Radiative transfer theory
(Pure gas atmosphere)

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Radiative transfer equation

The radiative transfer equation states that the specific intensity of radiation $I(s)$ (defined as the energy flux per unit time, unit frequency, unit solid angle and unit area normal to the direction of propagation, as a function of the optical frequency s) during its propagation in a medium is subject to losses due to extinction and to gains due to emission:

$$\frac{dI(s)}{dx} = -m(s) \cdot I(s) + r \cdot j(s)$$

where x is the co-ordinate along the optical path, $m(s)$ is the extinction coefficient, r is the mass density $j(s)$ is the emission coefficient per unit mass.

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Pure gas atmosphere

Extinction

In general, the extinction coefficient (s) includes both the absorption coefficient (s) and the scattering coefficient $s(s)$, of both the gas and the aerosols suspended in the gas:

$$m(s)=a(s)^{gas}+s(s)^{gas}+a(s)^{aerosol}+s(s)^{aerosol}$$

In the MIR the assumption of a pure gas atmosphere with no-scattering is a reasonable assumption and:

$$m(s)=a(s)^{gas}=a(s)$$

Pure gas atmosphere

Emission

In absence of scattering and for local thermal equilibrium (LTE), the source function is equal to :

$$r\cdot j(s)=a(s)B(s,T)$$

where (s) is the absorption coefficient (equal to the emission coefficient, Kirchhoff's Law) and $B(s,T)$ is the Plank function at frequency s and temperature T.

Radiative transfer equation

for pure gas atmosphere

For an atmosphere with no scattering and in LTE the radiative transfer equation is reduced to:

$$\frac{dI(s)}{dx} = -a(s)\cdot I(s) + a(s)\cdot B(s,T)$$

This equation can be easily integrated leading to the integral equation of radiative transfer.

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Integral equation of Radiative Transfer

$$\underset{\text{Spectral intensity observed at L}}{I(s,L)} = \underbrace{\overset{\text{Intensity of the background source}}{I(s,0)}\;\overset{\text{“Transmittance” between } 0 \text{ and } L}{e^{-t_s(0,L)}}}_{\text{Absorption term}} + \underbrace{\int_0^{t_s(0,L)} B(s,T(l))\,\overset{\text{“Transmittance” between } l \text{ and } L}{e^{-t_s(l,L)}}}_{\text{Emission term}}\,dt_s$$

“Optical depth” ⟶ $t_s(l,L) = \int_l^L a_s(l')dl'$

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Radiative Transfer for emission instruments

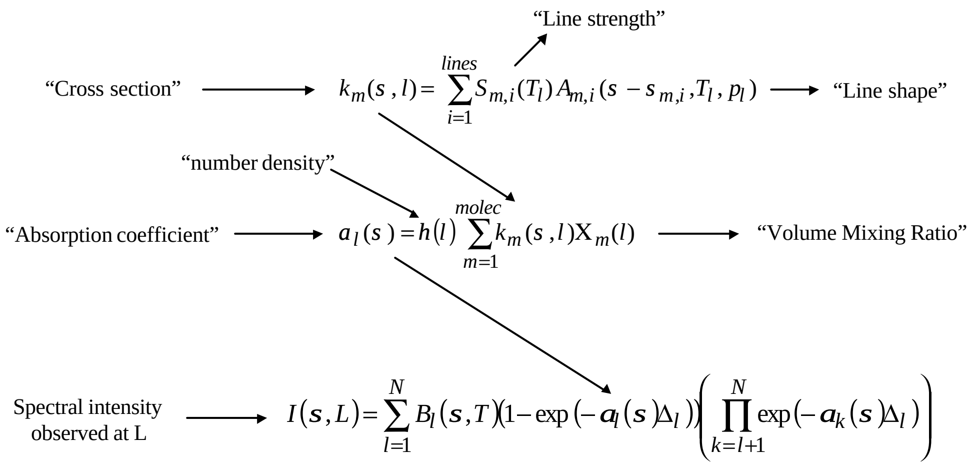
In the case of MIPAS only the emission term is relevant in the integral equation of radiative transfer

$$I(s,L)=\int_0^{t_s(0,L)} B(s,T(l))e^{-t_s(l,L)}dt_s$$

This integral is numerically performed as:

$$I(s,L)=\sum_{l=1}^{N} B_l(s,T)(1-\exp(-a_l(s)\Delta_l))\left(\prod_{k=l+1}^{N}\exp(-a_k(s)\Delta_l)\right)$$

Tree of operations for Radiative Transfer calculation



"Line strength"

"Cross section"

$$k_m(s,l)=\sum_{i=1}^{lines} S_{m,i}(T_l)A_{m,i}(s-s_{m,i},T_l,p_l)$$

"Line shape"

"number density"

"Absorption coefficient"

$$a_l(s)=h(l)\sum_{m=1}^{molec} k_m(s,l)X_m(l)$$

"Volume Mixing Ratio"

Spectral intensity
observed at L

$$I(s,L)=\sum_{l=1}^{N} B_l(s,T)(1-\exp(-a_l(s)\Delta_l))\left(\prod_{k=l+1}^{N}\exp(-a_k(s)\Delta_l)\right)$$

Forward Model of the measurements

The forward model calculates the measured quantities.

The measured signal is equal to the atmospheric spectral intensity $I(s, q, L)$, obtained with the radiative transfer model, convoluted with instrument effects:

$$S(s,q,L)=\iint\left(I(s,J,L)\cdot AILS(s-s')\,ds'\right)\cdot FOV(J-q')\,dJ'$$

Where AILS is the "apodized instrument line shape" and FOV is the "field of view " of the instrument.

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Optimised Forward Model (OFM)

- For the analysis of MIPAS measurements a dedicated code (named Optimised Forward Model) was developed for fast and accurate computation.
- For the validation of the OFM comparisons were made with reference models (Oxford RFM) and reference measurements (ATMOS).
- Several numerical and physical optimisations were used in the OFM.

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Numerical and physical choices in OFM

Spectroscopic cross sections

- In the code, the cross-sections can either be calculated line-by-line (LBL) using pre-selected spectroscopic data and fast Voigt profile computations or be read from look-up tables (LUTs).
- The relative speed of the two approaches depends on the access time of the memory used to store LUTs.
- The baseline is to use Singular Value Decomposition to compress the LUTs so that they can be read from RAM.

Numerical and physical choices in OFM

Radiative transfer

- The radiative transfer occurs along the line of sight, but in the case of a **stratified atmosphere** (the atmospheric properties depend only on the altitude z) the radiative transfer integral can be performed in the altitude domain

$$dl = (dl/dz)\, dz$$

Numerical and physical choices in OFM

Segmentation

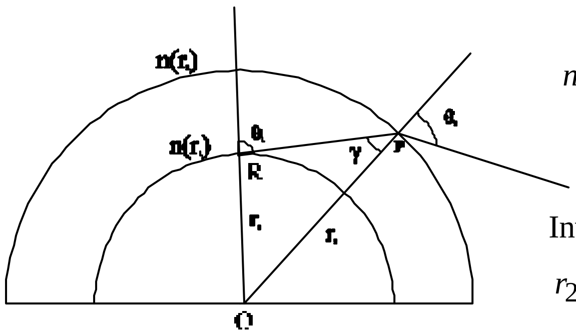
- use of relatively thick atmospheric layers for the “segmentation” of the radiative transfer and of Curtis-Godson approximation for the calculation of pressure and temperature (weighted averages).

$$p^{e}_{m,l,g} = \frac{\int_{z_{l-1}}^{z_l} p(z)\cdot X_m(z)\cdot h\left(p(z),T(z)\right)\cdot\frac{dl^g}{dz}\cdot dz}{\int_{z_{l-1}}^{z_l} X_m(z)\cdot h\left(p(z),T(z)\right)\cdot\frac{dl^g}{dz}\cdot dz} \qquad T^{e}_{m,l,g} = \frac{\int_{z_{l-1}}^{z_l} T(z)\cdot X_m(z)\cdot h\left(p(z),T(z)\right)\cdot\frac{dl^g}{dz}\cdot dz}{\int_{z_{l-1}}^{z_l} X_m(z)\cdot h\left(p(z),T(z)\right)\cdot\frac{dl^g}{dz}\cdot dz}$$

Numerical and physical choices in OFM

Optical path

- Use of Snell’s law for optical ray tracing in the atmosphere



$$n(r_2)\cdot\sin q_2 = n(r_1)\cdot\sin g$$

Invariant along the optical path

$$r_2\cdot n(r_2)\cdot\sin q_2 = r_1\cdot n(r_1)\cdot\sin q_1$$

Numerical and physical choices in OFM

Apodized Instrument Line Shape

The ILS (instrument line shape) of the instrument has lobes that extend in a wide spectral interval. In order to limit the calculations to a small interval (micro-window) a convolution with an apodizing function is applied to both the measured and the simulated spectrum.

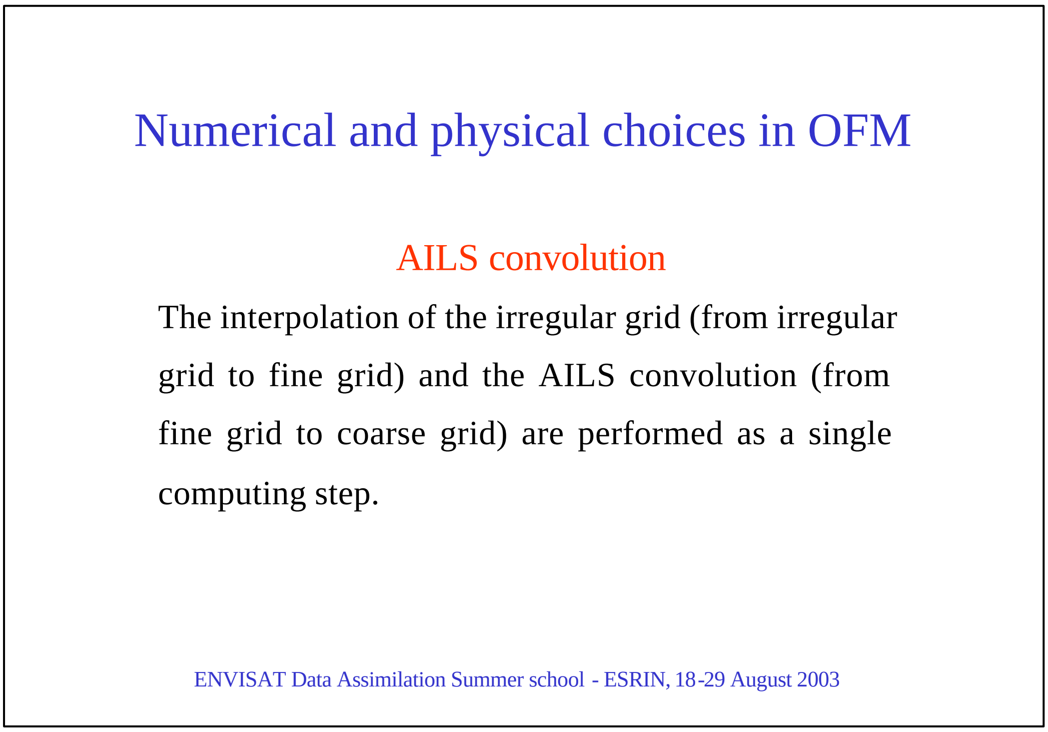
The AILS is equal to the convolution of the ILS with the apodizing function.

Numerical and physical choices in OFM

Dependence on spectral frequency

The Forward Model is required at the instrument resolution (“coarse grid” of 0.025 cm^{-1}).

Radiative transfer calculations require a “fine grid” which may be as small as 0.0005 cm^{-1}, but only a subset of fine grid points is used (“irregular grid”).



Numerical and physical choices in OFM

AILS convolution

The interpolation of the irregular grid (from irregular grid to fine grid) and the AILS convolution (from fine grid to coarse grid) are performed as a single computing step.

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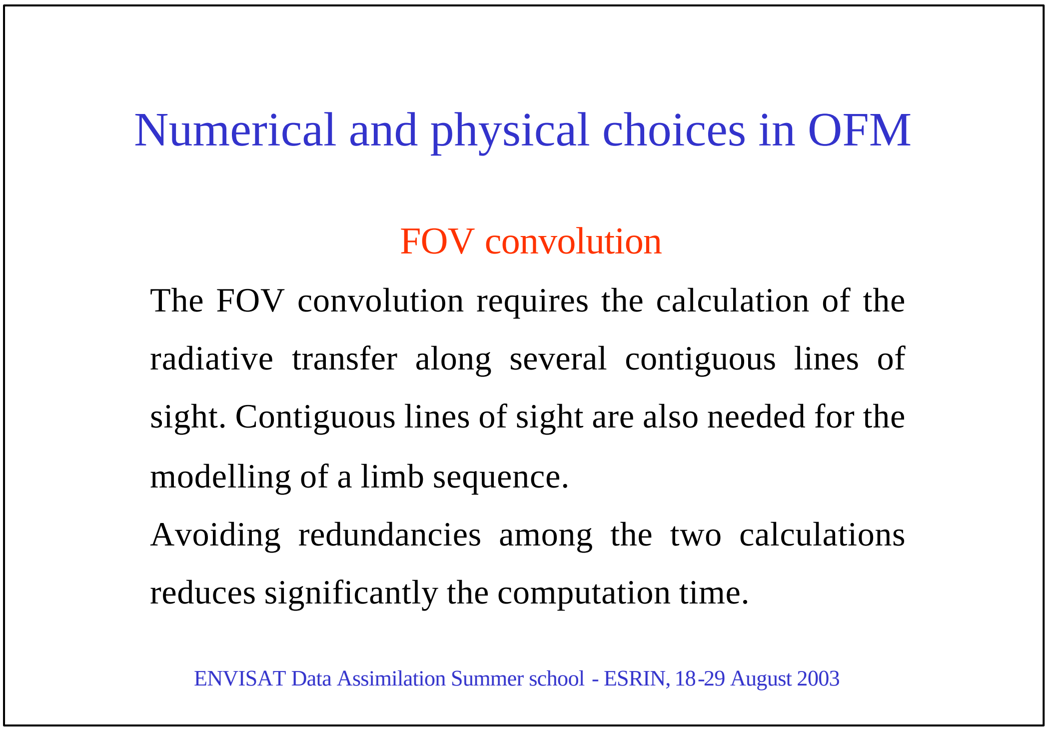

Numerical and physical choices in OFM

FOV convolution

The FOV convolution requires the calculation of the radiative transfer along several contiguous lines of sight. Contiguous lines of sight are also needed for the modelling of a limb sequence.

Avoiding redundancies among the two calculations reduces significantly the computation time.

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Numerical and physical choices in OFM

NLTE

- Non-LTE (NLTE) occurs when the excitation temperature of the emitting gas is different from the thermal temperature
- NLTE effects are not modelled in the OFM
- NLTE is, however, a source of error which is considered in the micro-window selection

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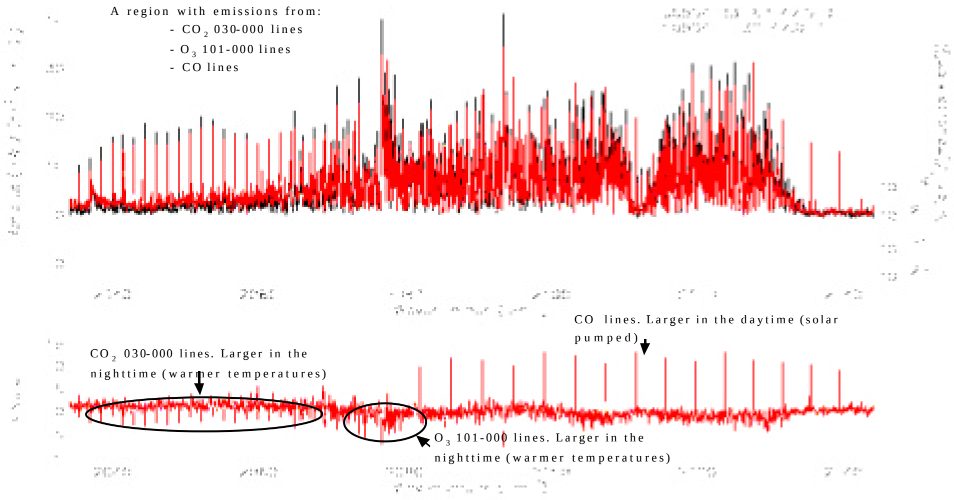
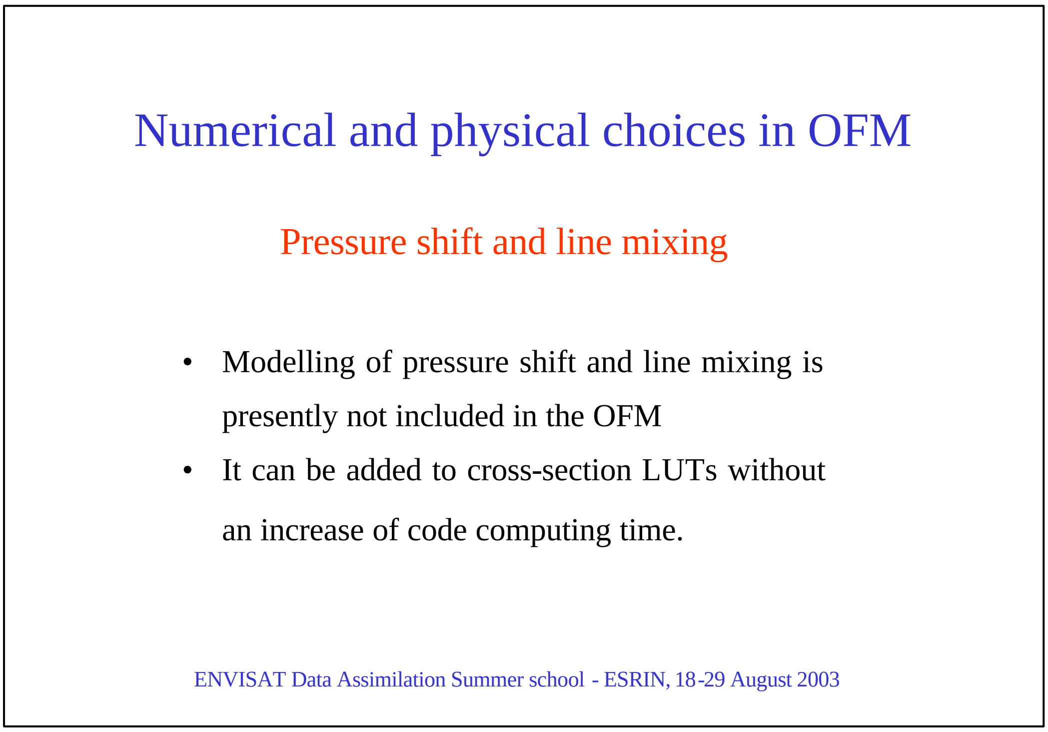


A region with emissions from:
- CO_2 030-000 lines
- O_3 101-000 lines
- CO lines

CO lines. Larger in the daytime (solar pumped)

CO_2 030-000 lines. Larger in the nighttime (warmer temperatures)

O_3 101-000 lines. Larger in the nighttime (warmer temperatures)



Numerical and physical choices in OFM

Pressure shift and line mixing

- Modelling of pressure shift and line mixing is presently not included in the OFM
- It can be added to cross-section LUTs without an increase of code computing time.

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