Combining Line-By-Line and Pre-Frequency-Averaged Models in Radiative Transfer

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The Observing Instrument

The Microwave Limb Sounder (MLS) is an instrument on the NASA Earth Observing System Aura satellite, which was launched 14 July 2004 into a near-polar 700 km orbit. It passively observes thermal emission from the limb of the atmosphere, in about 1000 channels. The antenna scans from about 100 km at the limb, to the surface, every 26 seconds, with 148 integration periods per scan. About 500 million measurements are taken every day. From these we compute about five million estimates of atmospheric parameters such as temperature and concentration of minor constituents of the atmosphere, at 72 levels on 3500 profiles in the orbit plane, every day.

An overview of data analysis methods used for this instrument was presented in the *Frontiers in Geomathematics* section of the 2011 Joint Mathematics Meeting, in New Orleans.

See `http://mls.jpl.nasa.gov` for more information.

Radiative Transfer Equation

The clear-sky non-scattering radiative-transfer equation, in the form we use it, is

$$\frac{\mathrm{d}I(s;\nu)}{\mathrm{d}s} + \alpha(s;\nu)\, I(s;\nu) = \alpha(s;\nu)\, B(s;\nu)$$

where

- $I(s;\nu)$ is radiative intensity,
- $\alpha(s;\nu)$ is the bulk absorption coefficient, which also depends upon temperature, pressure, and composition at s,
- $B(s;\nu)$ is the Planck radiation function, which also depends upon temperature at s,
- s is position along the path of radiation propagation, and
- ν is frequency.

Radiative Transfer Equation (cont.)

The Planck radiation function, in the form we use it, is

$$B(s;\nu) = \frac{h\nu}{k\left(\exp\left(\frac{h\nu}{kT(s)}\right) - 1\right)}$$

where

- h is Planck's constant,
- k is Boltzmann's constant, and
- $T(s)$ is temperature.

From here onward, s and ν are frequently suppressed for clarity.

Radiative Transfer Equation (cont.)

The bulk absorption coefficient is

$$\alpha(s;\nu) = \sum_{n=1}^{N_f} f_n(s)\,\beta_n(s;\nu)$$

where

- $f_n(s)$ is the volume mixing ratio of the nth chemical species,
- $\beta_n(s;\nu)$ is the absorption cross section for the nth chemical species, and
- N_f is the number of chemical species.

$\beta_n(s;\nu)$ also depends upon the temperature and pressure at s, upon spectroscopic properties of the nth chemical species, and upon $f_n(s)$ for some species, e.g., H_2O.

Radiative Transfer Equation (cont.)

The absorption cross section β_n for the nth chemical species is

$$\beta_n = \mathcal{R}_n \sqrt{\frac{\ln 2}{\pi}} P \left[\sum_{j=1}^{N_{\text{lines}}} 10^{S_{nj}} L(x_{nj}, y_{nj}, z_{nj}) \right]$$

where

$$\begin{aligned} S_{nj} = & \mathcal{I}_{nj}(300) \frac{hcE\ell_{nj}}{k} \left(\frac{1}{300} - \frac{1}{T} \right) \\ & \log \left[\frac{Q_n(300) \tanh(h\nu/kT)(1 + \exp(-h\nu/(kT)}{Q_n(T)(1 - \exp(-h\nu_{0nj}/(k\,300)))} \right], \end{aligned}$$

and j ranges over all spectral lines that have significant contribution at frequency ν.

Radiative Transfer Equation (cont.)

The spectral line shape function

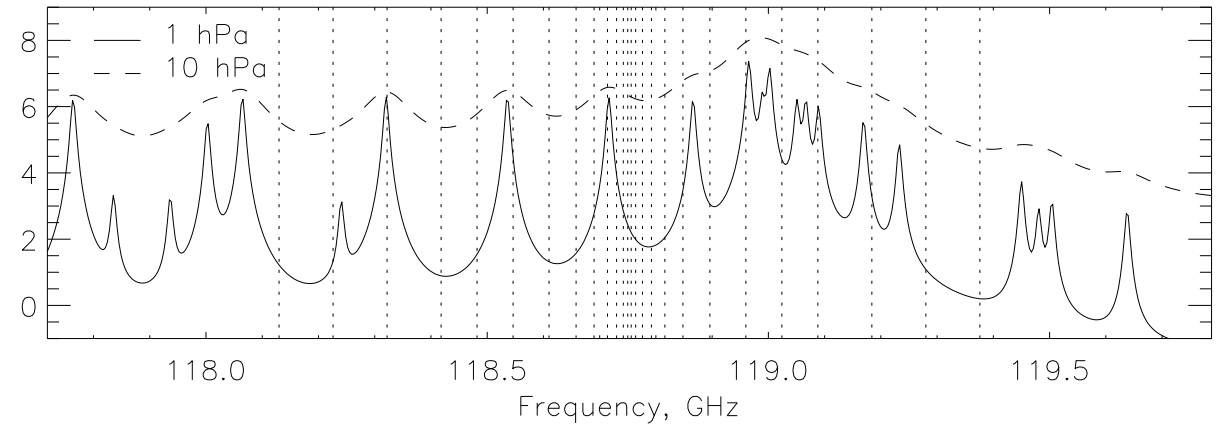
$$L(x_{nj}, y_{nj}, z_{nj}) = \frac{\nu}{\nu_0} \left\{ \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{[y_{nj} - Y_{nj}(x_{nj} - t)] \exp\left(-t^2\right)}{y_{nj}^2 + (x_{nj} - t)^2} \, \mathrm{d}t + \frac{1}{\pi} \frac{y_{nj} - Y_{nj} z_{nj}}{z_{nj}^2 + y_{nj}^2} \right\}$$

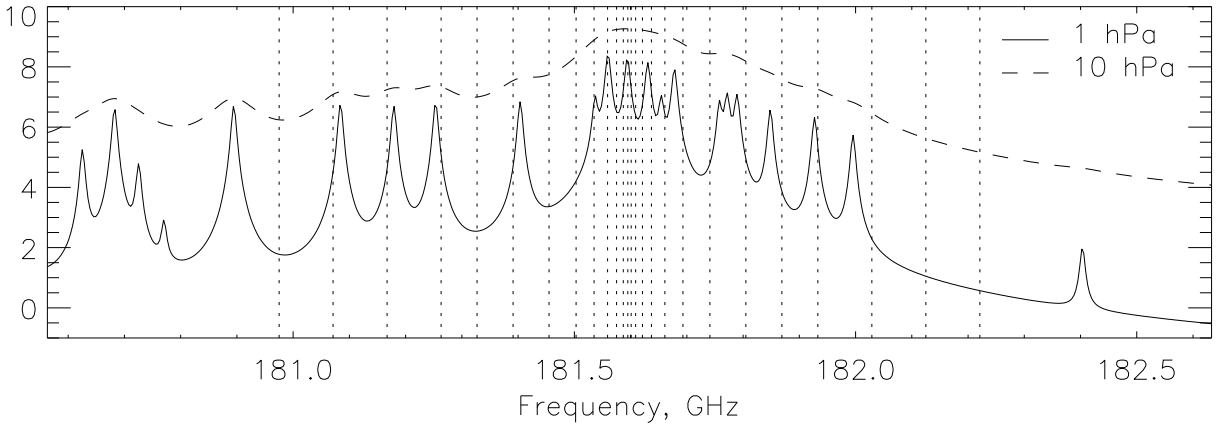
is related to the Voigt function, the real part of the Fadeeva function $w(z) = exp\left(-z^2\right) \operatorname{erfc}(-iz)$, which is the complex generalization of the error function.

The point here is not for you to understand all the parameters and details, but to be convinced that computing $\beta(s; \nu)$ is quite expensive.

ln β for HNO_3 at 200 K

The variation of β as a function of frequency is very different at different frequencies. Features are broadened at higher pressures and higher temperatures. Dotted lines are channel boundaries in the MLS instrument.





Solution of Radiative Transfer Equation

The solution of the radiative transfer equation, for one frequency, can be written

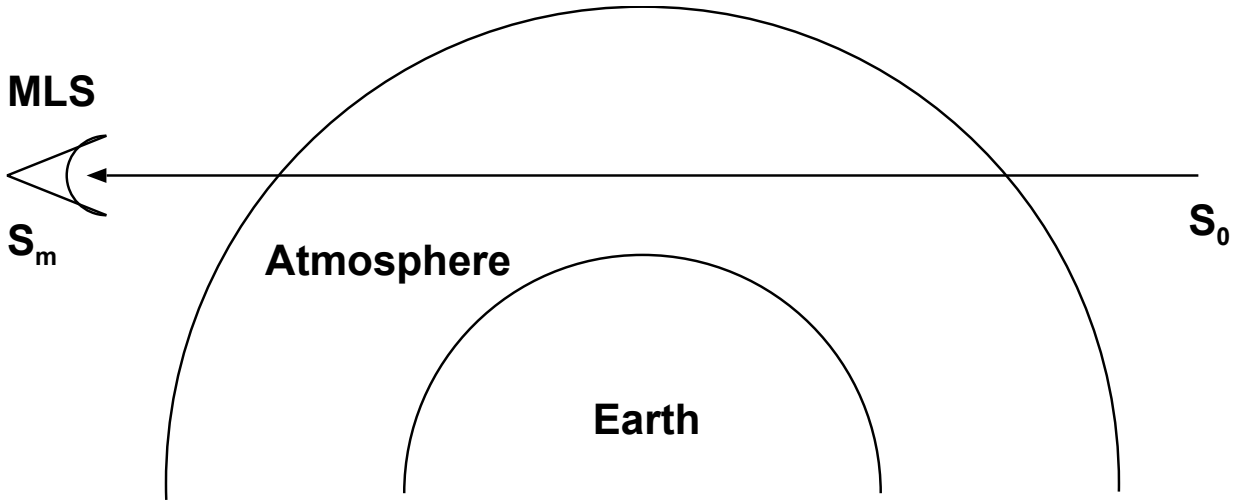
$$I(s_m) = I(s_0)\mathcal{T}(s_0, s_m) + \int_{s_0}^{s_m} \mathcal{T}(s, s_m)\,\alpha(s)\,B(s)\,\mathrm{d}s\,,$$

where

$$\mathcal{T}(s, s_m) = \exp\left(-\int_{s}^{s_m} \alpha(\sigma)\,\mathrm{d}\sigma\right)\,,$$

- $I(s_0)$ is space radiance, about 2.3 K,
- s_m is the position of the observing instrument, and
- s_0 is deep space at the other end of the observing path.

MLS Viewing geometry



Solution of Radiative Transfer Equation (cont.)

We integrate by parts, giving

$$I(s_m) = I(s_0)\mathcal{T}(s_0, s_m) + \int_{s_0}^{s_m} \mathcal{T}(s, s_m) \frac{\mathrm{d}B(s)}{\mathrm{d}s} \, \mathrm{d}s \, .$$

This is then approximated by a quadrature

$$I(s_m) \approx I(s_0)\mathcal{T}(s_0, s_m) + \sum_{i=1}^{N_p} \mathcal{T}(s, s_m) \, \Delta B_i \, ,$$

where N_p is the number of points on the path of integration.

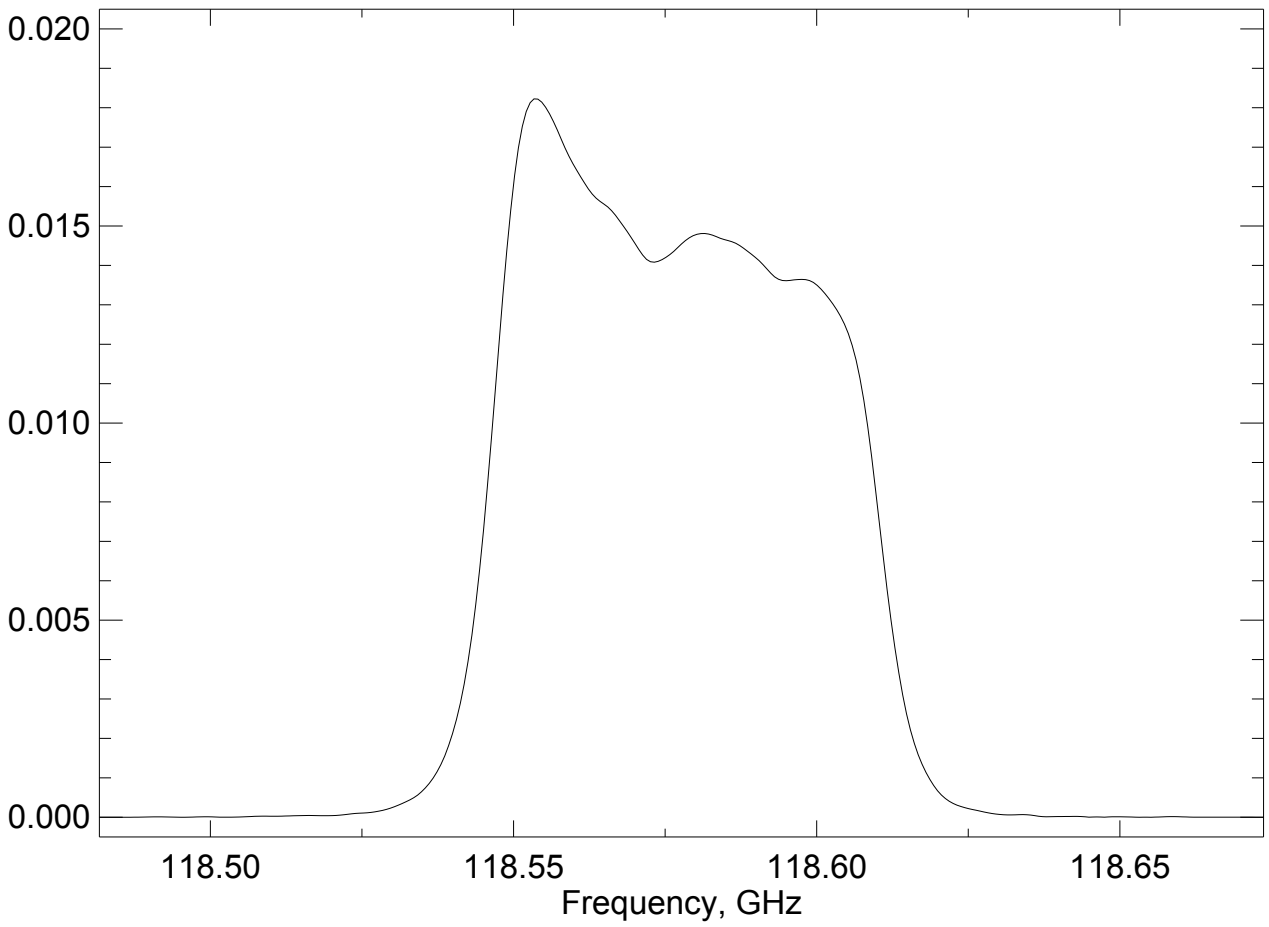
What The Instrument Observes

The instrument channels are not infinitesimally narrow. Each channel measures radiation over a range of frequencies. The response of each channel, as a function of frequency, was measured in the laboratory before the instrument was launched. What the instrument observes in a single channel is the average of the incident radiation $I(s_m;\nu)$, weighted with the channel's filter function, $\phi_c(\nu)$:

$$\hat{I}_c = \int_{\nu_1}^{\nu_2} \phi_c(\nu) I(s_m;\nu)\,\mathrm{d}\,\nu \approx \sum_{\ell=1}^{N_\nu} \phi_c(\nu_\ell)\Delta\nu_\ell\, I(s_m,\nu_\ell)\,,$$

We call this *frequency averaging*.

Filter shape example



Pre-frequency Averaging

Returning to the solution of the radiative transfer equation, in the transmissivity integral for one frequency

$$\mathcal{T}(s, s_m) = \exp\left(-\int_s^{s_m} \alpha(\sigma)\,\mathrm{d}\sigma\right)$$

we decompose the bulk absorption coefficient $\alpha(\sigma)$ into two parts, $\alpha^s(\sigma)$ for chemical species for which β, and therefore α, have strong variation as a function of frequency, and $\alpha^w(\sigma)$ for those having weak variation, giving

$$\mathcal{T}(s, s_m) = \exp\left(-\int_s^{s_m} \left(\alpha^s(\sigma) + \alpha^w(\sigma)\right)\,\mathrm{d}\sigma\right) .$$

We abbreviate $\mathcal{T}(s, s_m)$ to $\mathcal{T}$ for clarity from now on.

Pre-frequency Averaging (cont.)

Expanding, we have

$$\mathcal{T} = \mathcal{T}^s \mathcal{T}^w = \exp\left(-\int \alpha^s(\sigma)\,\mathrm{d}\sigma\right) \exp\left(-\int \alpha^w(\sigma)\,\mathrm{d}\sigma\right) .$$

Omitting the initial condition $I(s_0)\mathcal{T}(s_0, s_m)$ in the expression for $I(s_m;\nu)$, for clarity, the computed radiance approximation for channel c, *viz.* $\sum_\ell \phi_c(\nu_\ell)\Delta\nu_\ell \sum_i \mathcal{T}_i(\nu_\ell)\Delta B_i$, thereby becomes, after exchanging the order of summation,

$$\hat{I}_c \approx \sum_{i=1}^{N_p} \sum_{\ell=1}^{N_\nu} \left(\phi_c(\nu_\ell)\Delta\nu_\ell \Delta B_i(\nu_\ell)\mathcal{T}_i^s(\nu_\ell)\right) \mathcal{T}_i^w(\nu_\ell) .$$

Pre-frequency Averaging (cont.)

Although the channels are not infinitesimally narrow, the Planck function nonetheless has very little variation within one channel – $\frac{\mathrm{d}B}{\mathrm{d}\nu} \approx -2.377 \times 10^{-11}$ K/Hz at 118 GHz and 200K, or -2.28×10^{-3} K across a 96 MHz channel – so the factor $\Delta B_i(\nu_\ell)$ can be approximated by ΔB_{ic} evaluated at the channel center, and then removed from under the inner summation.

Considering the strong case alone, one can compute a frequency-averaged incremental radiance due to species with strongly-varying spectral features, at each point along the path, giving, for the parenthesized term in the earlier inner sum

$$\overline{I_{ic}^s} \approx \sum_{\ell=1}^{N_\nu} \Delta B_i(\nu_\ell)\phi_c(\nu_\ell)\Delta\nu_\ell \mathcal{T}_i^s(\nu_\ell) \approx \Delta B_{ic} \sum_{\ell=1}^{N_\nu} \phi_c(\nu_\ell)\Delta\nu_\ell \mathcal{T}_i^s(\nu_\ell)\,.$$

Pre-frequency Averaging (cont.)

We define "weak" to mean that β^w, and therefore $\mathcal{T}_i^w(\nu_\ell)$, do not vary strongly within one channel as a function of frequency. Without significant loss of accuracy, we can approximate $\mathcal{T}_i^w(\nu_\ell)$ by $\mathcal{T}_{ic}^w$, which is evaluated using some representative average β_{ic}^w for channel c, and remove $\mathcal{T}_{ic}^w$ from under the inner sum, giving

$$\begin{aligned}\hat{I}_c &\approx \sum_{i=1}^{N_p} \Delta B_{ic} \sum_{\ell=1}^{N_\nu} \phi_c(\nu_\ell) \Delta\nu_\ell \mathcal{T}_i^s(\nu_\ell) \mathcal{T}_i^w(\nu_\ell) \\ &\approx \sum_{i=1}^{N_p} \mathcal{T}_{ic}^w \Delta B_{ic} \sum_{\ell=1}^{N_\nu} \phi_c(\nu_\ell) \Delta\nu_\ell \mathcal{T}_i^s(\nu_\ell)\,.\end{aligned}$$

Pre-frequency Averaging (cont.)

Substituting the previous result, we have the approximation used in practice:

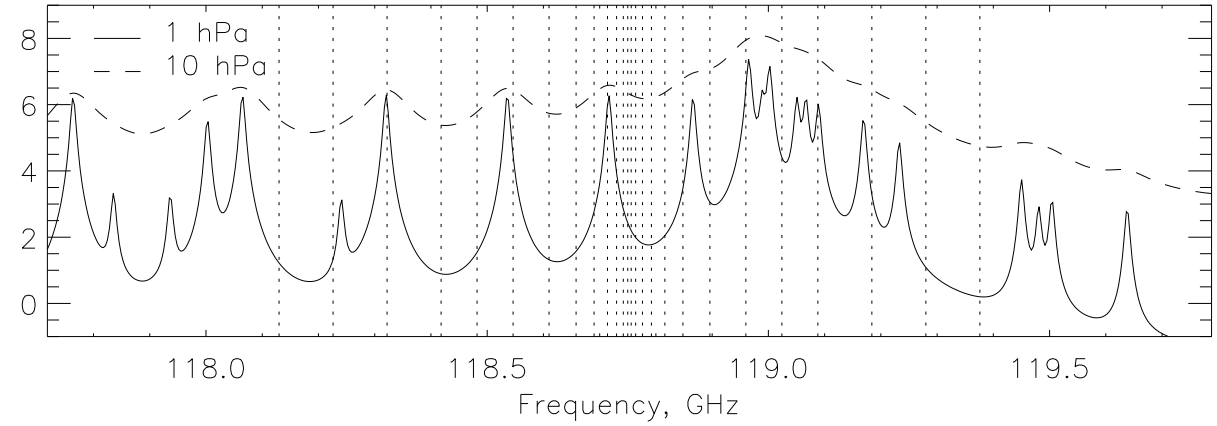
$$\hat{I}_c \approx \sum_{i=1}^{N_p} \overline{I_{ic}^s} \mathcal{T}_{ic}^w \, .$$

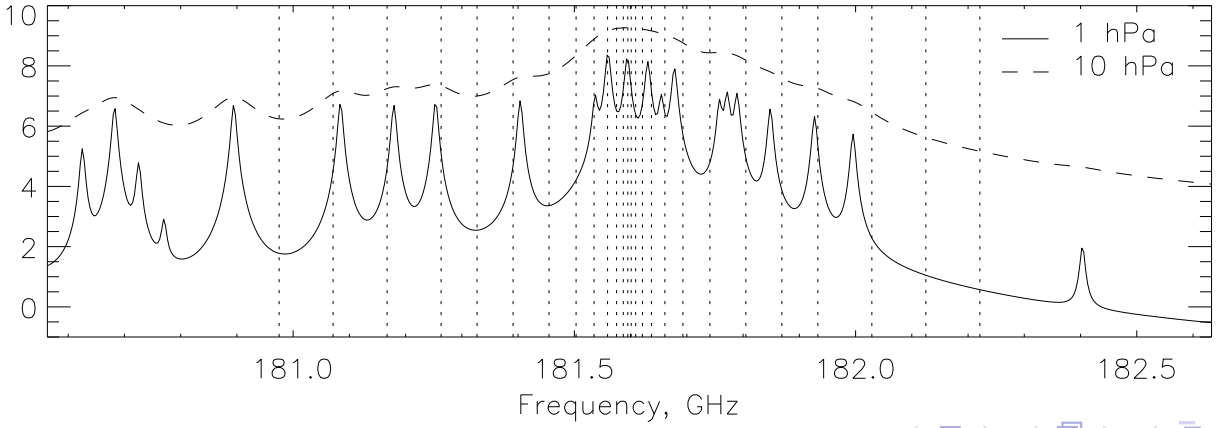
The calculation of $\hat{I}_c$ thus consists of

- computing incremental radiances $I_i^s(\nu_\ell)$ due to chemical species with strongly-varying $\beta_{ni}^s(\nu_\ell)$, along the path for several frequencies $\{\nu_\ell\}$,
- averaging those incremental radiances at each point on the path to get post-frequency-averaged incremental radiances $\overline{I_{ic}^s}$,
- computing transmissivity $\mathcal{T}_{ic}^w$ due to chemical species with weakly-varying β_{nic}^w, using pre-frequency-averaged β_{nic}^w, and
- combining those results as shown here.

ln β for HNO_3 at 200 K (again)

β for some species can be accurately modeled at some frequencies using channel averaging, and for some it cannot. For example, β for HNO_3 cannot be accurately modeled as a channel average at 119 GHz, but it can be at 119.35 and 182.2 GHz.





Computing $\mathcal{T}_{ic}^{w}$

Return to

$$\mathcal{T}_i^w(\nu) = \exp\left(-\int_{s_0}^{s_i} \alpha^w(\sigma;\nu)\,\mathrm{d}\sigma\right)$$

and

$$\alpha^w(s;\nu) = \sum_{n=1}^{N_f} f_n(s)\beta_n^w(s;\nu)\,.$$

We replace $\alpha^w(s;\nu)$ by the channel-averaged approximation

$$\alpha_c^w(s) \approx \sum_{n=1}^{N_f} f_n(s)\beta_{nc}^w(s)$$

where

$$\beta_{nc}^w(s) = \sum_{\ell=1}^{N_\nu} \phi_c(\nu_\ell)\beta_n^w(\nu_\ell, T(s), P(s))\,.$$

Computing $\mathcal{T}_{ic}^{w}$ (cont.)

To compute $\beta_{nc}^{w}(T(s), P(s))$, we evaluate and tabulate $\beta_{n}^{w}(\nu_\ell)$ at the same frequencies at which the channel response was measured, using the full line-by-line model, and average using the channel response function, for several values of pressure and temperature. We call this *Pre-Frequency Averaging*, or *PFA*.

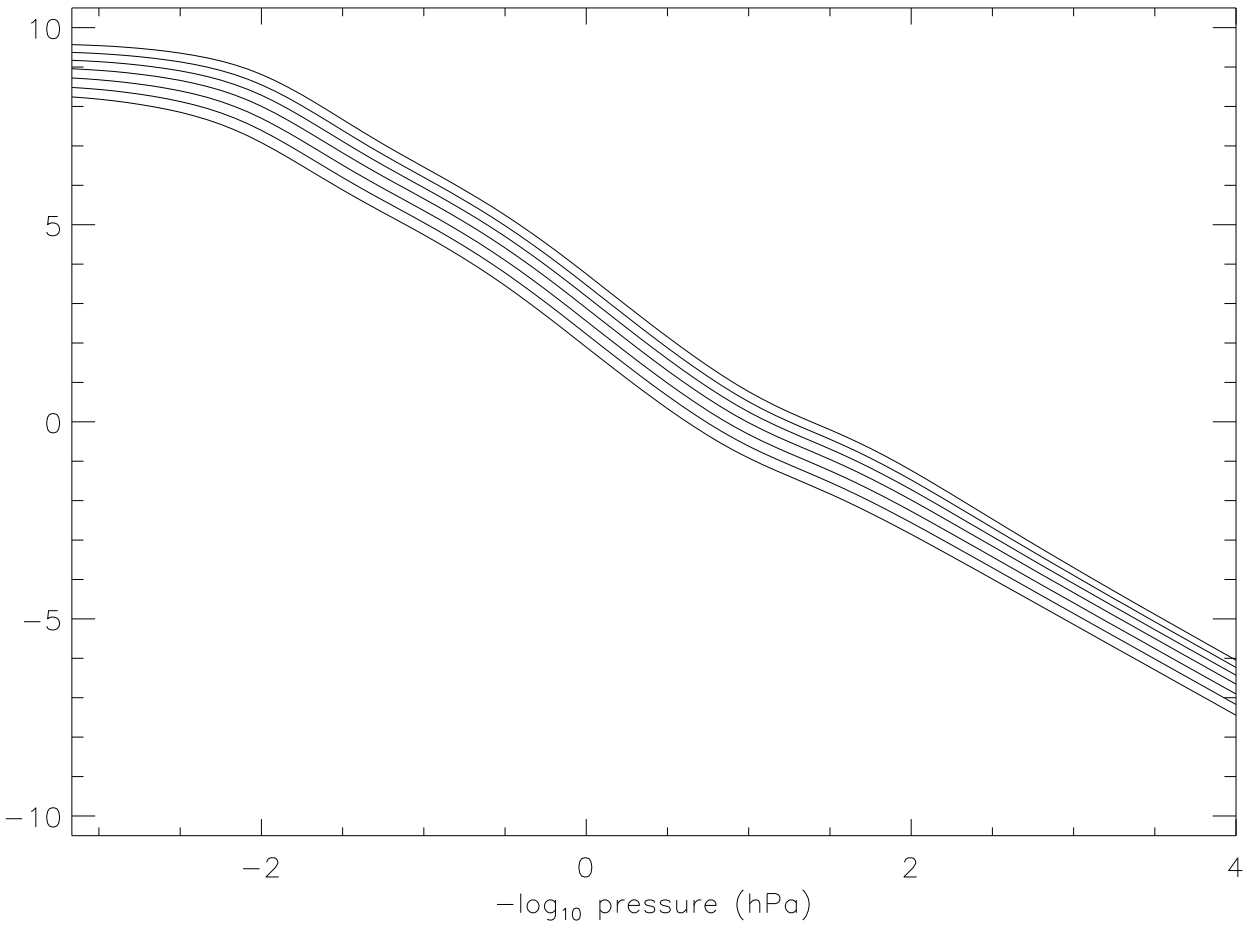
$\alpha_{c}^{w}(s)$ is evaluated by interpolating in those tables of $\beta_{nc}^{w}(T(s), P(s))$ using $T(s)$ and $P(s)$.

Evaluating $\beta_{n}^{w}(\nu_\ell)$ is quite expensive (billions are needed), but computing the tables of $\beta_{nc}^{w}(T(s), P(s))$ is an offline calculation, repeated only when new laboratory measurements of spectral characteristics are developed.

Example of frequency-averaged β^w

β^w is a smoothly-varying function of pressure and temperature.

$\ln \beta^w_{nc}$ for HNO_3 at $181.391 - 181.455$ GHz and $180 - 300$ K



Derivatives

To retrieve atmospheric parameters by solving the radiative transfer equation, we use a Gauss-Newton method, as described in the *Frontiers in Geomathematics* section of the Joint Mathematics Meeting in 2011, in New Orleans. This requires derivatives of radiance with respect to those parameters.

We solve for parameters on a specified grid, the points of which are not necessarily on the integration path. We therefore interpolate from a point p to a point s on the path using, for example,

$$f_n(s) = \sum_p \mu_{np}(s) f_{np}$$

Derivatives (cont.)

Returning to the solution of the radiative transfer equation, and taking the derivative with respect to an atmospheric parameter x_p at the point p, we have

$$\frac{\partial I(s_m)}{\partial x_p} = I(s_0)\frac{\partial \mathcal{T}(s_0, s_m)}{\partial x_p} + \int_{s_0}^{s_m} \frac{\partial \mathcal{T}(s, s_m)}{\partial x_p} \frac{\mathrm{d}B(s)}{\mathrm{d}s}\,\mathrm{d}s + \int_{s_0}^{s_m} \mathcal{T}(s, s_m)\,\frac{\partial^2 B(s)}{\partial x_p\,\partial s}\,\mathrm{d}s\,.$$

Derivatives (cont.)

Returning to the definitions of $\mathcal{T}$ and α, we have

$$\frac{\partial \mathcal{T}(s, s_m)}{\partial x_p} = -\mathcal{T}(s, s_m) \int_s^{s_m} \frac{\partial \alpha(\sigma)}{\partial x_p} \mathrm{d}\sigma \,.$$

In the case of x_p being the volume mixing ratio f_{np} of the nth chemical species at p, where β_n does not depend upon f_n, $\alpha(s) = \sum_n \beta_n(s) \sum_p \mu_{np}(s) f_{np}$, so the derivative with respect to f_{np} simplifies to

$$\frac{\partial \mathcal{T}(s, s_m)}{\partial f_{np}} = -\mathcal{T}(s, s_m) \int_s^{s_m} \mu_{np}(\sigma)\, \beta_n(\sigma)\, \mathrm{d}\sigma \,.$$

Derivatives (cont.)

The derivative with respect to temperature is slightly more complicated:

$$\frac{\partial \mathcal{T}(s, s_m)}{\partial T_p} = -\mathcal{T}(s, s_m) \int_s^{s_m} \sum_{n=1}^{N_f} f_n(\sigma)\, \mu_{Tp}(\sigma)\, \frac{\partial \beta_n(\sigma)}{\partial T}\, \mathrm{d}\sigma\,.$$

Therefore, to compute $\frac{\partial \mathcal{T}_c^w}{\partial T_p}$, we also tabulate $\frac{\partial \beta_{nc}^w}{\partial T}$ for several values of temperature and pressure, and interpolate in those tables using $T(s)$ and $P(s)$.

Example timings

Phase	PFA per iteration	LBL per iteration	PFA/LBL
InitPTAN	0.33	0.33	1.0
InitR2	16.99	17.48	0.972
FinalPTAN	214.87	316.47	0.679
InitRHI	0.576	0.578	1.0
InitUTH	14.321	29.72	0.482
CorePlusR3	93.87	151.33	0.620
CorePlusR2	97.31	189.66	0.513
CorePlusR4AB14	146.15	405.17	0.361
CorePlusR4AB14B	148.42	413.17	0.359
Methanol	68.906	279.32	0.247
CorePlusR4AB13	52.84	103.42	0.511
CorePlusR4B	22.036	40.869	0.539
CorePlusR5	54.077	54.337	1.0

Conclusion

On one hand, we

- compute $\mathcal{T}$ using a line-by-line method for every β, then
- frequency average radiance only at the instrument.

On the other hand, we

- compute $\mathcal{T}^s$ using a line-by-line method for β^s, and $\mathcal{T}^w$ by interpolating in tables of pre-frequency-averaged β^w,
- compute frequency averaged incremental radiance $\overline{I^s_{ic}}$ due to $\mathcal{T}^s$ at every point along the path of integration, then
- compute $\overline{I^s_{ic}}\mathcal{T}^w_{ic}$ and integrate along the path.

Exchanging the first for the second has been a profitable bargain, and a sufficiently accurate approximation.

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