Limbed Scattering Radiative Transfer Model Development in Support of the Ozone Mapping and Profiler Suite (OMPS) Limb Profiler Mission

R. Loughman1, D. Flittner2, E. Nyaku1, and P.K. Bhartia3

Abstract
The Gauss-Seidel Limbed Scattering (GSLS) radiative transfer (RT) model has been tested through comparison with several other RT models, including the Siro, MCG++, CDP1, LIMBTRAN, and SASKTRAN. To address deficiencies in the GSLS radiance calculations revealed in earlier comparisons, several recent changes have been added that improve the accuracy and flexibility of the GSLS model, including:

1. Introduction of variable atmospheric and surface properties along the limb line of sight.
2. Improved treatment of the variation of the extinction coefficient within atmospheric layers.
3. Re-introduction of the ability to simulate vector (polarized) radiances.
4. Addition of the ability to model multiple aerosol types within the model atmosphere.

These model improvements are verified by comparison to standard radiance tables, demonstrating significant improvement in cases for which previous versions of the model performed poorly. The GSLS model is implemented in a new retrieval algorithm used to process data from the Ozone Mapping and Profiler Suite (OMPS) Limb Profiler, which was recently launched on the Suomi NPP satellite. The significance of the GSLS RT model improvements for the OMPS LP retrievals will be illustrated by several examples.

Optical Path Length Improvement
A previous radiance comparison study (called L04 herein) notes a bias in the GSLS single-scattered (SS) radiances relative to the SS radiances calculated with the Siro model. This bias arises from the approximated use of the Gauss optical path length $r$ through a layer, based on the layer geometric path length $s$ and the extinction coefficients at layer top ($\beta_i$) and layer bottom ($\beta_f$): $r = s \beta_s$ ($\beta_f$)/2

The Siro model used the average $\beta$ within each layer (except the tangent layer), while Siro explicitly integrates $\beta$ along the path (treating $\beta$ as a linear function of altitude within each layer).

Multiple MS Zeniths
The L04 GSLS model also computes the multiple-scattering (MS) source function for the single zenith (GT above) that intersects the tangent limb, with atmospheric properties of interest. The current GSLS model can instead compute MS source functions at several zeniths (e.g., $\alpha_i, \alpha_o, \alpha_{i o}$, $\alpha_{oe}$ above). This modification allows better representation of the MS source function, as shown below in improved total-scatter (TS = SS + MS) radiance agreement with Siro, at the cost of $8$ times the run time (for unrolled RT at 17 MS zeniths).

TS Radiance Comparison
The figures above compare Siro TS radiances to L04 GSLS (left) and current GSLS (right) TS radiance for SAZ = 60° (thinner lines) and 80° (thicker lines). The line styles and colors have the same meaning as in the previous SLS comparisons. The Lambertian surface reflectivity $R = 0.3$, and the current GSLS model uses 17 MS zeniths along the LOS.

The improvement in TS radiance due to adding MS zeniths is significant when SAZ = 0° or SAZ = 80°, but these conditions minimize the TS variation of the solar illumination along the LOS. The current GSLS model is not yet capable of accurate MS source function calculations when SAZ = 90°. In the future, the multi-zenith GSLS model will be tested for twilight conditions, as well as other scenarios that the L04 GSLS model cannot simulate (e.g., surface or atmospheric variation along the LOS).

Finally, the current GSLS TS radiances uniformly exceed the Siro values by a small amount (1.2%) for the cases shown. The observed overestimate increases with increasing $R$, and requires further study. It may occur because RT models using flat (or pseudo-spherical, like GSLS) atmospheres for MS calculations over-estimate upwelling radiation.

Polarization Discussion
The figure in the previous column shows the unpolarized TS radiance error as a function of SS angle for a simulated OMPS LP orbit. The tangent height $h = 40$ km, $R = 0$, and the circles indicate the error associated with SAZ = 30°, 45°, 60°, 80°, 90° (solid lines) and 602, 676, 756, 869, 1023° (dashed lines). The overall behavior of these curves follows the expected pattern1, with largest errors appearing at 345°, when:

- Rayleigh scattering dominates
- Just a low scattering events are likely for a typical photon (vertical optical depth = 1)
- Absorption weak
- Surface reflectivity is small

Improved ASD Capability
Stratospheric aerosol measurement campaigns clearly demonstrate that the aerosol size distribution (A(SD)) varies significantly with altitude (typical with smaller particles at higher altitudes)2. The current GSLS model has been updated to allow the MS source function to vary with altitude. As a rough indication of the significance of this variation, the TS 676 nm radiance change is shown below for a simulated OMPS LP orbit in which the aerosol phase function differs, but all other quantities (including aerosol extinction coefficient) are fixed.

OMPS Retrieval Simulation
An orbit of simulated OMPS radiances (including 17 cases, evenly spaced across the sunlit hemisphere) was generated to perform an initial assessment of the significance of the GSLS RT model changes for the ozone retrieval. To isolate the effect of the RT model changes, many simplifications are used relative to the nominal OMPS LP retrieval:

- Noise-free simulated OMPS LP measurements with $R = 0.3$ across the entire orbit
- Aerosol and NO2 profiles are known perfectly by the ozone retrieval algorithm
- Tangent height (h) registration and surface reflectivity retrievals occur as usual, prior to the ozone profile retrieval

OMPS Retrieval Characteristics
For the base case (not shown), the forward simulations and the retrieval algorithm use a RT model in which:

- Simulated radiances are scalar (unpolarized)
- A single zenith is used to calculate MS source function
- The L04 GSLS method is used to calculate $e$
- The other cases differ from the base case by:
  - Forward simulation RT model uses Siro method to simulate $e$
  - Vector (polarized) forward simulation radiances
  - Forward simulation uses 17 MS zeniths

Ozone Retrieval Error
The figures above show the retrieval error $\Delta R\sigma$ standard deviation for the base case $\sigma$ (dashed lines). The UV $\Delta R$ (left panel) has a small ($\leq 2\%$) bias in all cases, primarily due to ozone a-priori profile influence. The polarized and multi-zenith cases show higher $\sigma$ values, driven primarily by $R$ registration in both cases (see below).

For the Vis retrieval (right panel above), the Siro case shows slightly higher $\sigma$ (with a significant $\Delta R$ bias at the lowest $h$ values, primarily due to topological cases with very low ozone at $h > 20$ km). The multi-zenith case again shows larger $\sigma$ throughout the retrieved altitude range.

Summary
Improvements in the current GSLS RT model significantly improve the calculated radiances relative to the L04 GSLS model, with SS radiance error now generally $0.5\%$ and TS radiance error at the 1-2% level. As shown in previous work, the OMPS LP ozone retrieval algorithm is resilient, tolerating numerous RT approximations without significantly changing the retrieved profiles. This work suggests that using the multi-zenith GSLS model would significantly improve the OMPS LP registration for retrievals at large $h$, and should be considered.

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