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EOS MLS Forward Model Polarized Radiative Transfer for Zeeman-Split Oxygen Lines

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The Microwave Limb Sounder on Aura

- The EOS Microwave Limb Sounder (MLS) was launched on the NASA Aura satellite in August, 2004 and since that time has provided near-continuous, $\sim$3500 daily sets of atmospheric composition and temperature profiles from $\sim$8–90 km along the suborbital track.
- Design life was 5 years, but almost most of the system is still operating after 13+ years. (Exceptions are the 2.5 THz radiometer and 640 GHz N_2O band.)
- The Aura orbit is sun synchronous (83°S–83°N) with 1:30 and13:30 equator crossings.
- MLS scans the atmospheric limb along track 240 times per orbit and successive MLS along-track limb scans overlap, so we can do a 2-D optimal-estimation retrieval at 1.5° uniformly-spaced suborbital profiles, using a block of limb scans to retrieve a block of profiles.

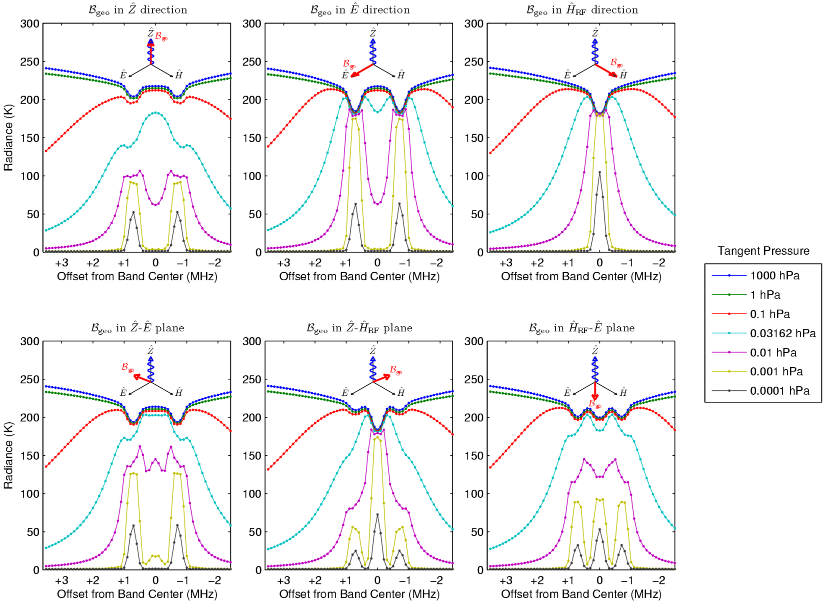
- The instrument has five radiometers:
  - 118 GHz: (two linear polarizations) Temperature, GPH, tangent pressure, IWC, IWP
  - 190 GHz: H_2O, HCN, HNO_3, N2O, RHI, CH_3CN, ClO, IWC, IWP, O_3, volcanic SO_2
  - 240 GHz: CO, UTLS HNO_3, IWC, IWP, O_3, volcanic SO_2, UT Temperature
  - 640 GHz: BrO, CH_3Cl, CH_3CN, CH_3OH, ClO, HCl, HO_2, HOCl, volcanic SO_2, CH_3CN HNO_3, IWC, IWP, N_2O, strat O_3
  - 2.5 THz: OH, O3
- Temperature is primarily inferred from emission by oxygen (O_2). Aura MLS middle atmosphere temperature retrievals use emission from the O_2 118.75 GHz line, but the retrieval code has also recently also been applied to the reprocessing of UARS MLS radiances from the 60-GHz band.

- The forward model is primarily a line-by-line calculation that provides the radiances and radiance derivatives (Jacobians) required by the optimal estimation retrieval.
- Aura MLS has two 100-kHz-resolution digital autocorrelator spectrometers (DACS) attached to two orthogonally linearly-polarized 118-GHz receivers. R1A couples to radiation with magnetic field vector ($\hat{\boldsymbol{H}}$) nearly horizontal at the tangent point of the limb path while R1B couples to radiation with $\hat{\boldsymbol{H}}$ nearly vertical.
- The R1B DACS is very rarely operated as the hardware is used on the 230-GHz CO line center.
- Starting in the upper mesosphere ($\gtrsim$70 km), this emission becomes increasingly polarized and non-isotropic due to Zeeman splitting of O_2 spectral lines by the geomagnetic field.

- The model accounts for polarization-dependent emission and for correlation between polarizations with complex 2x2 intensity and absorption matrices after Lenoir. This formalism is believed to be equivalent to the formalism of Stokes parameters used by ARTS. (Part of why we are here is to check!)
- The forward model is built into the retrieval system, with FORTRAN modules controlled by a complex configuration language, and it is quite cumbersome to use as a stand-alone radiative transfer model.
- Polarized forward mode algorithms were documented in a TGARS Aura special issue paper, Schwartz, et al. ”EOS MLS Forward Model Polarized Radiative Transfer for Zeeman-Split Oxygen Lines” and, more leisurely and pedagogically, in an ATBD, both of which are available on the MLS website.
- This rest of this talk is a brief summary of some highlights from these papers. I have hardcopies of the TGARS paper if you want some light reading.

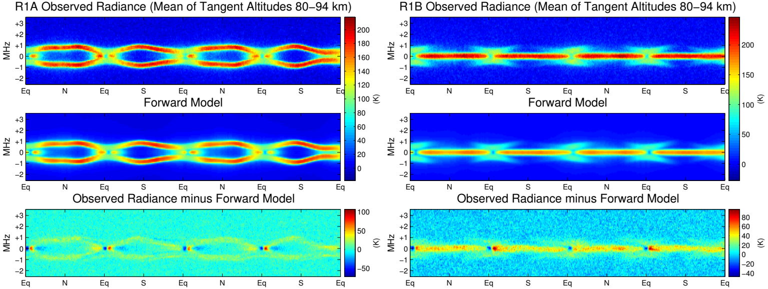
Modeled 118-GHz Limb Radiances

Canonical $\mathcal{B}_{\mathrm{geo}}(50\,\mu\mathrm{T})$ orientations



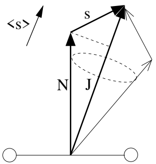
- The six panels show single-frequency, single-ray, modeled 118-GHz radiances for six orientations of $\mathcal{B}_{\text{geo}}(50\ \mu\text{T})$, with respect to the polarization and propagation directions of the linear polarization mode under consideration.
- Doppler-broadened cores of the lines are fully saturated at 0.001 hPa for some polarization, but not necessarily for that of the observation.
- In the top left panel, propagation is along $\mathcal{B}_{\text{geo}}$ and the σ_+ (higher frequency) and σ_- (lower frequency) lines are right and left circularly polarized respectively. Along the 0.001 hPa tangent-pressure ray, the line centers are opaque for one circular mode and transparent for the other. A linear polarization consists of half of each.
- In the top middle panel, $\mathcal{B}_{\text{geo}}$ is aligned with $\hat{\boldsymbol{E}}$ and the $\sigma_\pm$ lines are linearly co-polarized with the mode under consideration.
- In the top right panel, $\mathcal{B}_{\text{geo}}$ is aligned with the antenna's $\hat{\boldsymbol{H}}$ direction and the π line is co-polarized with the mode under consideration.

MLS Radiances, Forward model, and Residuals



- Two orbits of mean 80–94 km DACS radiances (R1A on top left, R1B on top right)
- Corresponding forward model calculations (middle)
- At high latitudes, $\mathcal{B}_{\text{geo}}$ is nearly normal to the earth's surface and R1A ($\hat{\boldsymbol{H}}$ horizontal) sees the $\sigma\pm$ lines while R1B ($\hat{\boldsymbol{H}}$ vertical) sees the π line.
- Residuals (bottom) include non-retrieved Doppler shifts due to mean wind.

The Spin-Rotational Microwave Spectrum of O_2

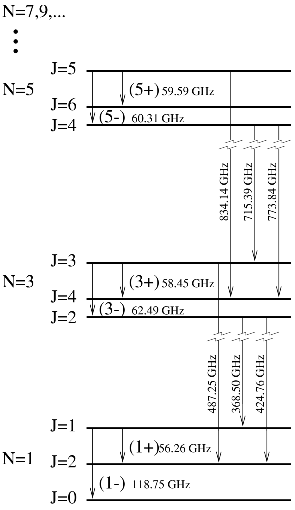


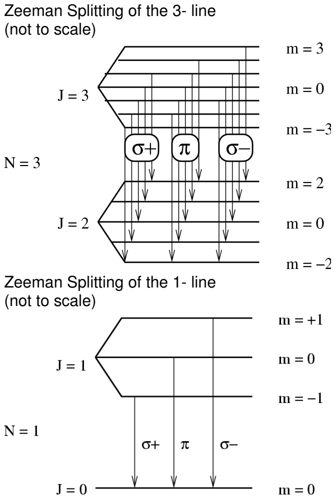
- The electronic ground state of diatomic oxygen (O_2) has a pair of aligned electronic spins (electronic spin quantum number $s = 1$) with an associated magnetic dipole moment.
- Oxygen's microwave spectrum consists of magnetic dipole transitions that reorient this spin relative to the molecule's end-over-end rotation (quantum number N).
- It is approximately "Hund's case (b)", where $\boldsymbol{s}$ adds to $\boldsymbol{N}$ to give total angular momentum, $\boldsymbol{J}$. Time-averaged $\langle \boldsymbol{s} \rangle$ is the projection of $\boldsymbol{s}$ on $\boldsymbol{J}$.

Zeeman Splitting of O_2 Spectral Lines

- The projection of $\boldsymbol{J}$ (and therefore of $\langle \boldsymbol{s} \rangle$) on $\mathcal{B}_{\text{geo}}$ has J(J+1) values denoted by the quantum number m.
- These J(J+1) states are shifted in energy by interaction with the $\mathcal{B}_{\text{geo}}$, $\Delta E = mg\mu_B|\mathcal{B}_{\text{geo}}|$.
- maximum shifts are $\sim \pm$140 kHz/μTesla, or less than 700 kHz in magnitude for typical terrestrial fields, $|\mathcal{B}_{\text{geo}}| \lesssim 50\mu$Tesla.
- Zeeman components with different ΔM couple to different radiation polarizations.

Diatomic Oxygen Spin-Rotation Spectrum





Polarization-dependent 3-D Magnetic Susceptibility

- Linearly-polarized radiation with its $\boldsymbol{H}$ vector along the imposed magnetic field couples only to π transitions
- Right and left-circular polarizations propagating along the external field couple only to σ_+ and σ_- transitions.
- In a Cartesian basis where $\hat{z}$ is the direction of $\boldsymbol{\mathcal{B}}_{\mathrm{geo}}$, the susceptibility tensor has the form

$$\boldsymbol{\chi}^{(\mathbf{3})} = \begin{bmatrix} (\chi_+ + \chi_-)/2 & -\imath(\chi_+ - \chi_-)/2 & 0 \\ \imath(\chi_+ - \chi_-)/2 & (\chi_+ + \chi_-)/2 & 0 \\ 0 & 0 & \chi_0 \end{bmatrix}.$$

where, χ_+, χ_- and χ_0 are the eigenvalues of $\boldsymbol{\chi}^{(\mathbf{3})}$.

Reduction to 2-D: ρ Matrices

- $\chi^{(3)}$ is a tensor, so we know how to rotate it ($\boldsymbol{R}\chi^{(3)}\boldsymbol{R}^{\dagger}$)
- We can rotate by θ to put make $\hat{z}$ the direction of propagation and by ϕ to put the the linear polarization of our receiver in the $\hat{x}$ direction.
- In the weak interaction limit, (Im$\{\chi\} \ll 1$), the EM fields are nearly transverse, the $\hat{z}$ dimension may be neglected, and the resulting 2x2 matrix, $\boldsymbol{\chi}$, may be written

$$\boldsymbol{\chi} = \chi_{+}\boldsymbol{\rho}_{+} + \chi_{0}\boldsymbol{\rho}_{\mathbf{0}} + \chi_{-}\boldsymbol{\rho}_{-} \ ,$$

where

$$\boldsymbol{\rho}_{\pm} = \boldsymbol{R}_{\phi} \begin{bmatrix} 1 & \mp\imath\cos\theta \\ \pm\imath\cos\theta & cos^2\theta \end{bmatrix} \boldsymbol{R}_{\phi}^{\dagger} \ ,$$

$$\boldsymbol{\rho}_{0} = \boldsymbol{R}_{\phi} \begin{bmatrix} 0 & 0 \\ 0 & \sin^2\theta \end{bmatrix} \boldsymbol{R}_{\phi}^{\dagger} \ ,$$

and the ϕ rotation is

$$\boldsymbol{R}_{\phi} = \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \ .$$

Reduction to 2-D: ρ Matrices (continued)

- The three complex 2x2 matrices, $\boldsymbol{\rho}_+$, $\boldsymbol{\rho}_\mathbf{0}$, $\boldsymbol{\rho}_-$, are functions only of θ and ϕ
  - θ is the angle between $\boldsymbol{\mathcal{B}}_{\text{geo}}$ and the propagation direction, $\hat{z}$.
  - ϕ is the angle between the radiation linear polarization direction and the $\boldsymbol{\mathcal{B}}_{\text{geo}}$-$\hat{z}$ plane.
- The coefficients χ_+, χ_- and χ_0 are complex scalars, sums of the lineshapes of all lines of a given Δm, while the $\boldsymbol{\rho_j}$ contain common polarization dependence for each set, Δm. (Wigner-Eckart Theorem)
- When Zeeman splitting is negligible ($|\boldsymbol{\mathcal{B}}_{\text{geo}}| = 0$ or far from line center), $\boldsymbol{\chi} = \chi_+\boldsymbol{\rho}_+ + \chi_0\boldsymbol{\rho}_\mathbf{0} + \chi_-\boldsymbol{\rho}_-$ is a multiple of the identity matrix and equations reduce to the scalar case for each diagonal.
- When Zeeman splitting is not negligible, matrices at different points along the propagation path do not generally commute.

Polarized Intensity: The Coherence Matrix

In the rotated, reduced-dimensionality basis, the 2x2 intensity coherence matrices are

$$\boldsymbol{I} = \begin{bmatrix} I_{\|} & I_{|} + \imath I_{\circ} \\ I_{|} - \imath I_{\circ} & I_{\perp} \end{bmatrix} ,$$

where $I_{\|}$ and $I_{\perp}$ are radiated power in linear polarizations respectively parallel and perpendicular to the direction of linear polarization of our receive and $I_{\circ}$ and $I_{|}$ are the circular and linear coherences of the polarizations.
This matrix has the same information as is in a Stokes vector.

Polarized Radiative Transfer

The differential equation of radiative transfer is

$$\frac{d\boldsymbol{I}}{ds} = \left(\frac{\imath\pi\nu}{c}\chi\right)\boldsymbol{I} + \boldsymbol{I}\left(\frac{\imath\pi\nu}{c}\chi\right)^{\dagger} \ .$$

This differential equation can be cast in a descretized integral form very similar to that of the differential temperature form in scalar case:

$$\boldsymbol{I} = \sum_{i=0}^{N} \mathcal{T}_{\boldsymbol{i}} \Delta B_i$$

where $\mathcal{T}_i$ is the power transmittance matrix from the ith layer boundary to the top of the atmosphere ΔB_i is a function of B_i, the Planck source function at layer-boundary temperature, T_i,

$$B_i = \frac{h\nu}{k(\exp\{\frac{h\nu}{kT_i}\} - 1)} \ .$$

$$\Delta B_i = \frac{B_{i+1} - B_{i-1}}{2}$$

Transmittance Matrices

$\mathcal{T}_i$, is built out of layer *field* transmittance matrices, $\boldsymbol{E}_j$,

$$\boldsymbol{E_i} = \exp\left(-\int_{s_i}^{s_{i-1}} \frac{\imath\pi\nu}{c}\chi\,\mathrm{d}s\right)$$

$$\mathcal{T}_i = \boldsymbol{E}_1\boldsymbol{E}_2\ldots\boldsymbol{E}_i\boldsymbol{E}_i^\dagger\ldots\boldsymbol{E}_2^\dagger\boldsymbol{E}_1^\dagger.$$

Order is important as the $\boldsymbol{E}_i$ matrices generally do not commute with one another.

$\mathcal{T}_i$ is manifestly Hermitian, composed of matrix pairs $\boldsymbol{E}_i$ and $\boldsymbol{E}_i^\dagger$ built up from the center outward, with the earliest times (largest indices) in the middle.

The contribution of isotropic (scalar) absorption from other molecules or from the wings of distant O_2 lines may be added to the argument of the exponential

$$\boldsymbol{E_i} = \exp\left(-\int_{s_i}^{s_{i-1}} \left(\frac{\imath\pi\nu}{c}\boldsymbol{\chi} - \sum_k \frac{1}{2}\alpha_k \mathbf{1}\right) \mathrm{d}s\right)$$

where k is the index over unpolarized contributions. The factor of $\frac{1}{2}$ makes these “field” absorption rather than “power” absorption.

A Note on Matrix Exponentiation

Matrix exponentiation has its usual definition as a power series:

$$\exp \chi = \mathbf{1} + \chi + \frac{1}{2}\chi^2 + \dots .$$

We assume that layers are thin enough that χ commutes with itself throughout a layer. Note, generally

$$\exp(\chi_\mathbf{1}) \exp(\chi_\mathbf{2}) \neq \exp(\chi_\mathbf{1} + \chi_\mathbf{2})$$

because all of the $\chi_\mathbf{1}$'s have to be on the left-hand side.

Derivatives (Jacobians)

- Jacobians are calculated analytically. In calculating derivatives with respect to mixing ratios or temperature, care must be taken to preserve matrix order.

$$\frac{\partial \boldsymbol{I}(x)}{\partial x} = \sum_{i=1}^{N} \frac{\partial \mathcal{T}_i}{\partial x} \Delta B_i + \mathcal{T}_i \frac{\partial \Delta B_i}{\partial x}$$

It is convenient to define $\boldsymbol{P_i} = \boldsymbol{E_1 E_2} \dots \boldsymbol{E_i}$, the field transmittance matrix to the i th layer boundary, so the power transmittance matrix may be written $\mathcal{T}_{\boldsymbol{i}} = \boldsymbol{P_i P_i^\dagger}$. Derivatives of $\boldsymbol{P_i}$ can be built up using the recurrence relation

$$\frac{\partial \boldsymbol{P_i}}{\partial x} = \frac{\partial \boldsymbol{P_{i-1}}}{\partial x} \boldsymbol{E_{i-1}} + \boldsymbol{P_{i-1}} \frac{\partial \boldsymbol{E_{i-1}}}{\partial x}$$

and used to evaluate

$$\frac{\partial \mathcal{T}_{\boldsymbol{i}}}{\partial x} = \frac{\partial \boldsymbol{P_i}}{\partial x} \boldsymbol{P_i^\dagger} + \left(\frac{\partial \boldsymbol{P_i}}{\partial x} \boldsymbol{P_i^\dagger} \right)^\dagger .$$

Complex Lineshape (Fadeeva with line interference)

$$
\begin{aligned}
\mathcal{F}(x_j, y_j) &= \frac{1}{\pi}\,\frac{\nu}{\nu_{0j}} \int_{-\infty}^{\infty} e^{-t^2} \left(\frac{y_j - Y_j(x_j - t)}{(x_j - t)^2 + y_j^2} + \frac{\imath(y_j Y_j + x_j - t)}{(x_j - t)^2 + y_j^2} \right) dt \\
&= \frac{\nu}{\nu_{0j}} (1 + \imath Y_j) F(x_j + \imath y_j),
\end{aligned} \tag{1}
$$

where

$$
\begin{aligned}
x_j &= \frac{\sqrt{\ln 2}\left(\nu - \nu_j^k - \Delta\nu_{j,m,\Delta m}\right)}{w_d^k}, \\
y_j &= \frac{\sqrt{\ln 2}\, w_{cj} P}{w_d^k} \left(\frac{T_0}{T}\right)^{n_{cj}^k}, \\
Y_j &= P \left[\delta_j^k \left(\frac{T_0}{T}\right)^{n_{\delta_j}^k} + \gamma_j^k \left(\frac{T_0}{T}\right)^{n_{\gamma_j}^k} \right], \\
w_d^k &= \sqrt{2 \ln 2\, \mathrm{k_B}/c} \sqrt{\frac{T}{\mathcal{M}^k}}\, \nu,
\end{aligned}
$$

and the shifted line-center frequency is

$$
\nu_j^k = \left[\nu_{0j}^k + \Delta\nu_{0j}^k P \left(\frac{T_0}{T}\right)^{n_{\Delta\nu_{0j}}^k} \right] \left(1 + \frac{v_{\mathrm{los}}}{c}\right). \tag{2}
$$

Line parameters tabulated in the MLS scalar forward model ATBD include

- unshifted line center frequency, ν_{0j}, from the JPL line database,
- collisional line width parameter, w_{cj}^{k},
- collisional line width temperature dependence exponent, n_{cj}^{k},
- line pressure shift parameter, $\Delta\nu_{0j}^{k}$
- line pressure shift temperature dependence exponent, $n_{\Delta\nu_{0j}}^{k}$
- line interference parameters, δ_j^k, $n_{\delta_j}^k$, γ_j^k, $n_{\gamma_j}^k$.
- A line pressure shift, $\Delta\nu_{0j}^{k}$, has been included in the model, but has been set to zero based upon recent measurements that indicate a line-shift magnitude of less than 0.1 MHz/hPa (Brian Drouin, Tretyakov 2004).