Data Simulation Using VLIDORT and PCRTM and its Use for Radiometric Calibration of Hyperspectral UV-NIR-SWIR Sensors

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Outline

- **Vector linearized discrete ordinate radiative transfer model (VLIDORT)**
  - A multiple-scattering multi-layer scattering code (inputs, output, some features and Supplemental Code packages)
  - An improved BRDF Model for hot-spot and its use to simulate hot-spot signature at top of atmosphere (TOA)

- **Principal component (PC) radiative transfer model (PCRTM) and the VLIDORT-PCRTM for Hyperspectral UV-NIR-SWIR Sensors**
  - Introduction of PCRTM
  - Flow chart of VLIDORT-PCRTM and look-up tables (LUTs)

    (Gas Absorption Coefficient LUT;   Aerosol/Dust/Cloud LUT)

- **Some Applications of VLIDORT-PCRTM for Radiometric Calibration**
  - Comparison of VLIDORT_PCRTM simulations with the observations from OMPS NP and EMIT

- **Summary**

VLIDORT Model

(Vector Linearized Discrete Ordinate Radiative Transfer)

- VLIDORT Version 2.8.3 is a multiple-scattering multi-layer discrete-ordinate scattering code with a simultaneous linearization facility for the generation of radiation fields and analytic Jacobians (partial derivatives with respect to any atmospheric or surface parameter).

- VLIDORT calculates Stokes 4-vectors [I, Q, U, V] or Stokes 3-vectors [I, Q, U] (linear polarization).
  - *Neglecting polarization altogether in VLIDORT gives identical results to those from the scalar LIDORT model*

- VLIDORT generates upwelling/downwelling output for any geometrical configuration at any level.

- Linearization is available for atmospheric profile Jacobians (e.g. O3 profiles) or atmospheric bulk-property Jacobians (e.g. total AOD), as well as for surface properties (e.g. albedo).

VLIDORT is a freely available; the code is written in Fortran 90 (Current Version is 2.8.3)

- *Code packages and User Guide available from Robert Spurr at RT Solutions Inc. (rtsolutions@verizon.net)*

VLIDORT Model (cont.)

- VLIDORT is a pure scattering RT model; it ingests total optical properties needed for vector RT:
  - *layer optical depths, single scattering albedos, the 4x4 phase matrix of scattering-matrix expansion coefficients in terms of generalized spherical functions, actual F-matrices for single scattering, and total surface properties (albedo, BRDFs)*
  - *Linearized optical properties (derivatives of the above quantities) must be prepared for calculations with Jacobians*
  - *VLIDORT does not distinguish individual atmospheric absorbers/scatterers, and (for surface BRDFs) type of surface.*

- VLIDORT treats multiple scattering (MS) in plane-parallel geometry, but for the single scattering (SS) field, solar and line-of-sight beams may be computed more accurately for curved spherical media.
  - *There is also a "sphericity correction" option for the MS fields*

- In addition to solar scattering, VLIDORT has a complete black-body atmospheric and surface thermal emission treatment, with a full linearization capability for thermal sources
  - *this includes temperature Jacobians through the use of Planck function derivatives.*

VLIDORT Model (cont.)

- VLIDORT has Four Supplemental Code packages
  - The Bidirectional Reflectance Distribution Function (BRDF) supplement is based on surface reflection kernels (semi-empirical reflectance matrices or scalar values developed for particular types of surfaces) and provides total BRDFs required for VLIDORT to execute; the supplement includes full surface property linearizations;
  - The SLEAVE (surface-leaving) supplement provides surface-leaving radiance sources (currently restricted to water-leaving or solar-induced fluorescence, this is scalar-only);
  - The SS (single-scatter) supplement holds externally-generated SS fields if these are to be ingested by VLIDORT as an alternative to an internal calculation of these fields;
  - The “VFZMAT” supplement based on the use of external F-matrix data sets for generating F-matrix and expansion-coefficient optical inputs required for VLIDORT calculations.

- VLIDORT also has a number of performance enhancements:
  - The delta-M scaling approximation for phase matrices indicative of sharply-peaked forward scattering;
  - The "solution-saving" and "boundary-value telescoping" options to avoid unnecessary computation for situations with contiguous cloud or aerosol layers embedded in a Rayleigh or isotropic atmosphere;

Surface BRDF Model

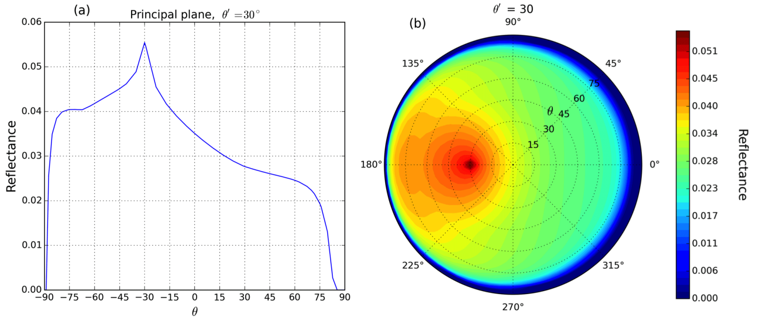
➢The RossThick-LiSparse-Reciprocal (RTLSR) kernel combination is the most common one used, in which the land surface reflectance function $B(\theta_i, \theta_r, \Delta\varphi)$ is represented as:

$$B(\theta_i, \theta_r, \Delta\varphi) = P_1 K_{Lamb} + P_2 K_{geo}(\theta_i, \theta_r, \Delta\varphi, P_4, P_5) + P_3 K_{vol}(\theta_i, \theta_r, \Delta\varphi)$$

P_1 is the Lambertian kernel amplitude with $K_{Lamb} \equiv 1$, P_2 and P_3 are the weights of the Li-Sparse-Reciprocal geometric scattering kernel K_{geo} and the Ross-Thick volume scattering kernel K_{vol} respectively. K_{vol} is :

$$K_{vol}(\theta_i, \theta_r, \Delta\varphi) = \frac{(\frac{\pi}{2} - \zeta) cos\zeta + sin\zeta}{cos\theta_r' + cos\theta_i'} - \frac{\pi}{4}. \qquad (1)$$

➢ It is observed a sharp increase of reflectance when incident (solar) and reflected (viewing) directions almost coincide in the backscatter Direction, i.e. hot-spot, in which K_{vol} needs to be corrected.



Courtesy of **Lorente** et al., AMT, 2018

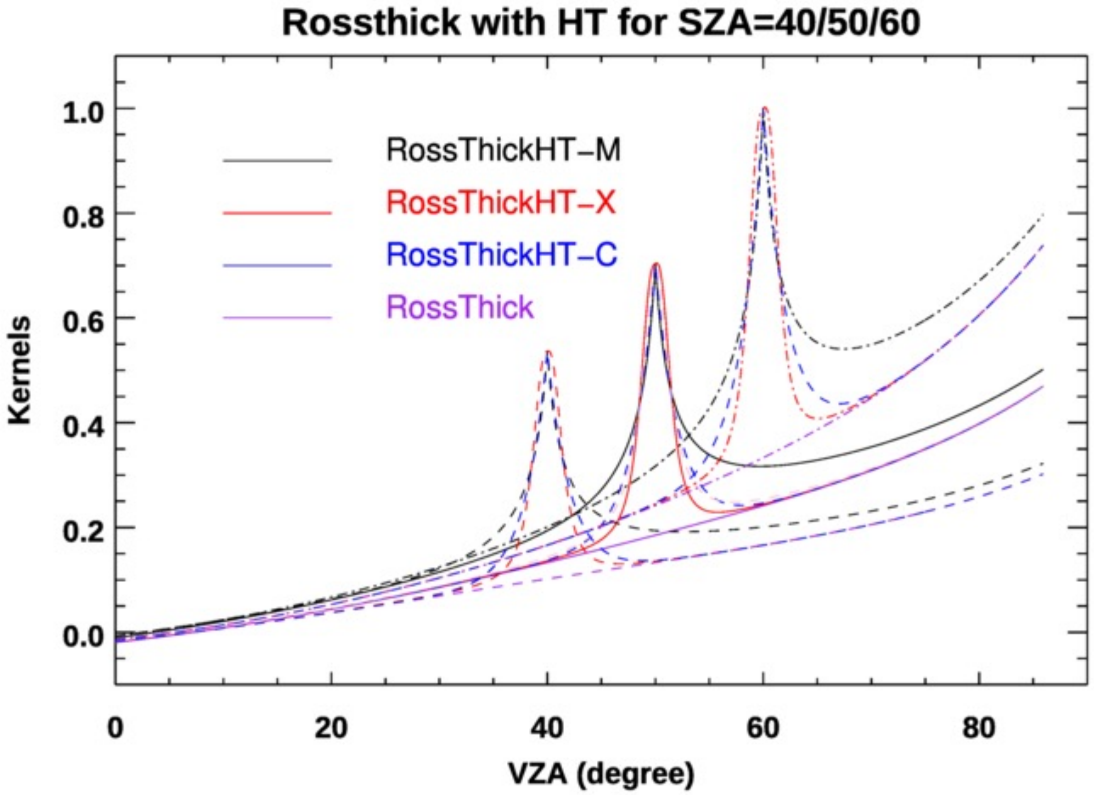
An Improved BRDF Hotspot Model and its Use in VLIDORT

Based on an analysis of POLarization and Directionality of Earth Reflectances (POLDER) measurements, Maignan et al.[2004] brought the hotspot correction into the Ross-Li model (referred as RossThickHT-M) as:

$$K_{vol} = 4\frac{3}{\pi}\frac{(\frac{\pi}{2}-\zeta)cos\zeta+sin\zeta}{cos\theta_r'+cos\theta_i'}(1.+\frac{1}{1+\zeta/\zeta_0})-\frac{1}{3}. \quad (2)$$

In a recent paper, we made improvement to this hot-spot model (referred as RossThickHT-X) as :

$$K_{vol} = 4\frac{3}{\pi}\frac{(\frac{\pi}{2}-\zeta)cos\zeta+sin\zeta}{cos\theta_r'+cos\theta_i'}(1+\frac{1}{1+sin^x(\zeta)*\frac{1}{sin^x(\zeta_0)}})$$



Xiong, X., Liu, X., Spurr, R., Zhao, M., Yang, Q., Wu, W., and Lei, L.: An improved BRDF hotspot model and its use in VLIDORT for studying the impact of atmospheric scattering on hotspot directional signatures in the atmosphere, Atmos. Meas. Tech., 17, 1965–1978, https://doi.org/10.5194/amt-17-1965-2024, 2024.

Improved BRDF Hotspot Model Converges much faster
-- need less terms of N_{BRDF} and $N_{FOURIER}$ to reconstruct a hotspot signature

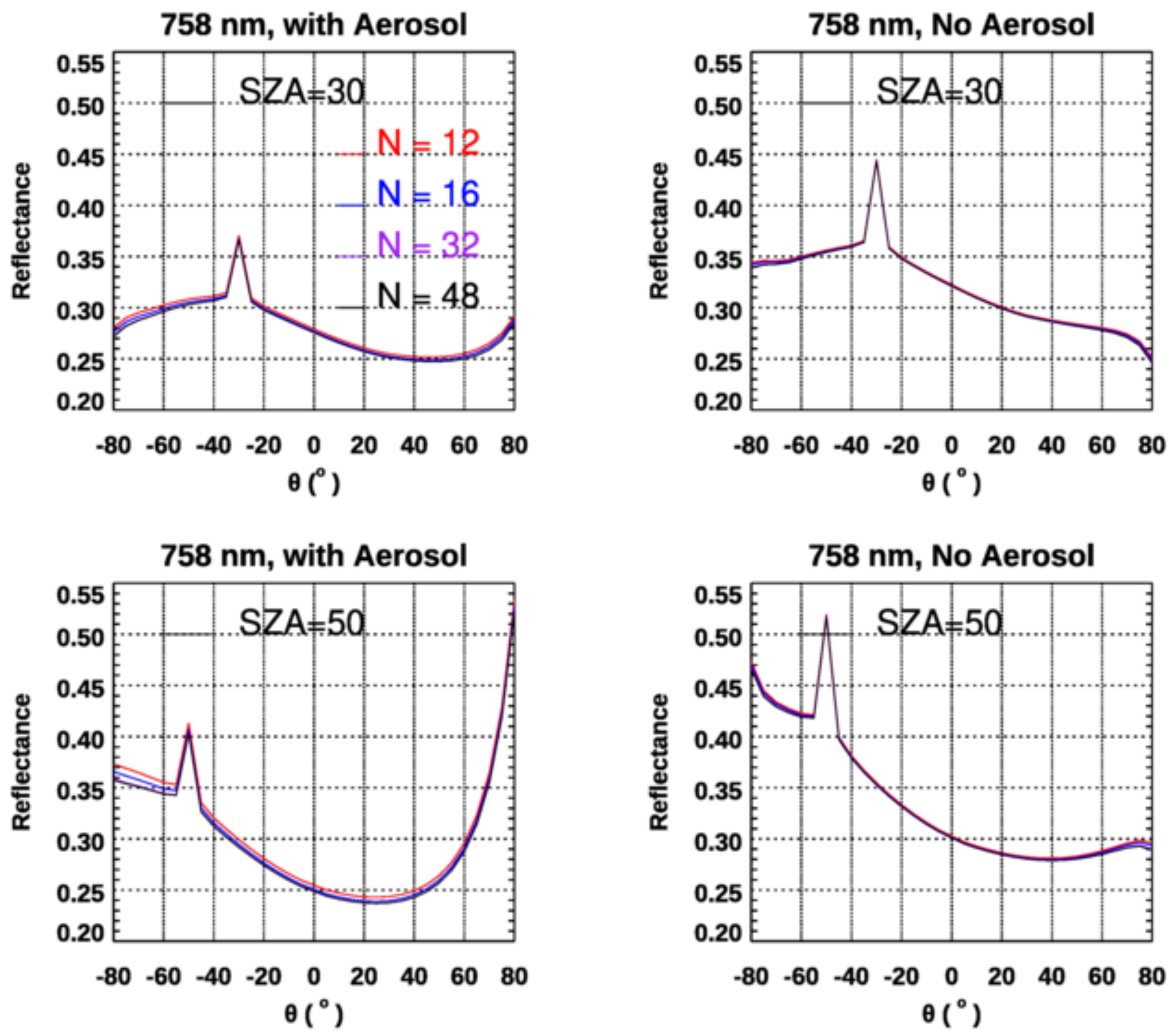
The Fourier components of the total BRDF are calculated through:

$$B^m(\mu,\mu') = \frac{1}{2\pi}\int_0^{2\pi} B(\mu,\mu',\varphi)\cos m\varphi \, d\varphi$$

		RossThickHT-M		RossThickHT-X	
#	Accuracy (%)	NBRDF	N_FOURIER	NBRDF	N_FOURIER
1	1	2810	1402	278	139
2	0.5	5620	2807	324	162
3	0.4	7020	3509	338	169
4	0.3	9360	4679	356	178
4	0.2	14040	7019	382	191
5	0.1	28080	14039	428	214

- For **a hotspot with ζ_0 = 1.5°**, the numbers of Gaussian points (N_{BRDF}) and Fourier Terms ($N_{FOURIER}$) are more than 10 times smaller than those needed with the original hotspot model from Maignan et al. [2004]; making our BRDF model much more practical for use with VLIDORT and other RTA models.
- In VLIDORT, as the direct-beam solar reflectance is calculated using the exact BRDF (rather than in a truncated Fourier-series form), an even smaller values of $N_{FOURIER}$ (i.e., 23 and 63 for atmospheres without and with aerosol scattering) can be used to obtain hotspot signature with acceptable accuracy.

TOA Hot-spot Signature Simulated by VLIDORT with RossThickHT-X-Li Model

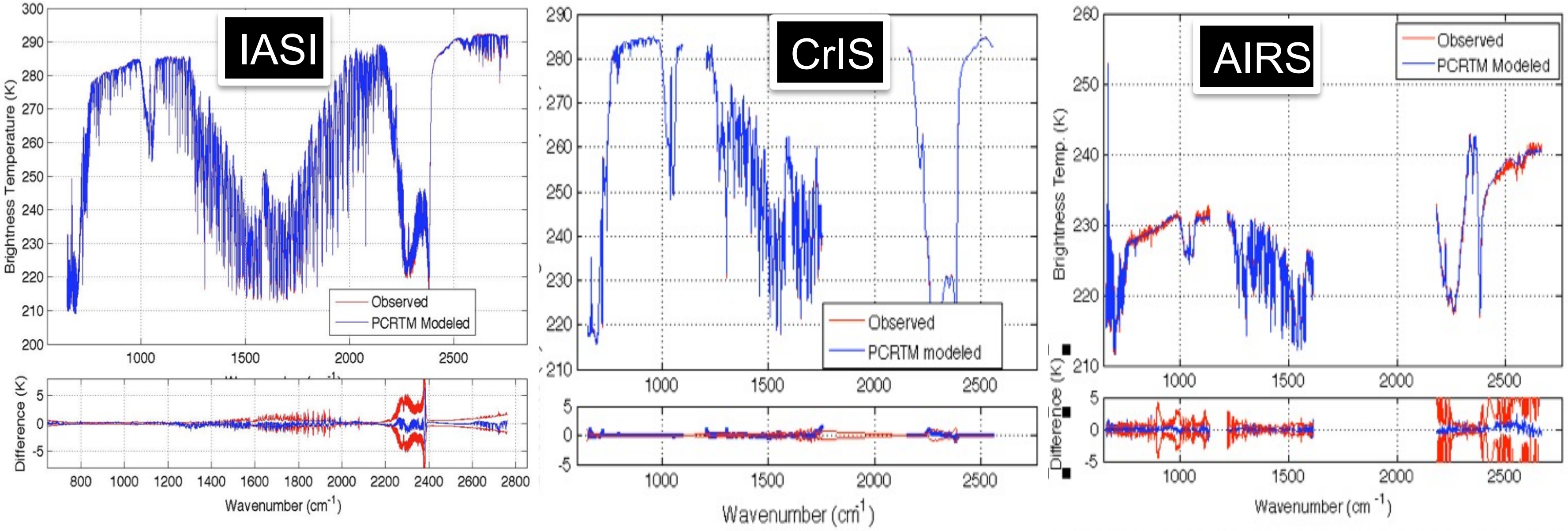


using $N_{STREAMS}$ = 12, 16, 32 and 48. Geometries are in the principal plane. For aerosol, optical depth is set as 0.2.

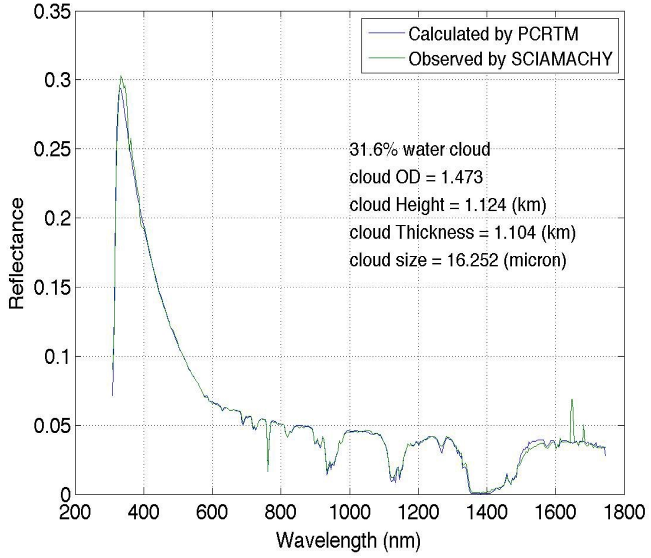
- ✓ *The hotspot amplitudes at TOA increase with solar zenith angle;*
- ✓ *Scattering by molecules and aerosols in the atmosphere tends to smooth out the hotspot signature at TOA, and the hotspot amplitude is reduced when aerosols are added to an otherwise clear (Rayleigh scattering only) atmosphere.*
- ✓ *The hotspot signatures in the near-infrared are larger than those in the visible as it is less impacted by molecules scattering, making it better to be used to derive the surface hotspot signature*

PCRTM (Principal Component based Radiative Transfer Model)

- PCRTM removes spectral redundancy by PC compression;
- PCRTM is a physics-based RTM which performs limited number of monochromatic RT calculations;
- PCRTM has been developed for many satellite remote sensors (AIRS, CrIS, IASI, NAST-I, CLARREO, CPF, SCIAMACHY, OMI, EMIT etc.) with many many application (forward model for operational L2/L3 algorithms, look-up table generations, AI algorithm training databases, sensor spectral calibrations, inter-satellite calibrations, high-fidelity simulators, RTM for climate related products….)



PCRTM simulated and IR sounder (AIRS, CrIS, and IASI) observed TOA radiance

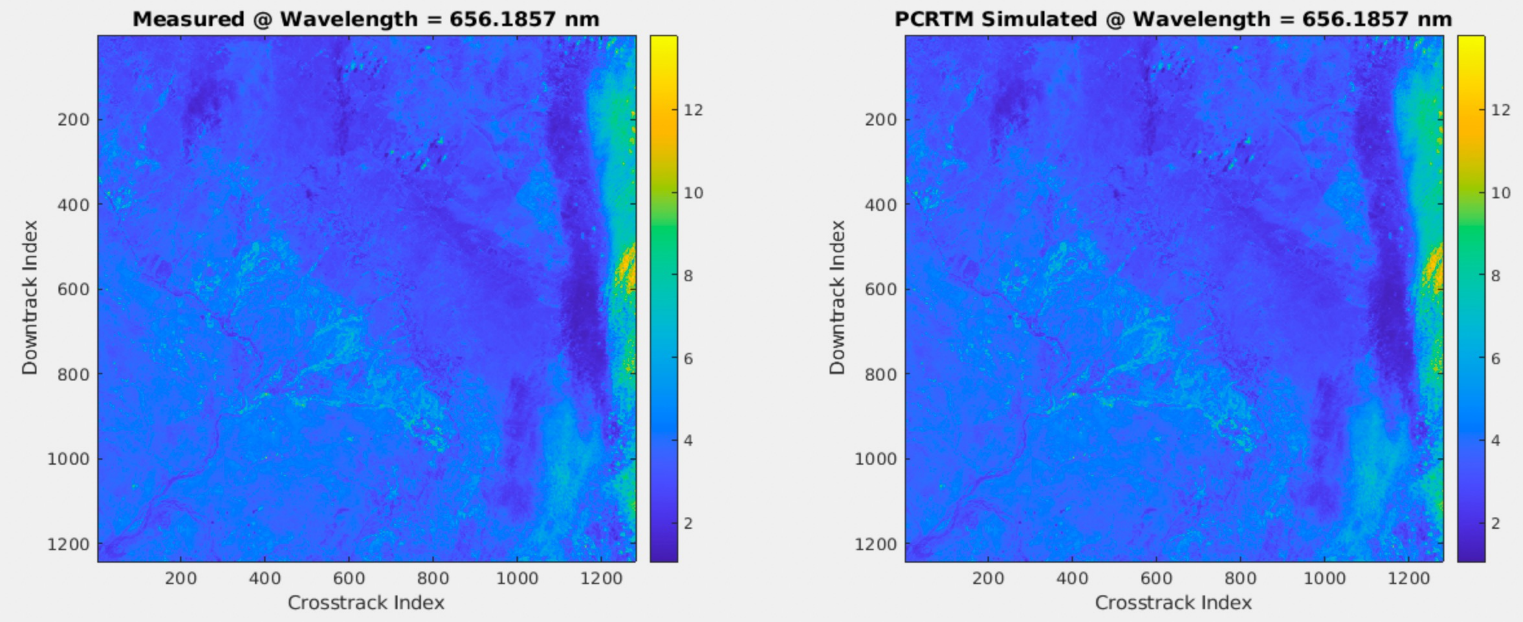


PCRTM simulated and SCIAMACHY solar Reflectance spectra

VLIDORT - PCRTM

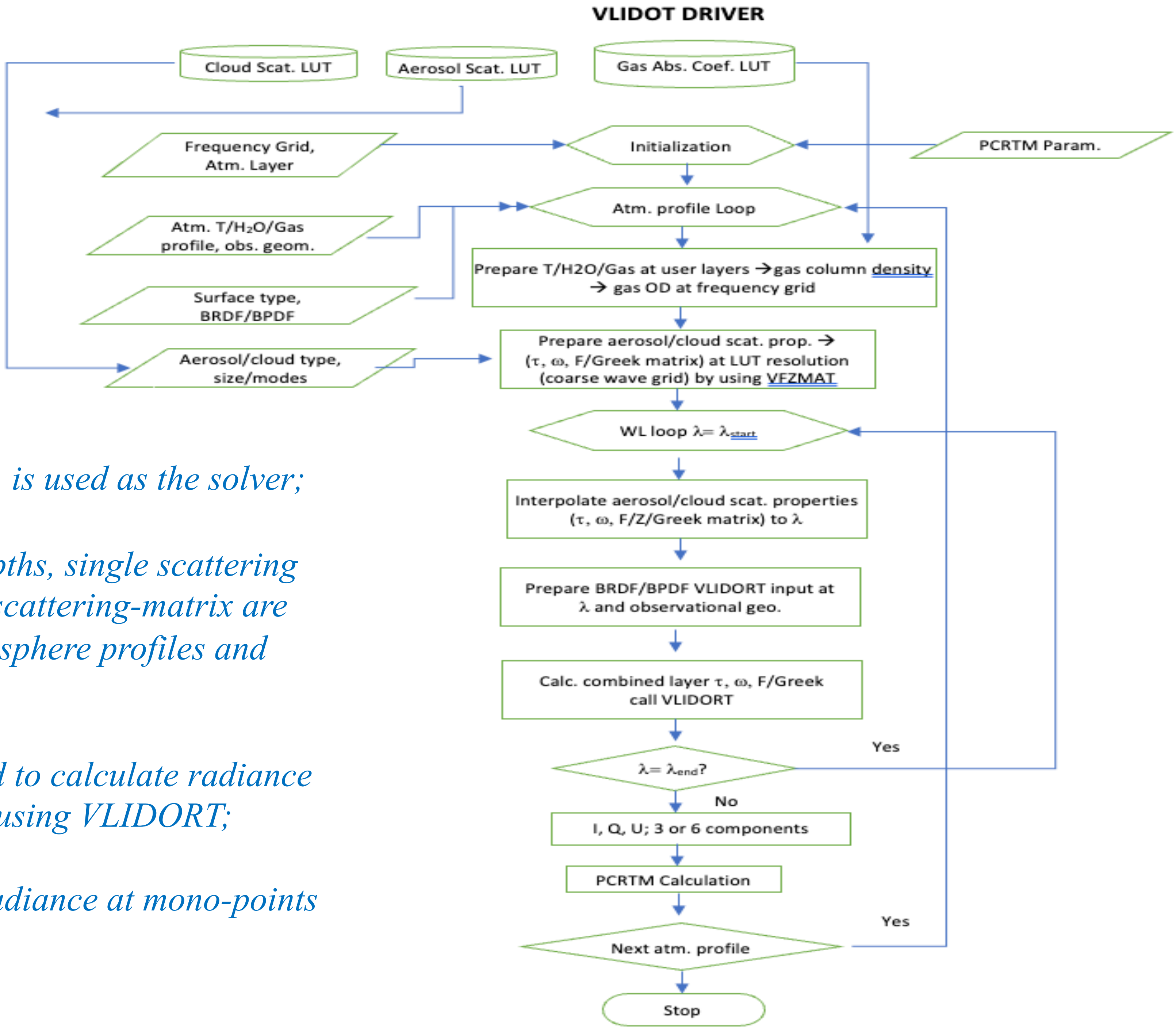
- PCRTM uses VLIDORT to account for polarized lights due to atmosphere gases/clouds/aerosols scatterings;
- PCRTM is super fast (4 orders of magnitude faster than LBL models); Conventional correlated-K based RTMs (e.g. MODTRAN) are too slow for efficient atmospheric correction algorithms;
- To building look-up table which can cover a diverse EMIT observation geometry and atmospheric condition only takes PCRTM 2.2 hours with 35 CPU cores.

EMIT observed radiance at 656.2 nm



PCRTM simulated radiance at 656.2 nm using EM L2 product as input

VLIDORT-PCRTM Flow Chart



1) *VLIDORT (version 3.8.3) is used as the solver;*

2) *Inputs of layer optical depths, single scattering albedos, phase matrix of scattering-matrix are calculated from real atmosphere profiles and multiple LUTs;*

3) *Interpolation to wave grid to calculate radiance of monochromatic points using VLIDORT;*

4) *Use PCRTM to convert radiance at mono-points to whole spectrum*

VLIDORT-PCRTM :Gas Absorption Coefficient LUT

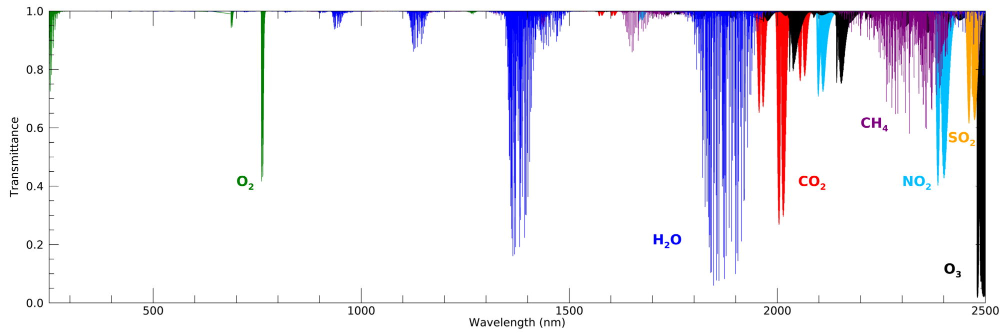
- Why LUT is needed

  - LBL method is the most accurate calculation but heavily time consuming.

  - Generating pre-calculated absorption coefficient for atmosphere trace gases at pre-defined pressure layer, temperature and spectra grid. (22 trace gases included in the VLIDORT-PCRTM)

- LUT's monochromatic spacing

  - Narrow enough to fully resolve line shapes of all absorption gases in each spectra band. Spacing varies from 0.002 to 0.5 cm-1



- LUT (l , p, T, vmr_{H2O}) for H2O, and LUT (l , p, T) for all other gases

  - 200~2500 nm, 100 pressure layer (0.005 ~ 1100 mb)

  - 29 temp. grid with 5K spacing and 3 H2O mixing ratio based on US STD profile, which can cover wide range of atm profiles.

    - LBLRTM is used to generate LBL molecules absorption coefficient.

- LUT interpolation

  - Linear interpolation for temperature and quadra interpolation for water mixing ratio.

VLIDORT-PCRTM : Aerosol/Dust/Cloud LUT

- Aerosol LUT

  - Single component aerosol: insoluble, water soluble, sea salt (accumulation or coarse mode), mineral (nuclei, accumulation or coarse mode), and sulfate;

  - Mixed aerosols : continental clean/average/polluted, urban, desert, maritime clean/polluted/tropical, Arctic, Antarctic - based on OPAC aerosol dataset.

  - Using Lorenz-Mie Look-Up Table (Chemyakin et al. 2021) to calculating bulk optical properties (ext/sca coeff. and phase matrix).

- Dust LUT

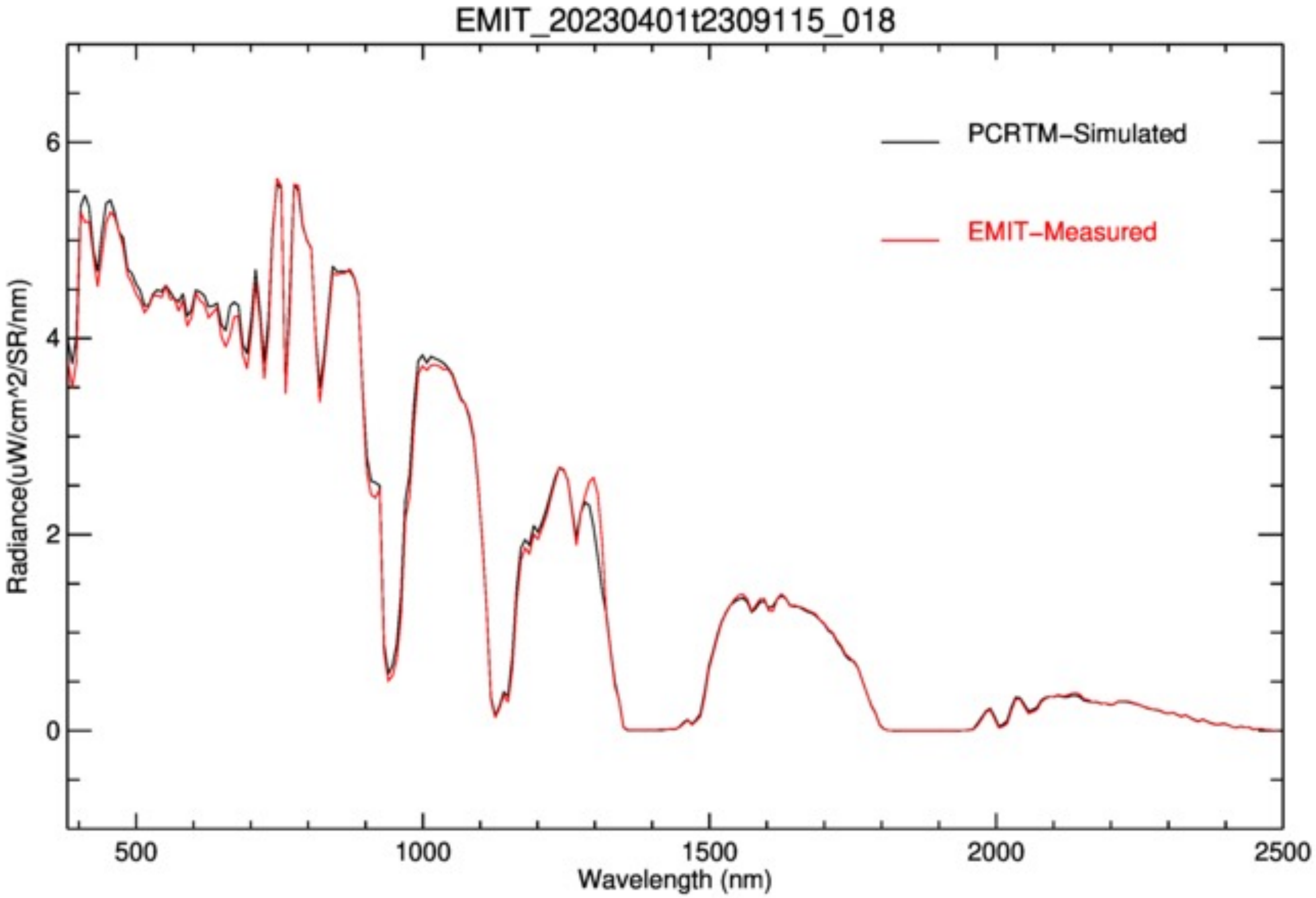
  - 19 dust types from different desert areas in northern Africa, Sahel, Eastern Africa and the Middle East, Eastern Asia, North America, South America, Southern Africa, and Australia.

  - Using TAMU-2020 dust dataset to calculating the dust bulk optical properties (ext/sca coeff. and phase matrix)

- Cloud LUT: water cloud and ice cloud

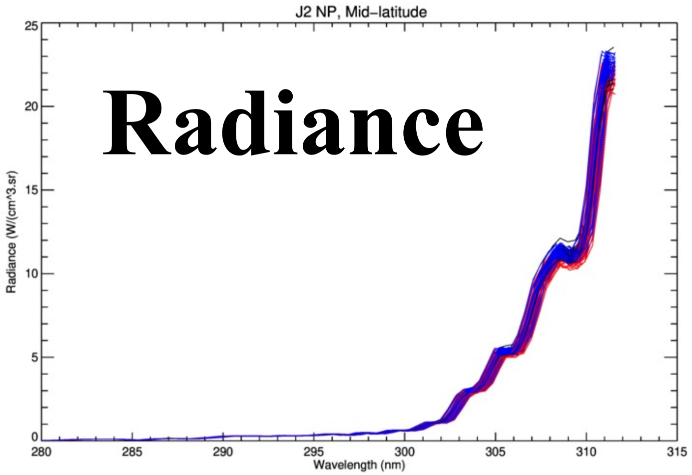
Example: VLIDORT-PCRTM Simulated Radiance with EMIT

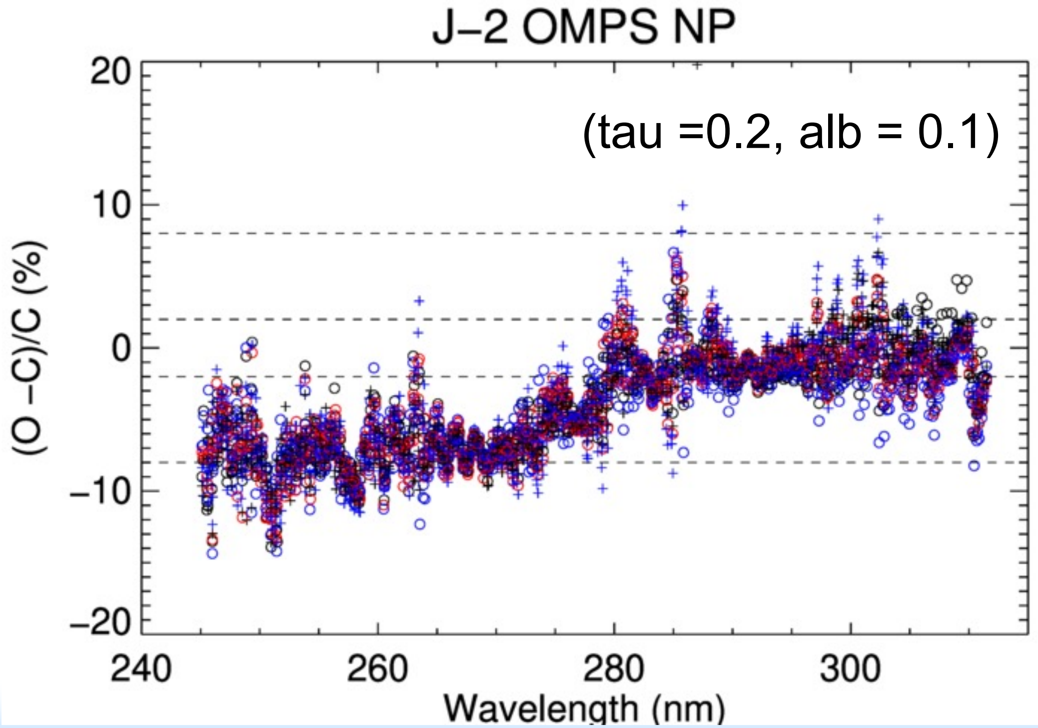
The NASA Earth Surface Mineral Dust Source Investigation (EMIT) instrument is an imaging spectrometer onboard ISS, launched on July 14, 2022, that measures light from the visible to the short wavelength.



Example: VLIDORT-PCRTM Simulated Radiance with OMPS-NP

Ozone Mapper Profiler Suite (OMPS) on JPSS-2 (or NOAA-21) was launched on November 9, 2022. It consists of two spectrometers each with different spectral and spatial coverage. The nadir mapper (NM) has spectral coverage from 300nm to 380nm with 198 channels, and the nadir profiler (NP) has spectral coverage from 250nm to 310nm with 158 channels.





- *VLIDORT-PCRTM simulation (C): input profiles of T, wv and Ozone are from the ERA5-matchup data. Other gases are from MERRA-2 climatology;*
- *The simulated radiance at 0.1 nm is convoluted using J-2 OMPS NP bandpass;*
- *Ring Effect is not considered;* Q/I ~3-5%; U/I ~ 10-15%
- *Lower right figure shows the O-C difference for one granule in the mid-troposphere,* SOMPS_j02_d20231018_t1327028_e1327403

Summary

1. A VLIDORT-PCTRM simulation system developed at NASA LaRC. It incorporates absorption by 22 gases and scattering by various aerosol and cloud models in the atmosphere;

2. One part we recently added is an improved surface BRDF model to calculate hotspot signature. This new BRDF hotspot model requires terms of 10 times less than previous model in VLIDORT to simulate the hotspot signature at the TOA, and this single model can be used in the condition with and without hotspot in applications;

3. By using this VLIDORT-PCTRM system, we simulate hyper-spectra of UV-NIR-SWIR Sensors very quickly, such as OMPS-NP and EMIT;

4. The VLIDORT-PCTRM simulated data can be used for Radiometric Calibration of any UV-NIR-SWIR sensors, as well as many more applications.

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