

A general purpose line-by-line model for infrared radiative transfer

Anu Dudhia, NCEO, AOPP, Dept. Physics, University of Oxford

## Introduction

The RFM is a free-to-use flexible radiative transfer model developed at the University of Oxford and currently supported by NCEO.

The main design aspects are

- Easy to use - probably its main advantage
- Robustness - you shouldn't be able to crash the program
- Portability - written in (almost) standard Fortran-77
- Efficient coding - attempts to maximise speed while minimising memory
- Self-documented code – just in case you need to make your own modifications
- On-line documentation and manuals – web page: [www.atm.ox.ac.uk/RFM/](http://www.atm.ox.ac.uk/RFM/) (or Google 'RFM Oxford')

The code will eventually be distributed via NCEO but for the moment email: [anu.dudhia@physics.ox.ac.uk](mailto:anu.dudhia@physics.ox.ac.uk)

## Features

- Spherical or plane-parallel atmospheres, or homogeneous paths
- Field-of-View & Instrument Line Shape convolutions
- CO2 Line mixing
- Continua for H2O, O2, N2 and CO2
- Non-LTE (via user-supplied vibrational temperatures)
- Collision-Induced Absorption
- Select lines of particular isotopes and/or bands
- Jacobians (Weighting functions) for p, T, VMR, line-of-sight pointing and surface temperature and emissivity
- Satellite/Balloon & Aircraft/Ground-based viewing geometries
- Surface reflections
- Output spectra of radiance, transmittance, absorption, cooling rates, optical depth and/or brightness temperature
- Output diagnostics from ray-tracing (including Curtis-Godson integrations)
- Output/Input absorption coefficient look-up tables  $k(v,p,T)$
- Horizontal structure in the atmosphere
- Flux calculations and matrices
- Different isotopic mixing ratio profiles.

What the RFM won't do: scattering

## Radiative Transfer

As with all (non-scattering) radiative transfer models, the RFM solves the radiative transfer equation along the line-of-sight:

$$L = \int B \, d\tau$$

where  $L(v)$  is the monochromatic radiance at wavenumber  $v$ ;  $B(v,T)$ , in the (usual) case of local thermodynamic equilibrium, is the Planck function which only depends on wavenumber and temperature  $T$ ; and  $\tau$  is the transmittance along the path, which is the difficult bit.

For monochromatic (as opposed to spectrally-averaged) models, Beer's Law can be used to decompose path transmittance into the product of the component transmittances of path segments  $i$  and individual absorbing species  $j$

$$\tau = \prod \tau_{ij} = \prod \exp(-\chi_{ij}) = \exp(-\sum \chi_{ij})$$

where  $\chi$  is the optical thickness of an absorber within a segment of the path, evaluated from

$$\chi = \int k \, u \, ds$$

where  $k$  is the absorption coefficient,  $u$  is the absorber density, integrated along the path segment  $ds$ . Again, evaluating  $k$  is the difficult part since it depends not only on the absorber and wavenumber, but also the local pressure,  $p$ , and temperature,  $T$ .

In a line-by-line model,  $k$  is evaluated as the sum of contributions of all local lines  $l$  centred at  $v_{0l}$  with strength  $S_l(T)$  and lineshape  $f(p,T,v-v_{0l})$

$$k = \sum S_l f(v-v_{0l})$$

where strength, position and additional parameters required to evaluate  $f$  for each line are listed in a spectroscopic database such as HITRAN.

However, for certain more complex molecules such as CFCs, individual transitions are not resolved and, instead, direct lab-measurements of absorption coefficient as a function of wavenumber  $v$ , for different  $(p,T)_j$  conditions, and tabulated in separate 'cross-section' files

$$k \equiv k(v,p,T_j)$$

In these cases the tabulated  $k$  values are simply interpolated for the required  $p,T$  conditions for each path segment and to the required spectral grid.

## Constructing Ray Paths

The RFM is designed to model spectra for a variety of applications varying from the simplest case of a homogeneous path (e.g. as gas-cell), where the path length, pressure, temperature and composition are all directly specified, to more complicated cases such as limb-viewing, where the atmospheric profile and tangent point may be specified, but the RFM itself has to determine the path of the ray through the atmosphere, taking local curvature and refraction into account.

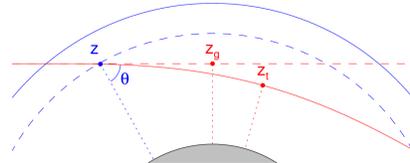
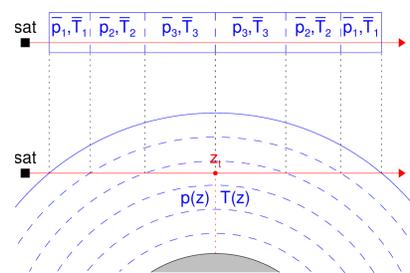


Illustration of the effect of refraction on a limb path. With the satellite to the left,  $z_g$  represents the geometric, or projected, tangent point (red dashed line) but refraction lowers the actual tangent point  $z_1$  and increases the overall path length (red solid line). The difference between projected and refracted tangent heights is several hundred metres for paths which intersect the troposphere.

Having corrected for any refraction effects, the RFM then splits the inhomogeneous atmospheric path into an equivalent series of homogeneous paths each of length specified by the ray-tracing and (Curtis-Godson) equivalent local  $p$  and  $T$



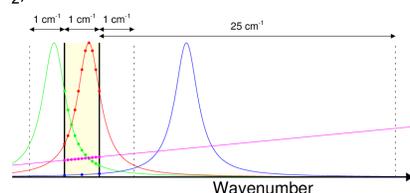
The lower plot shows the (inhomogeneous) atmospheric path specified by tangent height  $z$ , through a layered atmosphere defined by an altitude grid, while the upper plot shows the equivalent modelled path consisting of a series of homogeneous path segments defined by the intersections of the tangent path with the atmospheric layers. In this particular example, the atmosphere is assumed to have no variation in the horizontal, so the path segments are symmetric about the tangent point.

## Spectral Calculations

With the path calculation decomposed into a succession of homogeneous gas cells, the spectral absorption is then calculated for each cell.

In principle the line-by-line summation requires calculating the contribution of every spectral line over the entire required spectral range. Given that HITRAN contains several million lines, and a resolution of typically  $0.001 \text{ cm}^{-1}$  is required for Beer's Law to be valid, this is impractical. The RFM solves this problem by dividing the spectral range into  $1 \text{ cm}^{-1}$  intervals and assuming that, for the net contribution within each interval:

- Any line centred within the interval or adjacent intervals has to be calculated at full spectral resolution (i.e. typically  $0.001 \text{ cm}^{-1}$ )
- Any line centered from  $1-25 \text{ cm}^{-1}$  has a wing contribution which is smooth enough to be explicitly calculated at  $0.5 \text{ cm}^{-1}$  spacing and then interpolated with an inverse quadratic function
- Any line centred outside  $25 \text{ cm}^{-1}$  has either a negligible contribution or is represented by a separate continuum term ( $\text{H}_2\text{O}$ ,  $\text{CO}_2$ )



RfM calculations of absorption coefficient within each  $1 \text{ cm}^{-1}$  interval (yellow box) are performed at full spectral resolution for local lines (red, green), reduced resolution for other lines up to  $25 \text{ cm}^{-1}$  away (blue) and interpolated from tabulated continuum or cross-section data (pink).

## Look-Up Tables

While the line-by-line approach is regarded as the most accurate method of calculating absorption, it typically takes a few seconds per  $1 \text{ cm}^{-1}$  interval which is too slow, for example, if the RFM is to be used as the forward model component of a retrieval scheme where several iterations over  $100 \text{ cm}^{-1}$  interval might be required.

An obvious method to speed things up, while still maintaining the monochromatic approach, is to by-pass the line-by-line component by pre-tabulating  $k(v,p,T)$  as LUTs, similar to the representation of the heavy molecule absorption of cross-sections. However, to keep  $k$ -interpolation errors small, 'line' molecules requires a much higher density tabulation, particularly in the spectral domain, and the trick is to select tabulation points to maintain accuracy while keeping the data files to a reasonable size.

The RFM has the capacity both to generate and use such LUTs, giving a typical increase in speed of one or two orders of magnitude.

## Convolutions

The basic function of the RFM is to generate monochromatic spectra, typically at a spectral resolution of  $0.001 \text{ cm}^{-1}$  which is required to resolve high-altitude atmospheric spectral structure in the mid-infrared (limited by the Doppler broadening of absorption lines, which is approx  $10^{-6}$  of the frequency, with  $v=1000 \text{ cm}^{-1}$ ).

Satellite interferometers, such as MIPAS and IASI, have a much lower spectral resolution ( $0.025-0.5 \text{ cm}^{-1}$ ), so the measured radiance  $R$  at spectral point  $v_i$  represents a convolution of the 'real' high resolution spectrum  $L(v)$  with the (usually apodised) Instrument Line Shape  $\psi(v-v_i)$

$$R(v_i) = \int L(v) \psi(v-v_i) \, dv$$

Provided that the ILS is less than  $1 \text{ cm}^{-1}$  wide, the RFM can perform this convolution internally using a supplied ILS function, and also has a built-in triangular ILS function (AVG flag) to simply 'average' spectra to a coarser resolution.

For the limb-viewing geometry, a similar process can be applied to represent a finite vertical Field-of-View  $\Phi(z-z_j)$ , so that the measured radiance nominally from tangent height  $z_j$  can be modelled as a convolution of pencil-beam radiances  $L(z)$

$$R(z_j) = \int L(z) \Phi(z-z_j) \, dz$$

With a user-supplied FOV function, the RFM can also perform this convolution internally (in conjunction with any spectral convolution).

## How to get started ...

You will need ...

- The RFM source code
- A Fortran 77 compiler (or a compiler for any later version of Fortran)
- HITRAN spectroscopic data (from [www.hitran.com](http://www.hitran.com))
- An atmospheric profile (examples on RFM web-site)

The first step is to convert the HITRAN data (line parameters and cross-sections) into RFM-readable format using the (F77) tools available on the RFM web-site (fairly straightforward).

Compile the RFM, eg (linux): `gfortran *.for -o rfm` (no complications such as makefiles required)

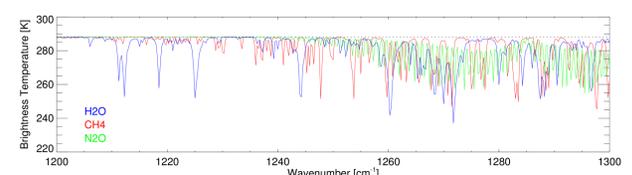
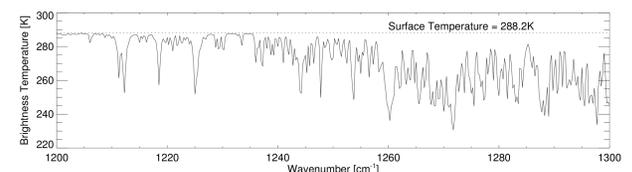
Use a text editor to create a file `rfm.drv` – this is the RFM input file which sets up the calculation. Examples for different applications are available on the RFM web-site, but in this case we'll take a simple example to simulate infrared radiance observed by a nadir-viewing instrument with IASI-like resolution.

```
*HDR          ! text for headers of output spectra
Example of nadir brightness spectrum
*FLG          ! flags defining type of calculation:
  NAD         ! nadir-viewing, plane-parallel atmosphere
  BBT         ! output Brightness Temperature spectra
  SFC         ! default surface temperature, emissivity=1
  AVG         ! apply triangular instrument line-shape
*SFC          ! define spectral range/resolution of output
  1200 1300 0.25
*GAS          ! list of absorbing molecules to consider
  CH4 H2O N2O
*ATM          ! atmospheric profile: T,p,VMRs on height grid
  ./atm/usa.atm
*SEC          ! Viewing angle, sec(theta)=1 is nadir
  1.0
*HIT          ! HITRAN data, in RFM binary format
  ./hit/hitran_2012.bin
*END
```

Example of an RFM driver file, used to generate the spectrum below

A more sophisticated IASI simulation would include additional molecules and continua, the IASI apodised ILS function, explicit surface temperature and emissivity, and a curved rather than plane-parallel atmosphere.

The RFM output is a text file containing a spectrum of brightness temperature at 401 points (1200-1300 inclusive at  $0.25$  spacing).



Top panel: spectrum generated using the above driver file; Lower panel: contributions from each molecule, created by running the RFM three more times selecting just one molecule for each run

## The Future

It is planned to release new versions of the RFM approximately every 6 months, with each new release containing a combination of bug fixes and new features, while making every attempt to make any new code backwardly compatible (i.e. so you can continue to use old driver tables and still get identical results)

Anticipated future updates include

- Speed-dependent line-shapes
- Improved  $\text{CO}_2$  and new  $\text{CH}_4$  line-mixing
- Single scattering