obs}} - \theta_i) + \cos \theta_{\odot}^{\text{obs}} \cos(\theta_{\text{obs}} - \theta_i) \quad \text{and} \quad (3.40)$$

$$\cos \Delta\phi_{\odot}^i = \left(\sin \theta_{\odot}^{\text{obs}} \cos \Delta\phi_{\odot}^{\text{obs}} \cos(\theta_{\text{obs}} - \theta_i) + \cos \theta_{\odot}^{\text{obs}} \sin(\theta_{\text{obs}} - \theta_i) \right) / \sin \theta_{\odot}^i. \quad (3.41)$$

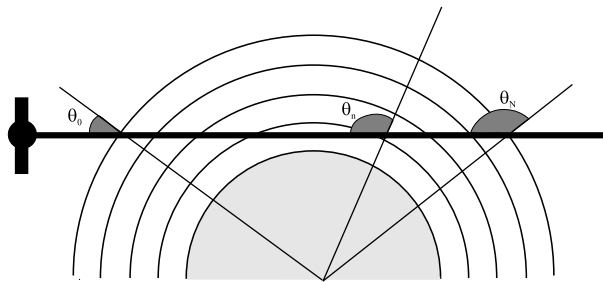


Figure 3.5: Zenith angle θ of the viewing direction is defined in a local coordinate system with local zenith direction as reference. Thus, θ varies along the LOS: $\theta_0 \neq \theta_n \neq \theta_N$. The same applies for solar zenith angle θ_{\odot} and azimuthal angles (not shown).

Related to changing solar angles along the LOS, the path of the solar beam from top-of-atmosphere to the LOS grid point and, thus, the solar transmission \mathcal{T}_{\odot} vary. With routines for the determination of the path of a ray through the atmosphere and calculation of optical depth along the path existing for the LOS, these can be used for the calculation of \mathcal{T}_{\odot} as well. Therefore, optical depth along the LOS of a virtual observer, placed at the “real” LOS and looking into sun direction, is calculated.

In contrast to the aforementioned sun geometry related quantities, the single scattering angle between solar beam and LOS is constant and is evaluated from Eq. (3.33) by using local directions at the observer. Finally, path lengths of the LOS segments are derived from Eq. (3.7).

3.6 Remarks and Outlook

The structure and principles of the RT model SARTre have been described. With SARTre, a consistent RT model taking emitted and scattered radiation from solar and terrestrial sources into account has been developed. Monochromatic intensity spectra for arbitrary observation geometries in a spherical shell atmosphere can be simulated, using the source function integration technique. Currently, instrumental characteristics like field-of-view and instrumental line shape or band pass features, respectively, can not be considered within SARTre, but have to be handled externally.

Deriving the incident radiation field, required to evaluate the multiple scattering source term, under the assumption of a locally planar atmosphere from the plane-parallel RT solver DISORT, does allow for the simulation of limb scattering observations. Limitations of the model due to “reduced” sphericity are examined within the following chapters. The plane-parallel assumption furthermore should allow for fast computation of scattered radiance spectra. However, currently SARTre lacks optimization in a wide variety of aspects and, thus, is by far not able to use its potentials concerning computation time.

In particular, the derivation of the incident radiation field $I(\boldsymbol{\Omega}')$ from a DISORT solution on each grid point along the LOS when solar radiation is taken into account extremely slows down the computation. Besides, for approximate spherical models it has been shown, that interpolation from a small number of radiation field solutions usually yields similarly accurate results (Loughman et al., 2004).

Using a discrete ordinate model to provide $I(\boldsymbol{\Omega}')$ restricts the maximum number of expansion terms in azimuth decomposition to the number of streams. Hence, representing strong forward

scattering patterns accurately can require a large number of streams N_{str} in the DISORT solution, where computation time is proportional to N_{str}^2 . Implementing another solver, e.g. a solver using matrix operator method, where the number of streams is independent of the number of expansion terms, might require a smaller number of streams to obtain the same accuracy. Similar computation time reduction may be achieved by implementing δ -scaling, which would allow to use a smaller number of expansion terms and streams for strongly peaked phase functions.

However, SARTre is a reasonable fast model for simulating spherical radiative transfer including scattering in the infrared and microwave spectral region.