Radiative Transfer and Second Order Model for the Microwave Limb Sounder (MLS)

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Contents

1 Hydrostatic Model **2**

2 Absorption Coefficient Calculations **4**

3 Radiative Transfer **5**

4 Derivatives **7**
4.1 Radiative Transfer Derivative 7
4.2 Radiative Transfer Second Derivative 8
4.3 Mixing Ratio Derivatives 9
4.4 Mixing Ratio Second Derivatives 9
4.5 Temperature Derivative 13
4.6 Temperature Second Derivative 16

5 Antenna Radiance **18**

6 Antenna Radiance Jacobians **19**
6.1 Mixing Ratios Antenna Radiance Jacobian 20
6.2 Mixing Ratios Antenna Radiance Hessian 20
6.3 Temperature Antenna Radiance Jacobian 20

7 Finite Difference Approximations for Jacobians **25**

8 Finite Difference Approximations for Hessians **26**

9 Frequency Averaging **26**

10 Polarized Radiative Transfer **27**

11 Polarized Derivatives **27**
11.1 General Form 27
11.2 Mixing Ratio Derivatives 28

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Theory of Radiative Transfer

1 Hydrostatic Model

The EOS MLS forward model assumes hydrostatic balance holds for the entire atmosphere. The hydrostatic function interrelates heights with pressure and only one of these (the latter) is independent.
h = height,
$g = 0.0098\,\mathrm{km/s^2}$,
$m = 29.864\,\mathrm{AMU} = 4.9590 * 10^{-26}\mathrm{kg}$,
$k = 1.3806503 \cdot 10^{-23}\mathrm{m^2 kg\,s^{-2} K^{-1}} = 1.3806503 \cdot 10^{-29}\mathrm{km^2 kg\,s^{-2} K^{-1}}$ is the Boltzmann constant.
$H^{\oplus}_{\mathrm{eff}} = 6372.0\,\mathrm{km}$ - the effective Earth radius,
$\frac{m}{k \ln 10} = 1.51288$

$$mgdh = \ln 10\, k\, T\, d\zeta$$

$$\zeta = -\log_{10} P$$

$$\zeta^{\oplus} = -\log_{10} 1000 = -3.00.$$

$$\log_b x = \frac{\log x}{\log b}.$$

$$P = e^{-\zeta \log 10}$$

$$\eta_q(\zeta) = \begin{cases} 0, & \zeta \le \zeta_{q-1} \\ \dfrac{\zeta - \zeta_{q-1}}{\zeta_q - \zeta_{q-1}}, & \zeta_{q-1} < \zeta < \zeta_q \\ \dfrac{\zeta_{q+1} - \zeta}{\zeta_{q+1} - \zeta_q}, & \zeta_q \le \zeta < \zeta_{q+1} \\ 0, & \zeta_{q+1} \le \zeta. \end{cases}$$

Note that $\eta_q(\zeta_q) = 1$.

$$\eta_1(\zeta) = \begin{cases} 1, & \zeta \le \zeta_1 \\ \dfrac{\zeta_2 - \zeta}{\zeta_2 - \zeta_1}, & \zeta_1 < \zeta < \zeta_2 \\ 0, & \zeta_2 \le \zeta. \end{cases}$$

$$\eta_Q(\zeta) = \begin{cases} 0, & \zeta \le \zeta_{Q-1} \\ \dfrac{\zeta - \zeta_{Q-1}}{\zeta_Q - \zeta_{Q-1}}, & \zeta_{Q-1} < \zeta < \zeta_Q \\ 1, & \zeta_Q \le \zeta. \end{cases}$$

$$T(\zeta) = \sum_{q=1}^{Q} \eta_q(\zeta) f_q^T$$

$$g \propto \frac{1}{r^2}$$

$$\int mg(h)\,dh = k \ln 10 \int T(\zeta) d\zeta$$

The hydrostatic relation is

$$h(\zeta) + H^{\oplus} = \frac{gH^{\oplus 2}}{gH^{\oplus} - k \log 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta)} \tag{1}$$

or

$$\frac{h(\zeta) + H^{\oplus}}{gH^{\oplus 2}} = \frac{1}{gH^{\oplus} - k \log 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta)}. \tag{2}$$

$$\begin{aligned} P_q(\zeta) &= \int_{\zeta^{\oplus}}^{\zeta} \frac{\eta_q(x)}{m}\,dx, \\ \frac{d}{d\zeta} P_q(\zeta) &= \frac{\eta_q(\zeta)}{m}. \end{aligned}$$

Notation: $H = h + H^{\oplus}$. H^s is the satellite height.
From hydrostatic relation (1), we have

$$\frac{dh}{d\zeta} = \frac{gH^{\oplus 2} k \log 10 \sum f_q^T \eta_q(\zeta)}{m\big[gH^{\oplus} - k \log 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta)\big]^2}. \tag{3}$$

Using relation (2), equation (3) can be rewritten as

$$\frac{dh}{d\zeta} = \frac{(h(\zeta) + H^{\oplus})^2 kT \log 10}{gH^{\oplus\,2} m}.$$

Also

$$\frac{dh}{df_q^T} = \frac{gH^{\oplus 2} k \log 10\, P_q(\zeta)}{\big[gH^{\oplus} - k \log 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta)\big]^2}. \tag{4}$$

Note that

$$\frac{dh}{df_q^T} = \frac{dH}{df_q^T}.$$

2 Absorption Coefficient Calculations

k - molecule
j - line

$$\mathcal{S}_j^k = \mathcal{I}_j^k(300) + \frac{\mathbf{h}cEl_j^k}{\log 10k}\left(\frac{1}{300} - \frac{1}{T}\right) + \log\left[\frac{Q^k(300)\cdot\tanh\{\mathbf{h}\nu/(2kT)\}\cdot\Big(1+\exp\big\{-\mathbf{h}\nu_j^k/(kT)\big\}\Big)}{Q^k(T)\cdot\Big(1-\exp\big\{-\mathbf{h}\nu_{0j}^k/(300k)\big\}\Big)}\right]$$

$$x_j^k(\nu) = \frac{\sqrt{\log 2}(\nu - \nu_j'^k)}{w_d^k}, \qquad y_j^k(\nu) = \frac{\sqrt{\log 2}w_{cj}^k P}{w_d^k}\left(\frac{300}{T}\right)^{n_{cj}^k}, \qquad z_j^k(\nu) = \frac{\sqrt{\log 2}(\nu + \nu_j'^k)}{w_d^k},$$

$$\begin{aligned}
\nu_j^k &= \left[\nu_{0j}^k + \triangle\nu_{0j}^k P\left(\frac{300}{T}\right)^{n_{\triangle\nu_{0j}^k}}\right], \\
\nu_j'^k &= \nu_j^k v_c, \\
v_c &= 1 + (-6.8\mathrm{km/s})/c
\end{aligned}$$

T is temperature in K,
P is pressure in hPa,
$\mathcal{R}^k$ is the isotopic fraction for the species,
$\mathcal{I}_j^k(300)$ is the logarithm of the integrated intensity in $\mathrm{nm}^2\mathrm{MHz}$ at 300K,
ν_{0j}^k is the unshifted rest line center frequency in MHz,
El_j^k is the ground state energy in cm^{-1},
$Q^k(T)$ is the partition function,
w_d^k is the Doppler width in MHz,

w_{cj}^k is the collision width in $\mathrm{MHz hPa}^{-1}$ at 300K, n_{cj}^k is its temperature dependence,
ν_j^k is the line position frequency in MHz
ν is the radiation frequency in MHz

v_c is the Doppler shift of the line position due to the z-axis component of the spacecraft and Earth velocities, $\mathbf{v}$,
$\triangle\nu_{0j}^k$ is the pressure shift parameter in $\mathrm{MHz\,hPa}^{-1}$, and $n_{\triangle\nu_{0j}^k}$ is its temperature dependence.

$$\mathrm{LineShape}\Big(x_j^k(\nu), y_j^k(\nu), z_j^k(\nu)\Big) = \left(\frac{\nu}{\nu_{0j}^k}\right)\left\{\frac{1}{\sqrt{\pi}}\frac{y_j^k(\nu)}{(y_j^k(\nu))^2 + (x_j^k(\nu))^2} + \frac{1}{\sqrt{\pi}}\frac{y_j^k(\nu)}{(z_j^k(\nu))^2 + (y_j^k(\nu))^2}\right\}$$

The cross-section β^k for the kth species is given by

$$\beta^k = \mathcal{R}^k\sqrt{\frac{\log 2}{\pi}}\frac{10^{-13}}{k}\frac{P}{T\cdot w_d^k}\left[\sum_j 10^{S_j^k}\mathrm{LineShape}\Big(x_j^k(\nu), y_j^k(\nu), z_j^k(\nu)\Big)\right]$$

3 Radiative Transfer

The atmospheric representation for the kth state vector component are function of the form

$$F^k = \sum_{q=1}^{Q} \eta_q^k(\zeta) f_q^k,$$

where k is a molecule, where F^k is the continuous representation, f_q^k are its values at breakpoints q, and M are the total number of vertical breakpoints. The functions $\eta_q^k(\zeta)$ represent a piecewise-linear interpolation. In this calculations, F^k represent **mixing ratios**. For example,

$$\begin{aligned} F^{O_3} &= \sum_{q=1}^{Q} \eta_q^{O_3}(\zeta) f_q^{O_3}, \\ F^{N_2} &= 0.8. \end{aligned}$$

The **temperature** representation is of the form

$$T(\zeta) = \sum_{q=1}^{Q} \eta_q^T(\zeta) f_q^T$$

For each of the levels $h_t = h_1,\ h_2,\ h_3, \ldots,$ the **path length** is given by

$$s = \pm\sqrt{(h + H^{\oplus})^2 - (h_t + H^{\oplus})^2}. \tag{5}$$

The choice of the sign depends on which side of the tangent h is.
The **incremental opacity** is given by

$$\triangle\delta_{i \to i-1} = \sum_{k=1}^{NS} \triangle\delta_{i \to i-1}^k,$$

where k is a molecule and NS is the total number of molecules considered. The **species incremental opacity** integral is

$$\triangle\delta_{i \to i-1}^k = \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\, \beta^k \frac{ds}{dh} \frac{dh}{d\zeta}\, d\zeta,$$

where

$$\frac{ds}{dh} = \frac{R}{\sqrt{R^2 - R_t^2}} = \frac{h + H^{\oplus}}{\sqrt{(h + H^{\oplus})^2 - (h_t + H^{\oplus})^2}}, \tag{6}$$

$$\frac{dh}{d\zeta} = \frac{(h + H^{\oplus})^2 kT \log 10}{g_0 H^{\oplus\,2} m}. \tag{7}$$

Here, we can write

$$\triangle\delta_{i \to i-1}^k = \int_{\zeta_i}^{\zeta_{i-1}} \alpha^k(s)\, ds,$$

where $\alpha^k = F^k \beta^k$ is **absorption coefficient** (with respect to molecule k), and

$$ds = \frac{ds}{dh}\frac{dh}{d\zeta} d\zeta.$$

The **transmission function** is defined as

$$\begin{aligned} \mathcal{T}_1 &= 1, \\ \mathcal{T}_2 &= \exp\big(-\triangle\delta_{2 \to 1}\big), \\ \mathcal{T}_3 &= \exp\big(-\triangle\delta_{2 \to 1} - \triangle\delta_{3 \to 2}\big), \\ \ldots & \quad \ldots \\ \mathcal{T}_i &= \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j \to j-1}\Big). \end{aligned}$$

The transmission function can be written in several alternative forms:

$$
\begin{aligned}
\mathcal{T}_i &= \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1}\Big) \\
&= \exp\Big(-\sum_{j=2}^{i}\sum_{k} \triangle\delta^k_{j\to j-1}\Big) \\
&= \exp\Big(-\sum_{j=2}^{i}\int_{\zeta_j}^{\zeta_{j-1}} \sum_k \underbrace{F^k(\zeta)\beta^k(\zeta,T)}_{\alpha^k} \underbrace{\frac{h+H^{\oplus}}{\sqrt{(h+H^{\oplus})^2-(h_t+H^{\oplus})^2}}\frac{(h+H^{\oplus})^2 kT\log 10}{g_0 H^{\oplus\,2} m}\,d\zeta}_{ds}\Big).
\end{aligned}
$$

The quantities can be calculated as follows:
h_t is calculated using Hydrostatic Model,
h is linearly interpolated / averaged (or can be calculated exactly),
T is linearly interpolated /averaged,
F_{O^3} is linearly interpolated,
$\beta^k(\zeta,T)$ is calculated using quadrature rule, with midpoint ζ evaluated exactly.

For each of the levels $h_t = h_1,\ h_2,\ h_3,\ldots$, the path length is given by

$$s_i = \pm\sqrt{(h_i+H^{\oplus})^2-(h_t+H^{\oplus})^2}, \qquad i=1,\ldots,N$$

Approximation: By convention, $\mathcal{T}_1 = 1$.

$$
\begin{aligned}
\triangle s_{i+1\to i} &\approx s_{i+1}-s_i \\
&= \pm\Big(\sqrt{(h_{i+1}+H^{\oplus})^2-(h_t+H^{\oplus})^2}-\sqrt{(h_i+H^{\oplus})^2-(h_t+H^{\oplus})^2}\Big), \qquad i=1,\ldots,N-1, \\
\triangle\delta^k_{i+1\to i} &\approx \frac{F^k_i\beta^k_i + F^k_{i+1}\beta_{i+1}}{2}\triangle s_{i+1\to i}, \qquad i=1,\ldots,N-1.
\end{aligned}
$$

Note that $\triangle s_{i+1\to i} > 0$.

The radiative transfer equation is

$$I(\mathbf{x}) = \sum_{i=1}^{2N}\triangle B_i \mathcal{T}_i,$$

where [1]

$$
\begin{aligned}
\mathcal{T}_1 &= 1, \\
\mathcal{T}_{i+1} &= \exp\Big(-\sum_{j=1}^{i}\triangle\delta_{j+1\to j}\Big), \qquad i\geq 1,
\end{aligned}
$$

and $\triangle B_i$ is the source function in differential temperature format given by

$$
\begin{aligned}
\triangle B_1 &= \frac{T_1+T_2}{2}, \\
\triangle B_i &= \frac{T_{i+1}-T_{i-1}}{2}, \\
\triangle B_{2N} &= T_{space} - \frac{T_{2N-1}+T_{2N}}{2},
\end{aligned}
$$

where $T_{space} = 2.7$.

[1]Notation: In the algorithm, $\triangle s_{j+1\to j} = \triangle s(j)$, $\triangle\delta_{j+1\to j} = \triangle\delta(j)$, and $\mathcal{T}(i+1) = \exp\Big(-\sum_{j=1}^{i}\triangle\delta(j)\Big)$.
Note, $\mathcal{T}(i) = \exp\big(-\big(\delta_{2\to 1}+\ldots\delta_{i\to i-1}\big)\big) = \exp\big(-\big(\triangle\delta(1)+\ldots+\triangle\delta(i-1)\big)\big) = \exp\Big(-\sum_{j=1}^{i-1}\triangle\delta(j)\Big)$.

Example: O_3 and N_2 molecules

$$\mathcal{T}_i = \exp\Bigg[-\sum_{j=2}^{i} \int_{\zeta_j}^{\zeta_{j-1}} \Big[\underbrace{F^{O_3}(\zeta)\beta^{O_3}(\zeta,T)}_{\alpha^{O_3}} + \underbrace{F^{N_2}(\zeta)\beta^{N_2}(\zeta,T)}_{\alpha^{N_2}} \Big] \underbrace{\frac{h+H^{\oplus}}{\sqrt{(h+H^{\oplus})^2-(h_t+H^{\oplus})^2}} \frac{(h+H^{\oplus})^2 kT\log 10}{g_0 H^{\oplus\,2} m}\, d\zeta}_{ds} \Bigg].$$

4 Derivatives

4.1 Radiative Transfer Derivative

Since

$$I(\mathbf{x}) = \sum_{i=1}^{2N} \triangle B_i \mathcal{T}_i,$$

with

$$\mathcal{T}_i = \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1} \Big),$$

the **derivative of the radiative transfer** is

$$\begin{aligned}
\frac{\partial I(\mathbf{x})}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{2N} \triangle B_i \mathcal{T}_i \\
&= \sum_{i=1}^{2N} \Big[\frac{\partial \triangle B_i}{\partial x_k} \mathcal{T}_i + \triangle B_i \frac{\partial \mathcal{T}_i}{\partial x_k} \Big] \\
&= \sum_{i=1}^{2N} \Big[\frac{\partial \triangle B_i}{\partial x_k} \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1} \Big) + \triangle B_i \frac{\partial}{\partial x_k} \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1} \Big) \Big] \\
&= \sum_{i=1}^{2N} \Big[\frac{\partial \triangle B_i}{\partial x_k} \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1} \Big) - \triangle B_i \Big(\sum_{j=2}^{i} \frac{\partial \triangle\delta_{j\to j-1}}{\partial x_k} \Big) \exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1} \Big) \Big] \\
&= \sum_{i=1}^{2N} \Big[\frac{\partial \triangle B_i}{\partial x_k} - \triangle B_i \Big(\sum_{j=2}^{i} \frac{\partial \triangle\delta_{j\to j-1}}{\partial x_k} \Big) \Big] \mathcal{T}_i \\
&= \sum_{i=1}^{2N} \Big[\frac{\partial \triangle B_i}{\partial x_k} - \triangle B_i \mathcal{W}_i \Big] \mathcal{T}_i,
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{W}_1 &= 0, \\
\mathcal{W}_i &= \sum_{j=2}^{i} \frac{\partial \triangle\delta_{j\to j-1}}{\partial x_k} \\
&= \sum_{j=2}^{i-1} \frac{\partial \triangle\delta_{j\to j-1}}{\partial x_k} + \frac{\partial \triangle\delta_{i\to i-1}}{\partial x_k} \\
&= \mathcal{W}_{i-1} + \frac{\partial \triangle\delta_{i\to i-1}}{\partial x_k}.
\end{aligned}$$

4.2 Radiative Transfer Second Derivative

The **second derivative of the radiative transfer** is

$$
\begin{aligned}
\frac{\partial^2 I(\mathbf{x})}{\partial x \partial y} &= \frac{\partial}{\partial y}\Big(\frac{\partial I}{\partial x}\Big) = \frac{\partial}{\partial y}\bigg(\sum_{i=1}^{2N}\bigg[\frac{\partial \triangle B_i}{\partial x} - \triangle B_i \sum_{j=2}^{i} \frac{\partial \triangle \delta_{j\to j-1}}{\partial x}\bigg]\mathcal{T}_i\bigg) \\
&= \sum_{i=1}^{2N}\Bigg(\bigg[\frac{\partial \triangle^2 B_i}{\partial x \partial y} - \frac{\partial \triangle B_i}{\partial y}\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x} - \triangle B_i \sum_{j=2}^{i}\frac{\partial^2 \triangle \delta_{j\to j-1}}{\partial x \partial y}\bigg]\mathcal{T}_i \\
&\qquad -\bigg[\frac{\partial \triangle B_i}{\partial x} - \triangle B_i \sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x}\bigg]\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial y}\,\mathcal{T}_i \\
&= \sum_{i=1}^{2N}\bigg[\frac{\partial \triangle^2 B_i}{\partial x \partial y} - \frac{\partial \triangle B_i}{\partial y}\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x} - \frac{\partial \triangle B_i}{\partial x}\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial y} \\
&\qquad + \triangle B_i\bigg(\Big(\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x}\Big)\Big(\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial y}\Big) - \sum_{j=2}^{i}\frac{\partial^2 \triangle \delta_{j\to j-1}}{\partial x \partial y}\bigg)\bigg]\mathcal{T}_i,
\end{aligned}
$$

or

$$
\frac{\partial^2 I(\mathbf{x})}{\partial x \partial y} = \sum_{i=1}^{2N}\bigg[\frac{\partial \triangle^2 B_i}{\partial x \partial y} - \frac{\partial \triangle B_i}{\partial y}\mathcal{W}_i^x - \frac{\partial \triangle B_i}{\partial x}\mathcal{W}_i^y + \triangle B_i\Big(\mathcal{W}_i^x\,\mathcal{W}_i^y - \partial \mathcal{W}_i^{x,y}\Big)\bigg]\mathcal{T}_i,
$$

where

$$
\begin{aligned}
\mathcal{W}_1^x &= 0, \quad \mathcal{W}_1^y = 0, \quad \partial\mathcal{W}_1^{x,y} = 0, \\
\mathcal{W}_i^x &= \sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x} = \sum_{j=2}^{i-1}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x} + \frac{\partial \triangle \delta_{i\to i-1}}{\partial x} \\
&= \mathcal{W}_{i-1}^x + \frac{\partial \triangle \delta_{i\to i-1}}{\partial x}, \\
\mathcal{W}_i^y &= \sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial y} = \sum_{j=2}^{i-1}\frac{\partial \triangle \delta_{j\to j-1}}{\partial y} + \frac{\partial \triangle \delta_{i\to i-1}}{\partial y} \\
&= \mathcal{W}_{i-1}^y + \frac{\partial \triangle \delta_{i\to i-1}}{\partial y}, \\
\partial\mathcal{W}_i^{x,y} &= \sum_{j=2}^{i}\frac{\partial^2 \triangle \delta_{j\to j-1}}{\partial x \partial y} \\
&= \partial\mathcal{W}_{i-1}^{x,y} + \frac{\partial^2 \triangle \delta_{i\to i-1}}{\partial x \partial y}.
\end{aligned}
$$

For $x = y$, the second derivative of the radiative transfer is

$$
\frac{\partial^2 I(\mathbf{x})}{\partial x^2} = \sum_{i=1}^{2N}\bigg[\frac{\partial \triangle^2 B_i}{\partial x^2} - 2\frac{\partial \triangle B_i}{\partial x}\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x} + \triangle B_i\bigg(\Big(\sum_{j=2}^{i}\frac{\partial \triangle \delta_{j\to j-1}}{\partial x}\Big)^2 - \sum_{j=2}^{i}\frac{\partial^2 \triangle \delta_{j\to j-1}}{\partial x^2}\bigg)\bigg]\mathcal{T}_i,
$$

or

$$
\frac{\partial^2 I(\mathbf{x})}{\partial x^2} = \sum_{i=1}^{2N}\bigg[\frac{\partial \triangle^2 B_i}{\partial x^2} - 2\frac{\partial \triangle B_i}{\partial x}\mathcal{W}_i + \triangle B_i\Big(\mathcal{W}_i^2 - \frac{\partial \mathcal{W}_i}{\partial x}\Big)\bigg]\mathcal{T}_i,
$$

where

$$
\begin{aligned}
\mathcal{W}_1^x &= 0, \qquad \partial\mathcal{W}_1^{x,x} \;=\; 0,\\
\mathcal{W}_i^x &= \sum_{j=2}^{i} \frac{\partial \triangle\delta_{j\to j-1}}{\partial x} \;=\; \sum_{j=2}^{i-1} \frac{\partial \triangle\delta_{j\to j-1}}{\partial x} + \frac{\partial \triangle\delta_{i\to i-1}}{\partial x}\\
&= \mathcal{W}_{i-1}^x + \frac{\partial \triangle\delta_{i\to i-1}}{\partial x},\\
\partial\mathcal{W}_i^{x,x} &= \sum_{j=2}^{i} \frac{\partial^2 \triangle\delta_{j\to j-1}}{\partial x^2}\\
&= \partial\mathcal{W}_{i-1}^{x,x} + \frac{\partial^2 \triangle\delta_{i\to i-1}}{\partial x^2}.
\end{aligned}
$$

4.3 Mixing Ratio Derivatives

For k and $\tilde{k}$ state vector components (mixing ratio species), $x = f_q^k$ and $y = f_{\tilde{q}}^{\tilde{k}}$ above. Here, q and $\tilde{q}$ are breakpoints where f^k and $f^{\tilde{k}}$ are known. Note that since $\dfrac{\partial \triangle B_i}{\partial f_q^k} = 0$ for all k and q, we have

$$
\frac{\partial I(\mathbf{x})}{\partial f_q^k} \;=\; -\sum_{i=1}^{2N} \triangle B_i \mathcal{W}_{i,q}^k \mathcal{T}_i, \tag{8}
$$

where

$$
\begin{aligned}
\mathcal{W}_{1,q}^k &= 0,\\
\mathcal{W}_{i,q}^k &= \mathcal{W}_{i-1,q}^k + \frac{\partial \triangle\delta_{i\to i-1}}{\partial f_q^k}.
\end{aligned}
$$

4.4 Mixing Ratio Second Derivatives

Note that since $\dfrac{\partial \triangle B_i}{\partial f_q^k} = 0$ and $\dfrac{\partial^2 \triangle B_i}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = 0$, we have

$$
\frac{\partial^2 I(\mathbf{x})}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} \;=\; \sum_{i=1}^{2N} \triangle B_i \left(\mathcal{W}_{i,q}^k \, \mathcal{W}_{i,\tilde{q}}^{\tilde{k}} - \partial\mathcal{W}_{i,q,\tilde{q}}^{k,\tilde{k}} \right) \mathcal{T}_i,
$$

where

$$
\begin{aligned}
\mathcal{W}_{1,q}^k &= 0, \quad \partial\mathcal{W}_{1,q,\tilde{q}}^k \;=\; 0,\\
\mathcal{W}_{i,q}^k &= \mathcal{W}_{i-1,q}^k + \frac{\partial \triangle\delta_{i\to i-1}}{\partial f_q^k},\\
\partial\mathcal{W}_{i,q,\tilde{q}}^{k,\tilde{k}} &= \partial\mathcal{W}_{i-1,q,\tilde{q}}^{k,\tilde{k}} + \frac{\partial^2 \triangle\delta_{i\to i-1}}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}}.
\end{aligned}
$$

Opacity Derivatives

The species incremental opacity integral is

$$
\triangle\delta_{i\to i-1}^k = \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k \,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,
$$

where mixing ratios are given by

$$
F^k(\zeta) \;=\; \sum_{q=1}^{Q} \eta_q^k(\zeta) f_q^k,
$$

and

$$\frac{\partial F^k}{\partial f_q^k} = \eta_q^k(\zeta),$$

$$\frac{\partial F^k}{\partial f_q^{\tilde{k}}} = 0, \quad \text{for } k \neq \tilde{k}.$$

The **opacity derivative** with respect to mixing ratio using the linear basis is

$$\frac{\partial \triangle\delta^k_{i\to i-1}}{\partial f_q^k} = \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^k(\zeta)\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,$$

$$\frac{\partial \triangle\delta^k_{i\to i-1}}{\partial f_q^{\tilde{k}}} = 0, \quad \text{for } k \neq \tilde{k},$$

where k and $\tilde{k}$ are molecules. Note that $\dfrac{\partial \triangle\delta_{i\to i-1}}{\partial f_q^k} = \dfrac{\partial}{\partial f_q^k}\Big(\sum_k \triangle\delta^k_{i\to i-1}\Big) = \dfrac{\partial \triangle\delta^k_{i\to i-1}}{\partial f_q^k}$.

Opacity Second Order Derivatives

The **opacity second order derivative** with respect to mixing ratios for molecules k and $\tilde{k}$ is identically 0:

$$\frac{\partial^2 \triangle\delta^k_{i\to i-1}}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = \int_{\zeta_i}^{\zeta_{i-1}} \frac{\partial \eta_q^k(\zeta)}{\partial f_{\tilde{q}}^{\tilde{k}}}\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta \;=\; 0,$$

for all k, $\tilde{k}$ and q, $\tilde{q}$. Thus,

$$\partial \mathcal{W}^{k,\tilde{k}}_{i,q,\tilde{q}} = 0,$$

and

$$\frac{\partial^2 I(\mathbf{x})}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = \sum_{i=1}^{2N} \triangle B_i \mathcal{W}^k_{i,q} \mathcal{W}^{\tilde{k}}_{i,\tilde{q}}\,\mathcal{T}_i. \tag{9}$$

Remark: Since

$$\frac{\partial I}{\partial f_q^k} = \sum_{i=1}^{2N} \triangle B_i \frac{\partial \mathcal{T}_i}{\partial f_q^k} \qquad \text{and} \qquad \frac{\partial^2 I}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = \sum_{i=1}^{2N} \triangle B_i \frac{\partial^2 \mathcal{T}_i}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}},$$

radiative transfer mixing ratio first and second derivatives can be computed after evaluating derivatives of $\mathcal{T}_i$:

$$\begin{aligned}
\frac{\partial \mathcal{T}_i}{\partial f_q^k} &= \frac{\partial}{\partial f_q^k}\Big[\exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1}\Big)\Big] \\
&= \frac{\partial}{\partial f_q^k}\Big[\exp\Big(-\sum_{j=2}^{i}\sum_k \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\Big)\Big] \\
&= -\mathcal{T}_i \sum_{j=2}^{i} \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^k \beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta, \\
\frac{\partial^2 \mathcal{T}_i}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} &= \mathcal{T}_i \left(\sum_{j=2}^{i} \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^k \beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\right)\left(\sum_{j=2}^{i} \int_{\zeta_i}^{\zeta_{i-1}} \eta_{\tilde{q}}^{\tilde{k}} \beta^{\tilde{k}}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\right),
\end{aligned}$$

which are consistent with results obtained in (8) and (9).

Examples

O_3 molecules

The opacity derivative with respect to O_3 mixing ratio using the linear basis is

$$\frac{\partial \triangle\delta^{O_3}_{i\to i-1}}{\partial f^{O_3}_q} = \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.$$

The **derivative of the radiative transfer** is

$$\frac{\partial I(\mathbf{x})}{\partial f^{O_3}_q} = -\sum_{i=1}^{2N} \triangle B_i \mathcal{W}^{O_3}_{i,q}\mathcal{T}_i,$$

where

$$\begin{aligned}
\mathcal{W}^{O_3}_{1,q} &= 0,\\
\mathcal{W}^{O_3}_{i,q} &= \mathcal{W}^{O_3}_{i-1,q} + \frac{\partial \triangle\delta_{i\to i-1}}{\partial f^{O_3}_q}.
\end{aligned}$$

For all i and q, calculate

$$\frac{\partial \triangle\delta^{O_3}_{i\to i-1}}{\partial f^{O_3}_q} = \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.$$

Given $W^{O_3}_{i,q}$, compute

$$\frac{\partial I_l}{\partial f^{O_3}_q} = -\sum_{i=1}^{2N} \triangle B_i \mathcal{W}^{O_3}_{i,q}\mathcal{T}_i,$$

where l is the level number (path) above the Earth surface. For a higher level l, there are more i's with $\mathcal{T}_i = 0$.

O_3 and N_2 molecules

The opacity derivatives with respect to O_3 and N_2 mixing ratios using the linear basis are

$$\begin{aligned}
\frac{\partial \triangle\delta^{O_3}_{i\to i-1}}{\partial f^{O_3}_q} &= \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,\\
\frac{\partial \triangle\delta^{N_2}_{i\to i-1}}{\partial f^{N_2}_q} &= \int_{\zeta_i}^{\zeta_{i-1}} \eta^{N_2}_q(\zeta)\,\beta^{N_2}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.
\end{aligned}$$

Since **incremental opacity** is given by

$$\triangle\delta_{i\to i-1} = \triangle\delta^{O_3}_{i\to i-1} + \triangle\delta^{N_2}_{i\to i-1},$$

we have

$$\begin{aligned}
\frac{\partial \triangle\delta_{i\to i-1}}{\partial f^{O_3}_q} &= \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,\\
\frac{\partial \triangle\delta_{i\to i-1}}{\partial f^{N_2}_q} &= \int_{\zeta_i}^{\zeta_{i-1}} \eta^{N_2}_q(\zeta)\beta^{N_2}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.
\end{aligned}$$

The derivative of the radiative transfer is

$$\frac{\partial I(\mathbf{x})}{\partial f^{k}_q} = -\sum_{i=1}^{2N} \triangle B_i \mathcal{W}^{k}_{i,q}\mathcal{T}_i,$$

where

$$
\begin{aligned}
\mathcal{W}_{1,q}^{k} &= 0, \\
\mathcal{W}_{i,q}^{k} &= \mathcal{W}_{i-1,q}^{k} + \frac{\partial \triangle \delta_{i \to i-1}}{\partial f_q^k},
\end{aligned}
$$

where k is either O_3 or N_2.

4.5 Temperature Derivative

The hydrostatic relation is

$$h(\zeta) = \frac{g^{\oplus} H^{\oplus 2}}{g^{\oplus} H^{\oplus} - k \ln 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta)} - H^{\oplus}$$

The **temperature** representation is of the form

$$T(\zeta) = \sum_{q=1}^{Q} \eta_q^T(\zeta) f_q^T.$$

The species incremental opacity integral is

$$\triangle\delta^k_{i\to i-1} = \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.$$

Substituting

$$\begin{aligned}
\frac{ds}{dh} &= \frac{R}{\sqrt{R^2 - R_t^2}} = \frac{h + H^{\oplus}}{\sqrt{(h+H^{\oplus})^2 - (h_t + H^{\oplus})^2}}, \\
\frac{dh}{d\zeta} &= \frac{(h+H^{\oplus})^2 kT \log 10}{g_0 H^{\oplus\,2} m},
\end{aligned}$$

into the species incremental opacity integral and differentiating with respect to f_q^T gives

$$\begin{aligned}
\frac{\partial \triangle\delta^k_{i\to i-1}}{\partial f_q^T} &= \frac{\partial}{\partial f_q^T} \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\big(P(\zeta), T(\zeta), \zeta\big)\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta \\
&= \frac{\partial}{\partial f_q^T} \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\big(P(\zeta), T(\zeta), \zeta\big)\,\frac{h + H^{\oplus}}{\sqrt{(h+H^{\oplus})^2 - (h_t + H^{\oplus})^2}}\,\frac{(h+H^{\oplus})^2 kT \log 10}{g_0 H^{\oplus\,2} m}\,d\zeta \\
&= \int_{\zeta_i}^{\zeta_{i-1}} \left\{ F^k \frac{\partial \beta^k}{\partial f_q^T}\,\frac{h + H^{\oplus}}{\sqrt{(h+H^{\oplus})^2 - (h_t + H^{\oplus})^2}}\,\frac{(h+H^{\oplus})^2 kT \log 10}{g_0 H^{\oplus\,2} m} \right. \\
&\quad + F^k \beta^k \frac{\partial}{\partial f_q^T}\left[\frac{(h+H^{\oplus})^3}{\sqrt{(h+H^{\oplus})^2 - (h_t + H^{\oplus})^2}}\right]\frac{kT \log 10}{g_0 H^{\oplus\,2} m} \\
&\quad \left. + F^k \beta^k \frac{(h+H^{\oplus})^3}{\sqrt{(h+H^{\oplus})^2 - (h_t + H^{\oplus})^2}}\,\frac{\partial}{\partial f_q^T}\left[\frac{kT \log 10}{g_0 H^{\oplus\,2} m}\right] \right\} d\zeta \\
&= \int_{\zeta_i}^{\zeta_{i-1}} \left\{ F^k \underbrace{\frac{\partial \beta^k}{\partial T}\,\frac{\partial T}{\partial f_q^T}}_{\partial\beta^k/\partial f_q^T}\,\frac{ds}{dh}\,\frac{dh}{d\zeta} \right. \\
&\quad + F^k \beta^k \frac{2(h+H^{\oplus})^2 \frac{\partial h}{\partial f_q^T} - 3(h_t+H^{\oplus})^2 \frac{\partial h}{\partial f_q^T} + (h+H^{\oplus})(h_t+H^{\oplus}) \frac{\partial h_t}{\partial f_q^T}}{\Big((h+H^{\oplus})^2 - (h_t+H^{\oplus})^2\Big)^{\frac{3}{2}}}(h+H^{\oplus})^2\,\frac{kT \log 10}{g_0 H^{\oplus\,2} m} \\
&\quad \left. + F^k \beta^k \underbrace{\frac{(h+H^{\oplus})^3}{\sqrt{(h+H^{\oplus})^2 - (h_t + H^{\oplus})^2}}}_{\frac{ds}{dh}(h+H^{\oplus})^2}\,\eta_q^T(\zeta)\,\underbrace{\left[\frac{k \log 10}{g_0 H^{\oplus\,2} m}\right]}_{\frac{dh}{d\zeta}/T/(h+H^{\oplus})^2} \right\} d\zeta.
\end{aligned}$$

Approximation:

$$\beta^k = \beta_0^k \left(\frac{T}{T_0}\right)^{n^k}.$$

Then,

$$\frac{\partial \beta^k}{\partial T} = n^k \beta_0^k \left(\frac{T}{T_0}\right)^{n^k-1} \frac{1}{T_0} = \frac{n^k \beta^k}{T}.$$

Here, n^k is calculated from

$$\begin{aligned}
\frac{\beta_1^k}{\beta_2^k} &= \left(\frac{T_1}{T_2}\right)^{n^k}, \qquad \text{or} \\
n^k &= \frac{\log \dfrac{\beta^k(T_0+\epsilon, P, \nu)}{\beta^k(T_0-\epsilon, P, \nu)}}{\log\left(\dfrac{T_0+\epsilon}{T_0-\epsilon}\right)},
\end{aligned}$$

with, for example, $T_0 = 230$ and $\epsilon = 5$.
Thus, the **temperature derivative of the incremental opacity** equation is

$$\begin{aligned}
\frac{\partial \triangle\delta^k_{i\to i-1}}{\partial f_q^T} &= \int_{\zeta_i}^{\zeta_{i-1}} \Bigg\{ F^k \beta^k \frac{n^k}{T} \eta_q^T(\zeta) \frac{ds}{dh}\frac{dh}{d\zeta} \\
&\quad + F^k\beta^k \frac{2(h+H^\oplus)^2 \dfrac{\partial h}{\partial f_q^T} - 3(h_t+H^\oplus)^2 \dfrac{\partial h}{\partial f_q^T} + (h+H^\oplus)(h_t+H^\oplus)\dfrac{\partial h_t}{\partial f_q^T}}{\left((h+H^\oplus)^2-(h_t+H^\oplus)^2\right)^{\frac{3}{2}}} \frac{dh}{d\zeta} \\
&\quad + F^k\beta^k \frac{\eta_q^T(\zeta)}{T}\frac{ds}{dh}\frac{dh}{d\zeta} \Bigg\} d\zeta.
\end{aligned}$$

$$\begin{aligned}
\frac{\partial h}{\partial f_q^T} &= \frac{g^\oplus {H^\oplus}^2 k \ \log 10 \ P_q(\zeta)}{\left[g^\oplus H^\oplus - k\log 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta)\right]^2}, \\
\frac{\partial h_t}{\partial f_q^T} &= \frac{g^\oplus {H^\oplus}^2 k \ \log 10 \ P_q(\zeta_t)}{\left[g^\oplus H^\oplus - k\log 10 \sum_{q=1}^{Q} f_q^T P_q(\zeta_t)\right]^2}.
\end{aligned}$$

Since **incremental opacity** is given by

$$\triangle\delta_{i\to i-1} = \triangle\delta^{O_3}_{i\to i-1} + \triangle\delta^{N_2}_{i\to i-1},$$

we have

$$\frac{\partial \triangle\delta_{i\to i-1}}{\partial f_q^T} = \frac{\partial \triangle\delta^{O_3}_{i\to i-1}}{\partial f_q^T} + \frac{\partial \triangle\delta^{N_2}_{i\to i-1}}{\partial f_q^T}.$$

The **temperature derivative** of radiance is given as

$$\frac{\partial I(\mathbf{x})}{\partial f_q^T} = \sum_{i=1}^{2N}\left[\frac{\partial \triangle B_i}{\partial f_q^T} - \triangle B_i \mathcal{W}_i\right]\mathcal{T}_i,$$

where

$$
\begin{aligned}
\mathcal{W}_{1,q} &= 0, \\
\mathcal{W}_{i,q} &= \sum_{j=2}^{i} \frac{\partial \triangle \delta_{j \to j-1}}{\partial f_q^T} \\
&= \sum_{j=2}^{i-1} \frac{\partial \triangle \delta_{j \to j-1}}{\partial f_q^T} + \frac{\partial \triangle \delta_{i \to i-1}}{\partial f_q^T} \\
&= \mathcal{W}_{i-1,q} + \frac{\partial \triangle \delta_{i \to i-1}}{\partial f_q^T}.
\end{aligned}
$$

4.6 Temperature Second Derivative

$$
\begin{aligned}
\frac{\partial^2 \triangle\delta^k_{i\to i-1}}{\partial f^T_q \partial f^T_{\tilde{q}}} &= \frac{\partial}{\partial f^T_{\tilde{q}}} \int_{\zeta_i}^{\zeta_{i-1}} \Bigg\{ F^k \beta^k \, \frac{n^k}{T} \, \eta^T_q(\zeta) \, \frac{ds}{dh} \, \frac{dh}{d\zeta} \\
&\quad + F^k \beta^k \frac{2(h+H^{\oplus})^2 \dfrac{\partial h}{\partial f^T_q} - 3(h_t+H^{\oplus})^2 \dfrac{\partial h}{\partial f^T_q} + (h+H^{\oplus})(h_t+H^{\oplus}) \dfrac{\partial h_t}{\partial f^T_q}}{\Big((h+H^{\oplus})^2 - (h_t+H^{\oplus})^2\Big)^{\frac{3}{2}}} \, \frac{dh}{d\zeta} \\
&\quad + F^k \beta^k \, \frac{\eta^T_q(\zeta)}{T} \frac{ds}{dh} \, \frac{dh}{d\zeta} \Bigg\} \, d\zeta
\end{aligned}
$$

$$
\begin{aligned}
&= \int_{\zeta_i}^{\zeta_{i-1}} \Bigg\{ \frac{\partial}{\partial f^T_{\tilde{q}}} \left[F^k \beta^k \, \frac{n^k}{T} \, \eta^T_q(\zeta) \, \frac{ds}{dh} \, \frac{dh}{d\zeta} \right] d\zeta \\
&\quad + \frac{\partial}{\partial f^T_{\tilde{q}}} \left[F^k \beta^k \frac{2(h+H^{\oplus})^2 \dfrac{\partial h}{\partial f^T_q} - 3(h_t+H^{\oplus})^2 \dfrac{\partial h}{\partial f^T_q} + (h+H^{\oplus})(h_t+H^{\oplus}) \dfrac{\partial h_t}{\partial f^T_q}}{\Big((h+H^{\oplus})^2 - (h_t+H^{\oplus})^2\Big)^{\frac{3}{2}}} \, \frac{dh}{d\zeta} \right] \\
&\quad + \frac{\partial}{\partial f^T_{\tilde{q}}} \left[F^k \beta^k \, \frac{\eta^T_q(\zeta)}{T} \frac{ds}{dh} \, \frac{dh}{d\zeta} \right] \Bigg\} \, d\zeta
\end{aligned}
$$

The Planck radiation function B expressed in temperature units is

$$B_i = \frac{\mathbf{h}\nu}{k\big[\exp\big(\frac{\mathbf{h}\nu}{kT_i}\big) - 1\big]},$$

where $\mathbf{h}$ is Planck's constant, k is Boltzmann's constant, ν is the radiation frequency, and T_i is temperature at the ith level. The differential source function is given by

$$\begin{aligned}
\triangle B_1 &= \frac{B_1 + B_2}{2}, \\
\triangle B_i &= \frac{B_{i+1} - B_{i-1}}{2}, \\
\triangle B_{2N} &= I_0 - \frac{B_{2N-1} + B_{2N}}{2},
\end{aligned}$$

where $I_0 = 2.7$ is the background cosmic radiance incident on the atmosphere.
The source function Jacobian for temperature is

$$\frac{\partial \triangle B_i}{\partial f_q^T} = \frac{\frac{\partial B_{i+1}}{\partial f_q^T} - \frac{\partial B_{i-1}}{\partial f_q^T}}{2},$$

where

$$\begin{aligned}
\frac{\partial B_i}{\partial f_q^T} &= -\frac{\mathbf{h}\nu}{k\big[\exp\big(\frac{\mathbf{h}\nu}{kT_i}\big) - 1\big]^2} \cdot \frac{-\mathbf{h}\nu}{kT_i^2} \exp\left(\frac{\mathbf{h}\nu}{kT_i}\right) \eta_q^T(\zeta_i) \\
&= \frac{B_i^2 \exp\big(\frac{\mathbf{h}\nu}{kT_i}\big)}{T_i^2} \eta_q^T(\zeta_i).
\end{aligned}$$

Approximation: The Planck radiation function B can be approximated by T. That is, $B_i \approx T_i$. Hence,

$$\begin{aligned}
\triangle B_1 &= \frac{T_1 + T_2}{2}, \\
\triangle B_i &= \frac{T_{i+1} - T_{i-1}}{2}, \\
\triangle B_{2N} &= T_{space} - \frac{T_{2N-1} + T_{2N}}{2},
\end{aligned}$$

where $T_{space} = 2.7$. Then, the source function Jacobian for temperature is

$$\begin{aligned}
\frac{\partial \triangle B_1}{\partial f_q^T} &= \frac{\eta_q^T(\zeta_1) + \eta_q^T(\zeta_2)}{2}, \\
\frac{\partial \triangle B_i}{\partial f_q^T} &= \frac{\dfrac{\partial T_{i+1}}{\partial f_q^T} - \dfrac{\partial T_{i-1}}{\partial f_q^T}}{2} \\
&= \frac{\eta_q^T(\zeta_{i+1}) - \eta_q^T(\zeta_{i-1})}{2}, \\
\frac{\partial \triangle B_{2N}}{\partial f_q^T} &= -\frac{\eta_q^T(\zeta_{2N-1}) + \eta_q^T(\zeta_{2N})}{2}.
\end{aligned}$$

5 Antenna Radiance

The channel radiance for each height is

$$I^A(\epsilon_t, \alpha_t) = \frac{\displaystyle\int_{-\pi}^{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon, \alpha)\, G(\epsilon_t - \epsilon, \alpha_t - \alpha) \cos\epsilon \, d\epsilon \, d\alpha}{\displaystyle\int_{-\pi}^{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} G(\epsilon_t - \epsilon, \alpha_t - \alpha) \cos\epsilon \, d\epsilon \, d\alpha}. \tag{10}$$

We have atmospheric information regarding the azimuth or α dimension. Therefore, we assume $I(\epsilon, \alpha)$ has no α dependence, so we write

$$I^A(\epsilon_t) = \frac{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon) \cos\epsilon \int_{-\pi}^{\pi} G(\epsilon_t - \epsilon, \alpha_t - \alpha) \, d\alpha \, d\epsilon}{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos\epsilon \int_{-\pi}^{\pi} G(\epsilon_t - \epsilon, \alpha_t - \alpha) \, d\alpha \, d\epsilon}.$$

Define

$$\overline{G}(\epsilon_t - \epsilon) \quad = \quad \frac{1}{2\pi} \int_{-\pi}^{\pi} G(\epsilon_t - \epsilon, \alpha_t - \alpha) \, d\alpha.$$

Then,

$$I^A(\epsilon_t) = \frac{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\, \overline{G}(\epsilon_t - \epsilon) \, \cos\epsilon \, d\epsilon}{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t - \epsilon) \, \cos\epsilon \, d\epsilon}. \tag{11}$$

Note that

$$4\pi = \int_{-\pi}^{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} G(\epsilon_t - \epsilon, \alpha_t - \alpha) \cos\epsilon \, d\epsilon \, d\alpha. \tag{12}$$

Then, we have

$$2 \quad = \quad \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t - \epsilon) \cos\epsilon \, d\epsilon,$$

and

$$I^A(\epsilon_t) \quad = \quad \frac{1}{2} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\, \overline{G}(\epsilon_t - \epsilon) \cos\epsilon \, d\epsilon. \tag{13}$$

However, we do not integrate over the entire range:

$$I^A(\epsilon_t) \quad = \quad \frac{1}{2} \int_{\epsilon_t - \epsilon_0}^{\epsilon_t + \epsilon_0} I(\epsilon)\, \overline{G}(\epsilon_t - \epsilon) \cos(\epsilon_t - \epsilon) \, d(\epsilon_t - \epsilon). \tag{14}$$

6 Antenna Radiance Jacobians

Given the expression of antenna radiance I^A in equation (11), the **antenna radiance Jacobian**, which considers the sensitivity of the antenna radiance to a state vector element at a fixed tangent pressure, is given by

$$
\begin{aligned}
\frac{\partial I^A}{\partial x_q} &= \frac{\partial}{\partial x_q} \frac{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon} \\
&= \frac{\partial}{\partial x_q}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \;\cdot\; \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon} \\
&\quad - \frac{\partial}{\partial x_q}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \;\cdot\; \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \;\cdot\; \frac{1}{\left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon\right]^2},
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial I^A}{\partial x_q} &= \left[\frac{\partial}{\partial x_q}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \right. \\
&\qquad \left. - I^A(\epsilon_t)\;\cdot\;\frac{\partial}{\partial x_q}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon\right] \cdot \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon} \\
&= \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial I(\epsilon)}{\partial x_q}\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\frac{\partial \overline{G}(\epsilon_t-\epsilon)}{\partial x_q}\,\cos\epsilon\,d\epsilon \right. \\
&\qquad + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\frac{\partial\cos\epsilon}{\partial x_q}\,d\epsilon + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,\frac{\partial}{\partial x_q}\,d\epsilon \\
&\qquad - I^A(\epsilon_t)\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial \overline{G}(\epsilon_t-\epsilon)}{\partial x_q}\,\cos\epsilon\,d\epsilon - I^A(\epsilon_t)\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\frac{\partial\cos\epsilon}{\partial x_q}\,d\epsilon \\
&\qquad \left. - I^A(\epsilon_t)\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,\frac{\partial}{\partial x_q}\,d\epsilon\right] \cdot \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}.
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
\frac{\partial I^A}{\partial x_q} &= \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left[\frac{\partial I}{\partial x_q} + (I(\epsilon) - I^A(\epsilon_t))\frac{d}{d\epsilon}\left(\frac{\partial\epsilon}{\partial x_q}\right)\right]\overline{G}(\epsilon_t-\epsilon)\cos\epsilon\,d\epsilon \right. \\
&\quad + \frac{\partial\epsilon_t}{\partial x_q}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} (I(\epsilon) - I^A(\epsilon_t))\,\frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\,\cos\epsilon\,d\epsilon - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} (I(\epsilon) - I^A(\epsilon_t))\,\frac{\partial\epsilon}{\partial x_q}\,\frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\,\cos\epsilon\,d\epsilon \\
&\quad \left. + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} (I(\epsilon) - I^A(\epsilon_t))\,\overline{G}(\epsilon_t-\epsilon)\,\frac{\partial\cos\epsilon}{\partial x_q}\,d\epsilon\right] \cdot \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}.
\end{aligned}
$$

where x_q is a state vector element and $I \equiv I(\mathbf{x}(\epsilon_t))$.

Geometric Quantities

Notation: $H = h + H^{\oplus}$. H^s is the satellite height.

$$\sin\epsilon = \left(\frac{h + H^{\oplus}}{H^s}\right), \tag{16}$$

$$\epsilon = \sin^{-1}\left(\frac{h + H^{\oplus}}{H^s}\right), \tag{17}$$

$$\frac{d\epsilon}{dh} = \frac{1}{\sqrt{1-\left(\frac{h+H^{\oplus}}{H^s}\right)^2}} \cdot \frac{1}{H^s} = \frac{1}{H^s \cos\epsilon}. \tag{18}$$

To convert to pressure integration coordinates:

$$d\epsilon = \frac{d\epsilon}{dh}\frac{dh}{d\zeta}d\zeta.$$

6.1 Mixing Ratios Antenna Radiance Jacobian

Since molecular concentrations have no effect on tangent pressure, we have $\partial\epsilon/\partial f_q^k = 0$ and $\partial\cos\epsilon/\partial f_q^k = -\sin\epsilon\,(\partial\epsilon/\partial f_q^k) = 0$, and mixing ratios antenna radiance Jacobian becomes

$$\frac{\partial I^A}{\partial f_q^k} = \frac{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial I(\epsilon)}{\partial f_q^k}\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}.$$

However, we do not integrate over the entire range:

$$\frac{\partial I^A}{\partial f_q^k} = \frac{\displaystyle\int_{\epsilon_t-\epsilon_0}^{\epsilon_t+\epsilon_0} \frac{\partial I(\epsilon)}{\partial f_q^k}\,\overline{G}(\epsilon_t-\epsilon)\,\cos(\epsilon_t-\epsilon)\,d(\epsilon_t-\epsilon)}{\displaystyle\int_{\epsilon_t-\epsilon_0}^{\epsilon_t+\epsilon_0} \overline{G}(\epsilon_t-\epsilon)\,\cos(\epsilon_t-\epsilon)\,d(\epsilon_t-\epsilon)}.$$

6.2 Mixing Ratios Antenna Radiance Hessian

Since molecular concentrations have no effect on tangent pressure, we have $\partial\epsilon/\partial f_q^k = 0$ and $\partial\cos\epsilon/\partial f_q^k = -\sin\epsilon\,(\partial\epsilon/\partial f_q^k) = 0$, and mixing ratios antenna radiance Hessian becomes

$$\frac{\partial^2 I^A}{\partial f_q^k \partial f_{\tilde{q}}^k} = \frac{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial^2 I(\epsilon)}{\partial f_q^k \partial f_{\tilde{q}}^k}\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}.$$

However, we do not integrate over the entire range:

$$\frac{\partial^2 I^A}{\partial f_q^k \partial f_{\tilde{q}}^k} = \frac{\displaystyle\int_{\epsilon_t-\epsilon_0}^{\epsilon_t+\epsilon_0} \frac{\partial^2 I(\epsilon)}{\partial f_q^k \partial f_{\tilde{q}}^k}\,\overline{G}(\epsilon_t-\epsilon)\,\cos(\epsilon_t-\epsilon)\,d(\epsilon_t-\epsilon)}{\displaystyle\int_{\epsilon_t-\epsilon_0}^{\epsilon_t+\epsilon_0} \overline{G}(\epsilon_t-\epsilon)\,\cos(\epsilon_t-\epsilon)\,d(\epsilon_t-\epsilon)}.$$

6.3 Temperature Antenna Radiance Jacobian

Temperature antenna radiance Jacobian:

$$\frac{\partial I^A}{\partial f_q^T} = \frac{\partial}{\partial f_q^T}\frac{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}{\displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}.$$

Derivation

The antenna temperature derivative can be written as

$$
\begin{aligned}
\frac{\partial I^A}{\partial f_q^T} &= \frac{\partial}{\partial f_q^T} \frac{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon} \\
&= \frac{\partial}{\partial f_q^T} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \;\cdot\; \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon} \\
&\quad - \frac{\partial}{\partial f_q^T} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \;\cdot\; \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \;\cdot\; \frac{1}{\left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon\right]^2},
\end{aligned}
$$

or

$$
\begin{aligned}
\frac{\partial I^A}{\partial f_q^T} = &\left[\underbrace{\frac{\partial}{\partial f_q^T} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}_{①}\right. \\
&\left. - I^A(\epsilon_t) \;\cdot\; \underbrace{\frac{\partial}{\partial f_q^T} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}_{②}\right] \;\cdot\; \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}.
\end{aligned} \tag{19}
$$

The first term in (19) can be written as

$$
\begin{aligned}
① = \frac{\partial}{\partial f_q^T} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon &= \underbrace{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial I(\epsilon)}{\partial f_q^T}\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon}_{❶} + \underbrace{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\frac{\partial \overline{G}(\epsilon_t-\epsilon)}{\partial f_q^T}\,\cos\epsilon\,d\epsilon}_{❷} \\
&+ \underbrace{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\frac{\partial\cos\epsilon}{\partial f_q^T}\,d\epsilon}_{❸} + \underbrace{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,\frac{\partial}{\partial f_q^T}\,d\epsilon}_{❹}.
\end{aligned}
$$

In order to derive an expression for ❷, we use equations (16) - (18) to write the following quantities:[2]

$$
\begin{aligned}
\frac{d\epsilon}{df_q^T} &= \frac{d\epsilon}{dH}\frac{dH}{df_q^T} = \frac{1}{H^s\cos\epsilon}\frac{dH}{df_q^T} = \frac{\tan\epsilon}{H}\frac{dH}{df_q^T}, \\
\frac{\partial\overline{G}(\epsilon_t-\epsilon)}{\partial f_q^T} &= \frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\frac{d(\epsilon_t-\epsilon)}{df_q^T} = \frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)} \cdot \left[\frac{d\epsilon_t}{dh_t}\frac{dh_t}{df_q^T} - \frac{d\epsilon}{dh}\frac{dh}{df_q^T}\right] \\
&= \frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)} \cdot \left[\frac{\tan\epsilon_t}{H_t}\frac{dH_t}{df_q^T} - \frac{\tan\epsilon}{H}\frac{dH}{df_q^T}\right].
\end{aligned}
$$

Thus,

$$
❷ = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\frac{\partial\overline{G}(\epsilon_t-\epsilon)}{\partial f_q^T}\,\cos\epsilon\,d\epsilon = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)} \cdot \left[\frac{\tan\epsilon_t}{H_t}\frac{dH_t}{df_q^T} - \frac{\tan\epsilon}{H}\frac{dH}{df_q^T}\right]\cos\epsilon\,d\epsilon. \quad \checkmark
$$

In order to derive an expression for ❸, we solve for

$$
\frac{d\cos\epsilon}{df_q^T} = -\sin\epsilon\frac{d\epsilon}{df_q^T} = -\sin\epsilon\frac{\tan\epsilon}{H}\frac{dH}{df_q^T} = -\frac{\tan^2\epsilon}{H}\frac{dH}{df_q^T}\cos\epsilon.
$$

[2] An expression for $\frac{dH}{df_q^T}$ is given by equation (4).

Thus,

$$❸ \;=\; \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\frac{\partial\cos\epsilon}{\partial f_q^T}\,d\epsilon \;=\; -\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\frac{\tan^2\epsilon}{H}\frac{dH}{df_q^T}\cos\epsilon\,d\epsilon. \quad \checkmark$$

In order to derive an expression for ❹, we solve for

$$\frac{d}{df_q^T}d\epsilon \;=\; \frac{d}{df_q^T}\frac{d\epsilon}{dh}\frac{dh}{d\zeta}d\zeta \;=\; \left[\frac{d^2\epsilon}{df_q^T dh}\frac{dh}{d\zeta}+\frac{d\epsilon}{dh}\frac{d^2h}{df_q^T d\zeta}\right]d\zeta,$$

where

$$\begin{aligned}\frac{d^2\epsilon}{df_q^T dh} &= \frac{d}{df_q^T}\left[\frac{1}{H^s\cos\epsilon}\right]=\frac{\sin\epsilon}{H^s\cos^2\epsilon}\frac{d\epsilon}{df_q^T}=\frac{\sin\epsilon}{H^s\cos^2\epsilon}\frac{d\epsilon}{df_q^T}=\frac{\sin\epsilon}{H^s\cos^2\epsilon}\frac{\tan\epsilon}{H}\frac{dH}{df_q^T}\\ &= \frac{\tan^2\epsilon}{H^sH\cos\epsilon}\frac{dH}{df_q^T} \;=\; \frac{\tan^2\epsilon}{H}\frac{dH}{df_q^T}\frac{d\epsilon}{dh}.\end{aligned}$$

From (3), we have

$$\begin{aligned}\frac{d^2h}{df_q^T d\zeta} &= \frac{d}{df_q^T}\left[\frac{gH^{\oplus 2}k\log 10\sum f_q^T\eta_q}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2}\right]\\
&= \frac{\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2 gH^{\oplus 2}k\,\eta_q\log 10}{\dfrac{+\,2gH^{\oplus 2}(k\log 10)^2P_q\sum f_q^T\eta_q\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^4}}\\
&= \frac{gH^{\oplus 2}k\,\eta_q\log 10}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2} + \frac{2gH^{\oplus 2}(k\log 10)^2TP_q\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^4}\\
&= \frac{gH^{\oplus 2}k\,\eta_q\log 10}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2} + \frac{2g^2H^{\oplus 4}(k\log 10)^2TP_q}{Hm\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^4}\\
&\qquad\left(\text{hydrostatic balance, } 1=\frac{gH^{\oplus 2}}{H\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q\big]}\right)\\
&= \frac{gH^{\oplus 2}kT\log 10}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2}\cdot\frac{\eta_q}{T}\\
&\quad+\frac{2}{H}\frac{gH^{\oplus 2}k\log 10\,T}{m\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2}\cdot\frac{gH^{\oplus 2}k\log 10\,P_q}{\big[gH^{\oplus}-k\log 10\sum_{q=1}^{Q}f_q^TP_q(\zeta)\big]^2}\\
&= \frac{dh}{d\zeta}\cdot\frac{\eta_q}{T}+\frac{2}{H}\frac{dh}{d\zeta}\frac{dh}{df_q^T}.\end{aligned}$$

Hence,

$$\begin{aligned}\frac{d}{df_q^T}d\epsilon &= \left[\frac{d^2\epsilon}{df_q^T dh}\frac{dh}{d\zeta}+\frac{d\epsilon}{dh}\frac{d^2h}{df_q^T d\zeta}\right]d\zeta\\
&= \left[\frac{\tan^2\epsilon}{H}\frac{dH}{df_q^T}\frac{d\epsilon}{dh}\frac{dh}{d\zeta}+\frac{d\epsilon}{dh}\left[\frac{dh}{d\zeta}\cdot\frac{\eta_q}{T}+\frac{2}{H}\frac{dh}{d\zeta}\frac{dh}{df_q^T}\right]\right]\frac{d\zeta}{dh}\frac{dh}{d\epsilon}d\epsilon\\
&= \left[\frac{\tan^2\epsilon}{H}\frac{dH}{df_q^T}+\left[\frac{\eta_q}{T}+\frac{2}{H}\frac{dh}{df_q^T}\right]\right]d\epsilon\\
&= \left[\frac{2+\tan^2\epsilon}{H}\frac{dh}{df_q^T}+\frac{\eta_q}{T}\right]d\epsilon.\end{aligned}$$

Thus,

$$❹ \;=\; \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,\frac{\partial}{\partial f_q^T}\,d\epsilon \;=\; \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\left[\frac{2+\tan^2\epsilon}{H}\frac{dh}{df_q^T}+\frac{\eta_q}{T}\right]d\epsilon. \quad ✓$$

Therefore,

$$\begin{aligned}
① = \frac{\partial}{\partial f_q^T}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \quad &= \quad \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial I(\epsilon)}{\partial f_q^T}\,\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \\
&\quad + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\left[\frac{\tan\epsilon_t}{H_t}\frac{dH_t}{df_q^T}-\frac{\tan\epsilon}{H}\frac{dH}{df_q^T}\right]\cos\epsilon\,d\epsilon \\
&\quad - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\overline{G}(\epsilon_t-\epsilon)\frac{\tan^2\epsilon}{H}\frac{dH}{df_q^T}\cos\epsilon\,d\epsilon \\
&\quad + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\overline{G}(\epsilon_t-\epsilon)\cos\epsilon\left[\frac{2+\tan^2\epsilon}{H}\frac{dh}{df_q^T}+\frac{\eta_q}{T}\right]d\epsilon \\
&= \quad \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left(\frac{\partial I}{\partial f_q^T}+I(\epsilon)\cdot\left(\frac{2}{H}\frac{dh}{df_q^T}+\frac{\eta_q}{T}\right)\right)\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \\
&\quad + \frac{\tan\epsilon_t}{H_t}\frac{dH_t}{df_q^T}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\,\cos\epsilon\,d\epsilon \\
&\quad - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} I(\epsilon)\frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\frac{\tan\epsilon}{H}\frac{dH}{df_q^T}\cos\epsilon\,d\epsilon.
\end{aligned}$$

The second term in (19) can be written as [3]

$$\begin{aligned}
② \;=\; \frac{\partial}{\partial f_q^T}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \quad &= \quad \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\partial\overline{G}(\epsilon_t-\epsilon)}{\partial f_q^T}\,\cos\epsilon\,d\epsilon \\
&\quad + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\frac{\partial\cos\epsilon}{\partial f_q^T}\,d\epsilon + \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,\frac{\partial}{\partial f_q^T}\,d\epsilon \\
&= \quad \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left(\frac{2}{H}\frac{dh}{df_q^T}+\frac{\eta_q}{T}\right)\overline{G}(\epsilon_t-\epsilon)\,\cos\epsilon\,d\epsilon \\
&\quad + \frac{\tan\epsilon_t}{H_t}\frac{dH_t}{df_q^T}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\,\cos\epsilon\,d\epsilon \\
&\quad - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d\overline{G}(\epsilon_t-\epsilon)}{d(\epsilon_t-\epsilon)}\frac{\tan\epsilon}{H}\frac{dH}{df_q^T}\cos\epsilon\,d\epsilon.
\end{aligned}$$

[3] Note that this is equivalent to ① with $I(\epsilon)=1$.

The antenna radiance temperature Jacobian, defined in equation (19), can be written as

$$
\begin{aligned}
\frac{\partial I^A(\epsilon_t)}{\partial f_q^T} \quad = \quad & \Bigg[\int \left(\frac{\partial I}{\partial f_q^T} + \big(I(\epsilon) - I^A(\epsilon_t)\big) \cdot \Big(\frac{2}{H} \frac{dh}{df_q^T} + \frac{\eta_q}{T} \Big) \right) \overline{G}(\epsilon_t - \epsilon)\, \cos\epsilon \, d\epsilon \\
& + \frac{\tan\epsilon_t}{H_t} \frac{dH_t}{df_q^T} \int \big(I(\epsilon) - I^A(\epsilon_t)\big) \frac{d\overline{G}(\epsilon_t - \epsilon)}{d(\epsilon_t - \epsilon)} \cos\epsilon \, d\epsilon \\
& - \int \big(I(\epsilon) - I^A(\epsilon_t)\big) \frac{d\overline{G}(\epsilon_t - \epsilon)}{d(\epsilon_t - \epsilon)} \frac{\tan\epsilon}{H} \frac{dH}{df_q^T} \cos\epsilon \, d\epsilon \Bigg] \cdot \frac{1}{\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \overline{G}(\epsilon_t - \epsilon)\, \cos\epsilon \, d\epsilon},
\end{aligned}
$$

where $I^A(\epsilon_t)$ is antenna radiance defined in (11).

Simplified equation

We assume no $\cos\epsilon$ and no normalization. Hence, the antenna radiance temperature Jacobian can be written as:

$$
\begin{aligned}
\frac{\partial I^A(\epsilon_t)}{\partial f_q^T} \quad = \quad & \int \left(\frac{\partial I}{\partial f_q^T} + (I(\epsilon) - I^A(\epsilon_t)) \cdot \Big(\frac{2 + \tan^2\epsilon}{H} \frac{dh}{df_q^T} + \frac{\eta_q}{T} \Big) \right) \overline{G}(\epsilon_t - \epsilon)\, d\epsilon \\
& + \frac{\tan\epsilon_t}{H_t} \frac{dH_t}{df_q^T} \int (I(\epsilon) - I^A(\epsilon_t)) \frac{d\overline{G}(\epsilon_t - \epsilon)}{d(\epsilon_t - \epsilon)} \, d\epsilon \\
& - \int (I(\epsilon) - I^A(\epsilon_t)) \frac{d\overline{G}(\epsilon_t - \epsilon)}{d(\epsilon_t - \epsilon)} \frac{\tan\epsilon}{H} \frac{dH}{df_q^T} \, d\epsilon.
\end{aligned}
$$

7 Finite Difference Approximations for Jacobians

Mixing Ratio Jacobian

$$\frac{\partial I_l}{\partial f_q^k} \approx \frac{I_l(f_q^k+\epsilon_q^k)-I_l(f_q^k)}{f_q^k+\epsilon_q^k-f_q^k} = \frac{I_l(f_q^k+\epsilon_q^k)-I_l(f_q^k)}{\epsilon_q^k},$$

where $\epsilon_q^k = 0.05 f_q^k$, i.e. is about 5% of the value of f_q^k. Hence,

$$\frac{\partial I_l}{\partial f_q^k} \approx \frac{I_l(1.05 f_q^k)-I_l(f_q^k)}{0.05 f_q^k}.$$

Temperature Jacobian

$$\frac{\partial I_l}{\partial f_q^T} \approx \frac{I_l(f_q^T+\epsilon_q^T)-I_l(f_q^T)}{f_q^T+\epsilon_q^T-f_q^T} = \frac{I_l(f_q^T+\epsilon_q^T)-I_l(f_q^T)}{\epsilon_q^T},$$

where $\epsilon_q^T = 0.05 f_q^T$.

$$\frac{\partial I_l}{\partial f_q^T} \approx \frac{I_l(1.05 f_q^T)-I_l(f_q^T)}{0.05 f_q^T}.$$

Antenna Radiance Mixing Ratio Jacobian

$$\frac{\partial I_l^A}{\partial f_q^k} \approx \frac{I_l^A(f_q^k+\epsilon_q^k)-I_l^A(f_q^k)}{\epsilon_q^k}.$$

Antenna Radiance Temperature Jacobian

$$\frac{\partial I_l^A}{\partial f_q^T} \approx \frac{I_l^A(f_q^T+\epsilon_q^T)-I_l^A(f_q^T)}{\epsilon_q^T}.$$

Derivative of Height with respect to Temperature

$$\frac{\partial h_l}{\partial f_q^T} \approx \frac{h_l(f_q^T+\epsilon_q^T)-h_l(f_q^T)}{f_q^T+\epsilon_q^T-f_q^T} = \frac{h_l(f_q^T+\epsilon_q^T)-h_l(f_q^T)}{\epsilon_q^T}.$$

Derivative of Absorption Coefficient with respect to Temperature

$$\frac{\partial \beta_l}{\partial f_q^T} \approx \frac{\beta_l(f_q^T+\epsilon_q^T)-\beta_l(f_q^T)}{f_q^T+\epsilon_q^T-f_q^T} = \frac{\beta_l(f_q^T+\epsilon_q^T)-\beta_l(f_q^T)}{\epsilon_q^T}.$$

Derivative of Source Function with respect to Temperature (has not been tested)

$$\frac{\partial \triangle B_i}{\partial f_q^T} \approx \frac{\triangle B_i(f_q^T+\epsilon_q^T)-\triangle B_i(f_q^T)}{f_q^T+\epsilon_q^T-f_q^T} = \frac{\triangle B_i(f_q^T+\epsilon_q^T)-\triangle B_i(f_q^T)}{\epsilon_q^T}.$$

8 Finite Difference Approximations for Hessians

Radiance Hessians

$$
\begin{aligned}
\frac{\partial^2 I_l}{\partial f_q^2} &\approx D_0^q\Big[\frac{\partial I_l}{\partial f_q}(\mathbf{f})\Big] = \frac{\frac{\partial I_l}{\partial f_q}(f_q+\epsilon_q) - \frac{\partial I_l}{\partial f_q}(f_q-\epsilon_q)}{2\epsilon_q} \\
&\approx D_-^q D_+^q\Big[I_l(\mathbf{f})\Big] = \frac{I_l(f_q+\epsilon_q) - 2I_l(f_q) + I_l(f_q-\epsilon_q)}{\epsilon_q^2}, \\
\frac{\partial^2 I_l}{\partial f_q \partial f_{\tilde{q}}} &\approx D_0^{\tilde{q}}\Big[\frac{\partial I_l}{\partial f_q}(\mathbf{f})\Big] = \frac{\frac{\partial I_l}{\partial f_q}(f_q, f_{\tilde{q}}+\epsilon_{\tilde{q}}) - \frac{\partial I_l}{\partial f_q}(f_q, f_{\tilde{q}}-\epsilon_{\tilde{q}})}{2\epsilon_{\tilde{q}}} \\
&\approx D_+^q D_+^{\tilde{q}}\Big[I_l(\mathbf{f})\Big] = \frac{I_l(f_q+\epsilon_q, f_{\tilde{q}}+\epsilon_{\tilde{q}}) - I_l(f_q, f_{\tilde{q}}+\epsilon_{\tilde{q}}) - I_l(f_q+\epsilon_q, f_{\tilde{q}}) + I_l(f_q, f_{\tilde{q}})}{\epsilon_q \epsilon_{\tilde{q}}} \\
&\approx D_0^q D_0^{\tilde{q}}\Big[I_l(\mathbf{f})\Big] = \frac{I_l(f_q+\epsilon_q, f_{\tilde{q}}+\epsilon_{\tilde{q}}) - I_l(f_q-\epsilon_q, f_{\tilde{q}}+\epsilon_{\tilde{q}}) - I_l(f_q+\epsilon_q, f_{\tilde{q}}-\epsilon_{\tilde{q}}) + I_l(f_q-\epsilon_q, f_{\tilde{q}}-\epsilon_{\tilde{q}})}{4\epsilon_q \epsilon_{\tilde{q}}},
\end{aligned}
$$

where $f_q = f_q^k$ for mixing ratios and $f_q = f_q^T$ for temperatures. If antenna radiance Jacobians are computed, then $I = I^A$ in the above formulas.

9 Frequency Averaging

$$
\begin{aligned}
\overline{\beta}_c^w(T,P) &= \frac{1}{\nu_1 - \nu_0}\int_{\nu_0}^{\nu_1} \phi_c(\nu)\beta^w(\nu)d\nu, \\
\tau_c^w &= \tau(\overline{\beta}_c^w),
\end{aligned}
$$

where $\overline{\beta}_c^w$ is an average β for a whole channel.

$$
\tau_c^{w\,k} = e^{-\int_0^z f^k \overline{\beta}_c^w(z)dz}
$$

For both PFA and LBL radiances for a particular channel c, we have

$$
\begin{aligned}
I_c &\approx \sum_{n=1}^{N_f} \phi_{cn} \sum_{i=1}^{N_p} \triangle B_{ni} \mathcal{T}_{cni}^s \mathcal{T}_{ci}^w \\
&= \sum_{i=1}^{N_p} \mathcal{T}_{ci}^w \sum_{n=1}^{N_f} \phi_{cn} \triangle B_{ni} \mathcal{T}_{cni}^s,
\end{aligned}
$$

where N_f is the number of frequencies in the channel, N_p is line-of-sight path length, s is a strong LBL, w is a weak PFA, and ϕ_c is the channel's filter function with

$$
\sum_{n=1}^{N_f} \phi_{cn} = 1.
$$

Since $\triangle B_{ni} \approx \triangle B_i$, we have

$$
\begin{aligned}
I_c &\approx \sum_{n=1}^{N_f} \phi_{cn} \sum_{i=1}^{N_p} \triangle B_i \mathcal{T}_{cni}^s \mathcal{T}_{ci}^w \\
&= \sum_{i=1}^{N_p} \mathcal{T}_{ci}^w \triangle B_i \sum_{n=1}^{N_f} \phi_{cn} \mathcal{T}_{cni}^s.
\end{aligned}
$$

10 Polarized Radiative Transfer

The radiative transfer equation is

$$\mathbf{I}(\mathbf{x}) = \sum_{i=1}^{2N} \triangle B_i \ \boldsymbol{\mathfrak{T}}_i,$$

where

$$\begin{aligned}
\boldsymbol{\mathfrak{T}}_i &= \mathbf{P}_i \mathbf{P}_i^*, \\
\mathbf{P}_i &= \mathbf{P}_{i-1} \mathbf{E}_i, \\
\mathbf{E}_i &= \exp\Big(- \int_{s_i}^{s_{i-1}} \mathbf{G}(s') ds' \Big) \ \equiv \ \exp\Big(- \sum_k \boldsymbol{\Delta\delta}_{i\to i-1}^k \Big) \ = \ \exp\big(- \boldsymbol{\Delta\delta}_{i\to i-1} \big).
\end{aligned}$$

In the sum over k, it explicitly allows the contributions of other species, with the field opacity of unpolarized species (half of their power opacities) added to $\mathbf{G}$ as multiple of the identity. Since

$$\mathbf{E}_1 = \mathbf{P}_1 = \mathbf{1},$$

we have

$$\boldsymbol{\mathfrak{T}}_1 = \mathbf{P}_1 \mathbf{P}_1^* = \mathbf{1}.$$

Also, for $i \geq 2$,

$$\begin{aligned}
\mathbf{P}_i &= \mathbf{P}_{i-1} \mathbf{E}_i \ = \ \mathbf{E}_2 \ldots \mathbf{E}_i \ = \ \exp\Big(- \sum_{j=2}^{i} \boldsymbol{\Delta\delta}_{j\to j-1} \Big), \\
\boldsymbol{\mathfrak{T}}_i &= \mathbf{P}_i \mathbf{P}_i^* \ = \ \mathbf{E}_2 \ldots \mathbf{E}_i \mathbf{E}_i^* \ldots \mathbf{E}_2^*.
\end{aligned}$$

The source function $\triangle B_i$ in differential temperature format is given by

$$\begin{aligned}
\triangle B_1 &= \frac{T_1 + T_2}{2}, \\
\triangle B_i &= \frac{T_{i+1} - T_{i-1}}{2}, \\
\triangle B_{2N} &= T_{space} - \frac{T_{2N-1} + T_{2N}}{2},
\end{aligned}$$

where $T_{space} = 2.7$.

The incremental opacity integral due to polarized O_2 lines is

$$\boldsymbol{\Delta\delta}_{i\to i-1}^{O_2} = \frac{\triangle s_{i\to i-1}^{\text{refr}}}{\triangle s_{i\to i-1}} \sum_{\triangle M=-1}^{+1} \boldsymbol{\rho}_{\triangle M}(\theta, \phi) \ \xi_{M,\triangle M} \int_{\zeta_i}^{\zeta_{i-1}} F^{O_2}\big(\zeta, \phi(\zeta)\big) \ \beta_{\triangle M}\big(\zeta, \mathcal{B}(\zeta), T(\zeta), \nu\big) \frac{ds}{dh} \frac{dh}{d\zeta} d\zeta,$$

where $\xi_{M,\triangle M}$ is the O_2 Zeeman component fractional intensity.

11 Polarized Derivatives

11.1 General Form

The **derivative of the polarized radiative transfer** is

$$\begin{aligned}
\frac{\partial \mathbf{I}(\mathbf{x})}{\partial x} &= \frac{\partial}{\partial x} \sum_{i=1}^{2N} \triangle B_i \boldsymbol{\mathfrak{T}}_i \\
&= \sum_{i=1}^{2N} \left[\frac{\partial \triangle B_i}{\partial x} \boldsymbol{\mathfrak{T}}_i + \triangle B_i \frac{\partial \boldsymbol{\mathfrak{T}}_i}{\partial x} \right].
\end{aligned}$$

The derivative of $\mathfrak{T}_i$ is given as

$$\frac{\partial \mathfrak{T}_i}{\partial x} \quad = \quad \frac{\partial(\mathbf{P}_i \mathbf{P}_i^*)}{\partial x} \;=\; \frac{\partial \mathbf{P}_i}{\partial x}\mathbf{P}_i^* + \mathbf{P}_i \frac{\partial \mathbf{P}_i^*}{\partial x} \;=\; \frac{\partial \mathbf{P}_i}{\partial x}\mathbf{P}_i^* + \left(\frac{\partial \mathbf{P}_i}{\partial x}\mathbf{P}_i^*\right)^*,$$

where

$$\frac{\partial \mathbf{P}_i}{\partial x} \quad = \quad \frac{\partial(\mathbf{P}_{i-1}\mathbf{E}_i)}{\partial x} \;=\; \frac{\partial \mathbf{P}_{i-1}}{\partial x}\mathbf{E}_i + \mathbf{P}_{i-1}\frac{\partial \mathbf{E}_i}{\partial x}.$$

11.2 Mixing Ratio Derivatives

Note that since

$$\frac{\partial \triangle B_i}{\partial f_q^k} = 0,$$

The mixing ratio derivative of the polarized radiative transfer is

$$\frac{\partial \mathbf{I}(\mathbf{x})}{\partial f_q^k} \quad = \quad \sum_{i=1}^{2N} \triangle B_i \frac{\partial \mathfrak{T}_i}{\partial f_q^k}.$$

The **incremental opacity derivative** with respect to mixing ratio is

$$\frac{\partial \boldsymbol{\Delta\delta}_{i\to i-1}^k}{\partial f_q^k} = \frac{\triangle s_{i\to i-1}^{\text{refr}}}{\triangle s_{i\to i-1}} \sum_{\triangle M=-1}^{+1} \boldsymbol{\rho}_{\triangle M}(\theta,\phi)\ \xi_{M,\triangle M} \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^k(\zeta)\,\beta_{\triangle M}^k\big(\zeta, \mathcal{B}(\zeta), T(\zeta), \nu\big)\ \frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,$$

where k is a molecule.