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A radiative transfer simulator for PACE: theoretical background, update, and potential use

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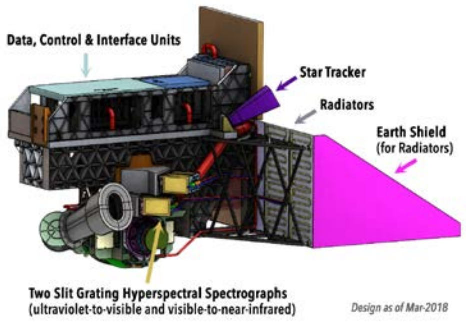
PACE: Plankton, Aerosol, Cloud, and ocean Ecosystem



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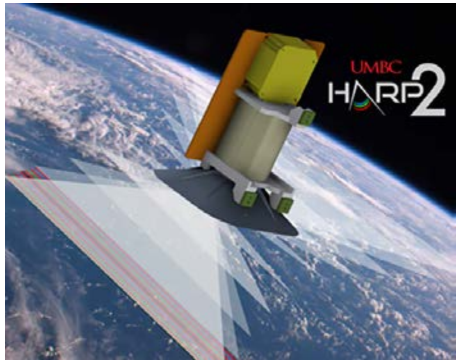
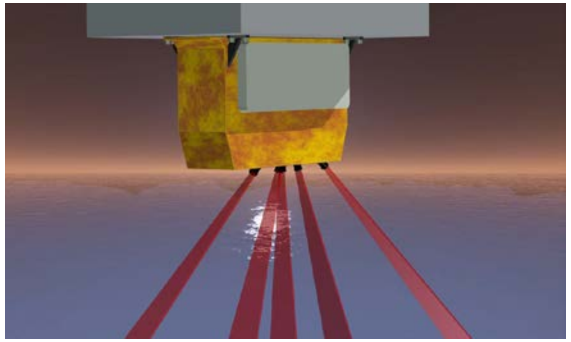




Ocean Color Instrument:

- Continuous wavelength coverage from 340 nm to 890 nm (5 nm resolution)
- SWIR bands: 940, 1038, 1250, 1378, 1615, 2130, and 2260 nm.
- 2-day global coverage at 1-km resolution.
- Calibration uncertainty <0.5%.

HARP2:

- 441, 549, 669, 873 nm
- Up to 60 viewing angles at 669 nm and up to 10 viewing angles at the other three bands.
- 2-day global coverage at 2.6 km resolution.
- 0.01 polarimetric

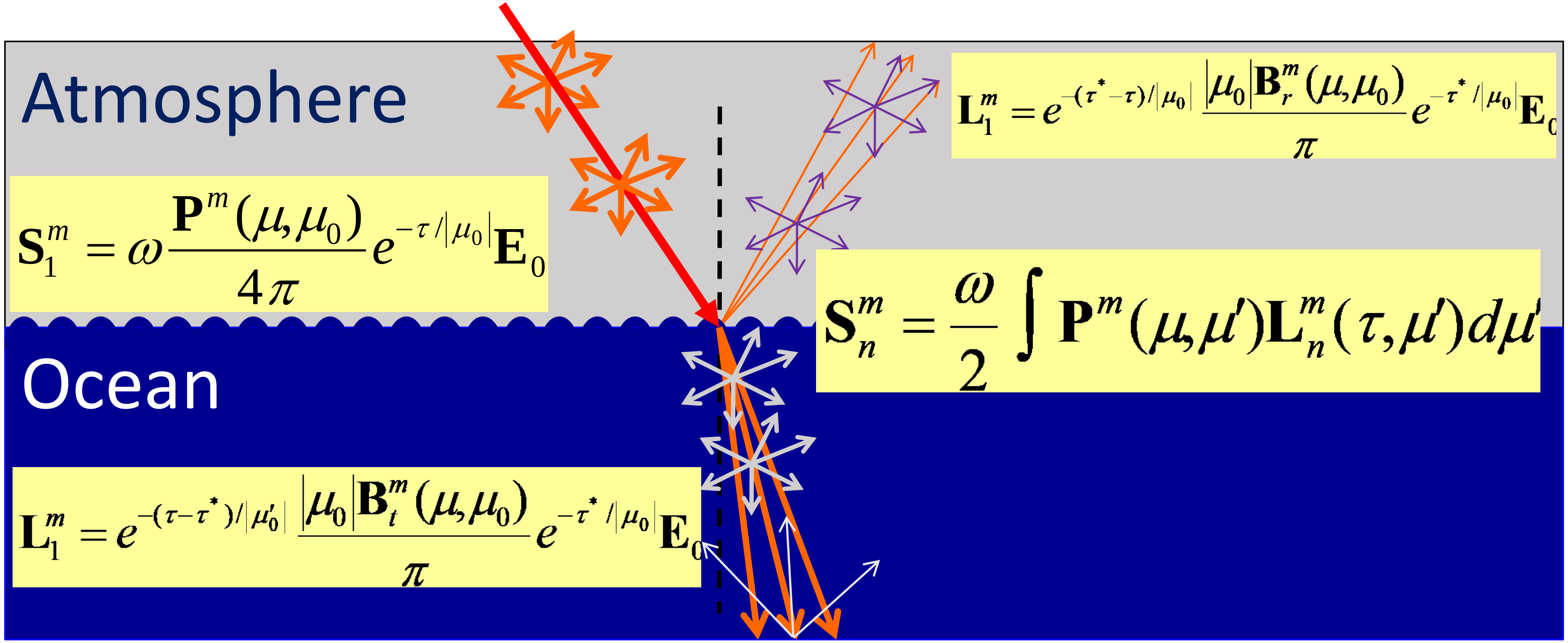
SpexOne:

- Continuous wavelength coverage from 385 nm to 770 nm (variable resolution)
- Five Viewing angles (0, ±20°, ± 58°)
- Swath: 100 km with 5.4 × 4.6 km^2 spatial resolution.
- radiometric uncertainty <2%; 0.003 polarimetric.

Building a PACE simulator: Key Components

- A monochromatic multiple scattering model
    - Atmosphere-ocean coupling;
    - Polarization;
    - Flexible atmospheric and ocean scattering properties;
    - Pseudo-spherical treatment of spherical shell.
- Atmospheric gas absorption:
    - H2O, CO2, O2, CH4: ARTS + HITRAN;
    - Ozone and NO_2: databases from Serdyuchenko et al. (2013); Bogumil et al. (2003).
- Flexible on wavelength ranges and relative spectral response functions.
- Inelastic scattering: Raman scattering and Fluorescence.

Elastic/monochromatic Radiative Transfer: the SOS Method



$$\mathbf{S}_1^m = \omega \frac{\mathbf{P}^m(\mu,\mu_0)}{4\pi} e^{-\tau/|\mu_0|}\mathbf{E}_0$$

$$\mathbf{L}_1^m = e^{-(\tau^*-\tau)/|\mu_0|} \frac{|\mu_0|\mathbf{B}_r^m(\mu,\mu_0)}{\pi} e^{-\tau^*/|\mu_0|}\mathbf{E}_0$$

$$\mathbf{S}_n^m = \frac{\omega}{2}\int \mathbf{P}^m(\mu,\mu')\mathbf{L}_n^m(\tau,\mu')d\mu'$$

$$\mathbf{L}_1^m = e^{-(\tau-\tau^*)/|\mu_0'|} \frac{|\mu_0|\mathbf{B}_t^m(\mu,\mu_0)}{\pi} e^{-\tau^*/|\mu_0|}\mathbf{E}_0$$

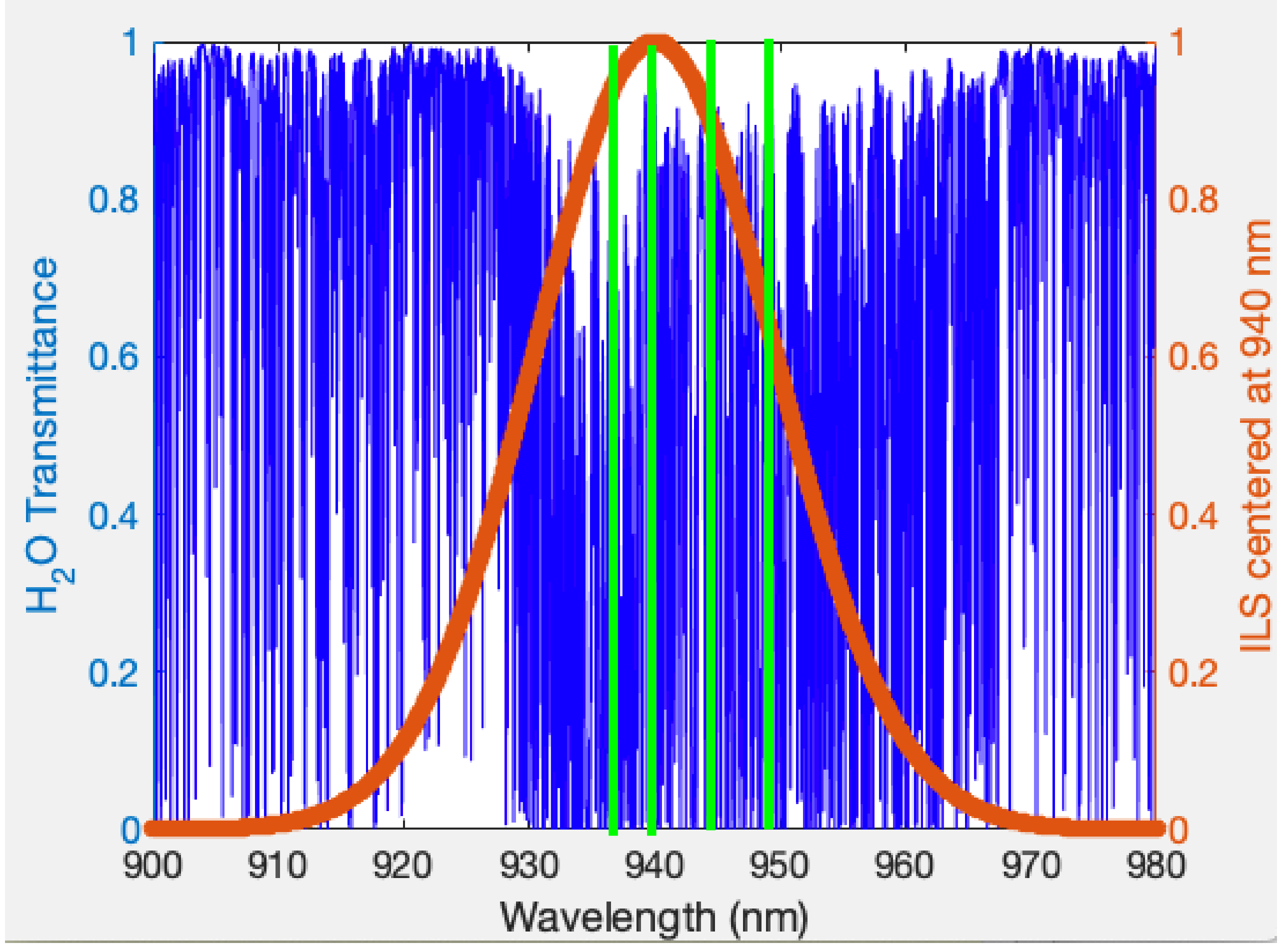
$$\mathbf{L}_n^m(\tau,\mu>0) = \int_{\tau}^{\tau_t} \exp\{-(\tau'-\tau)/\mu\}\mathbf{S}_n^m(\tau',\mu)d\tau/\mu$$

$$\mathbf{L}_n^m(\tau,\mu<0) = \int_{0}^{\tau} \exp\{-(\tau'-\tau)/\mu\}\mathbf{S}_n^m(\tau',\mu)d\tau/|\mu$$

Zhai, P, et al., “A vector radiative transfer model for coupled atmosphere and ocean systems with a rough interface,” J Quant Spectrosc Radiat Transf, **111**, 1025-1040 (2010).

Zhai, P, et al. "A vector radiative transfer model for coupled atmosphere and ocean systems based on successive order of scattering method," Opt. Express **17**, 2057-2079 (2009).

Gas and scattering interaction

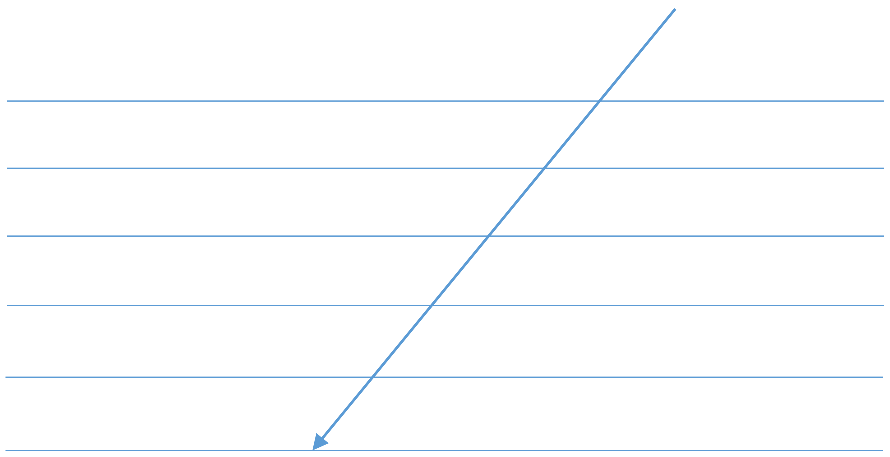


$$I(\tau_g) = I_c \begin{cases} \dfrac{1}{(\tau_g - \alpha)^{\beta+1}} & \tau_g \in (0,1) \\ \exp[-(\tau_g - \tau_g')] & \tau_g \in (1,\infty) \end{cases}$$

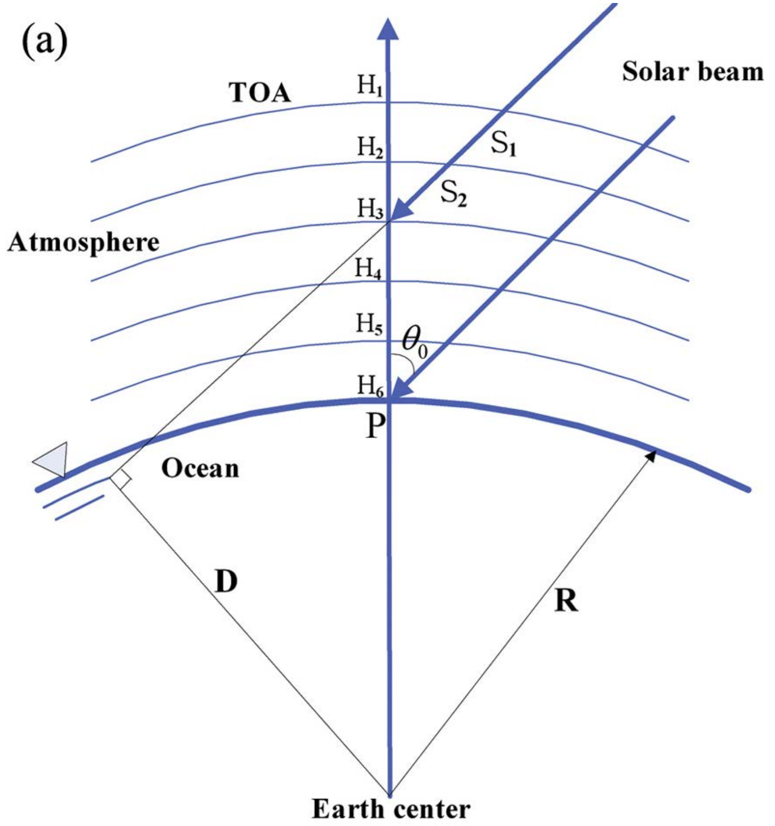
Advantages:
Efficient, Accurate, and flexible with different instrument RSR functions.

Method was first proposed by: Duan, M., Q. Min, and J. Li (2005), A fast radiative transfer model for simulating high-resolution absorption bands, J. Geophys. Res., 110, D15201, doi:10.1029/2004JD005590.

Pseudospherical treatment



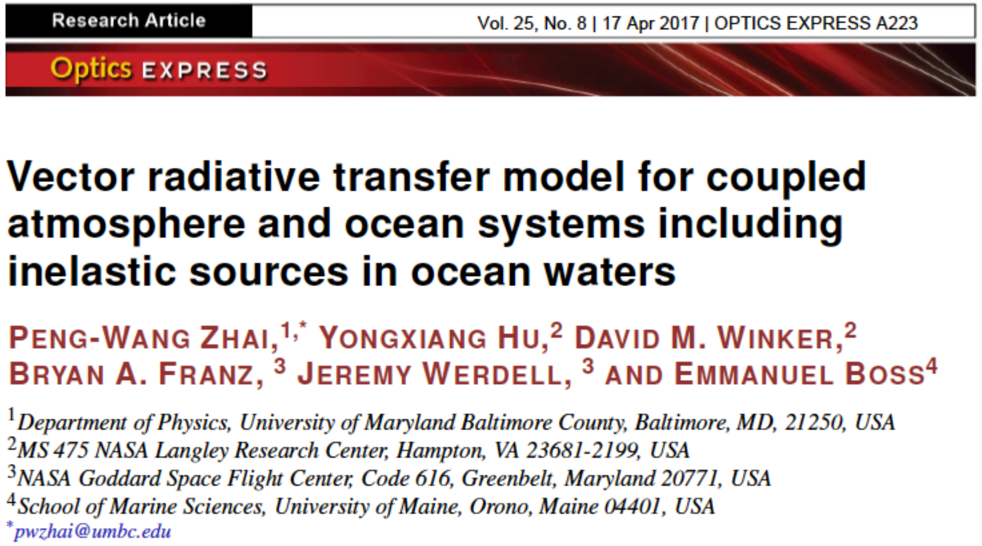
Plane parallel



Spherical Shell, Ref: He et al. RSE, 2018

Inelastic Scattering: a Important Component in Ocean Waters

- Raman Scattering by Water Molecules
- Fluorescence by Dissolved Organic Matter (FDOM)
- Fluorescence by Chlorophyll as a byproduct of Photosynthesis



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Vector radiative transfer model for coupled atmosphere and ocean systems including inelastic sources in ocean waters

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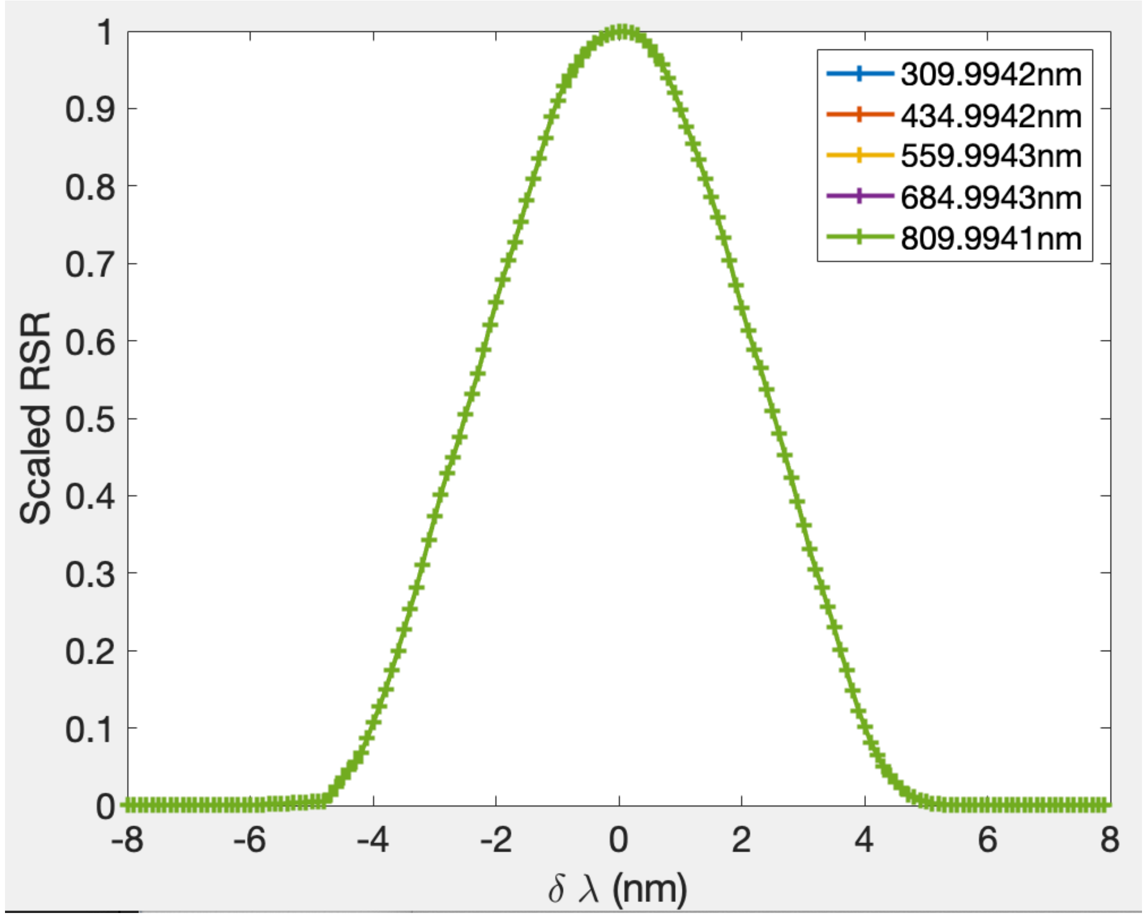
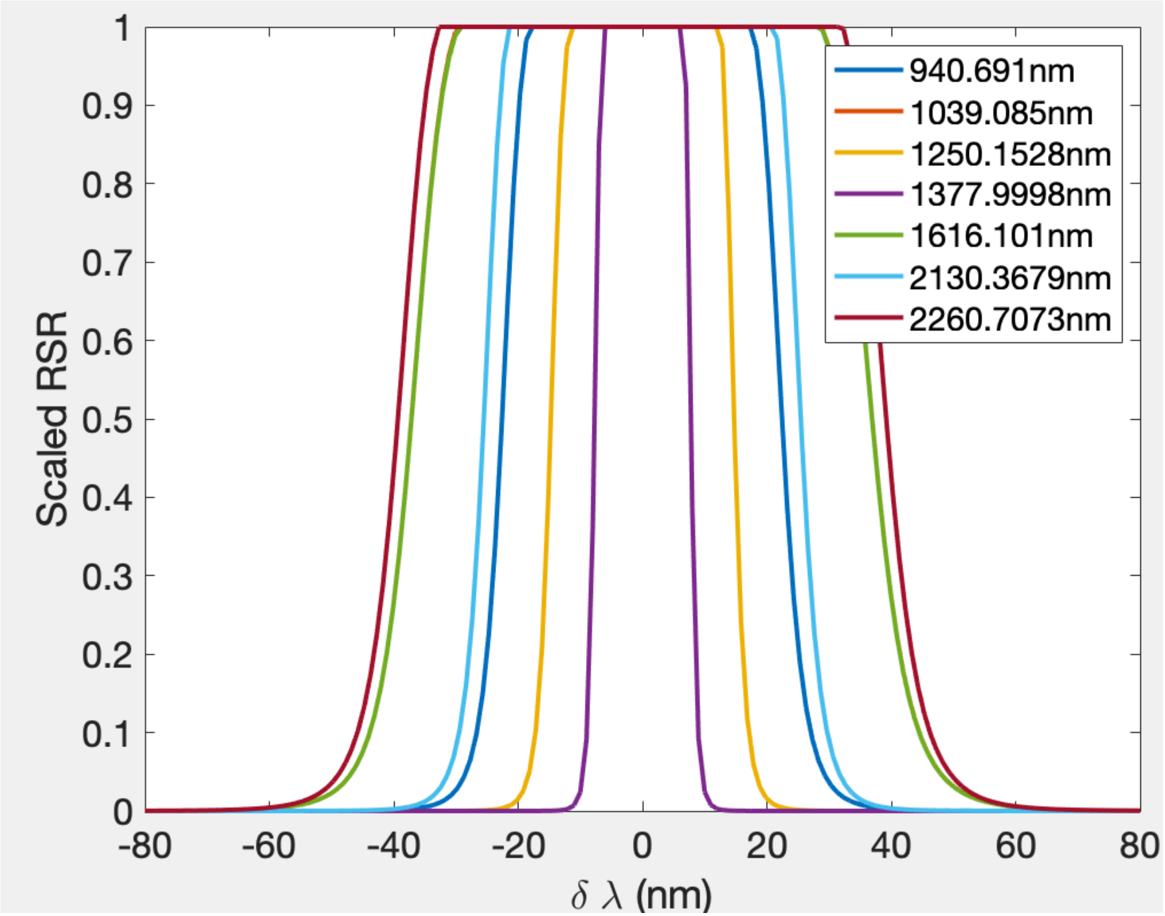
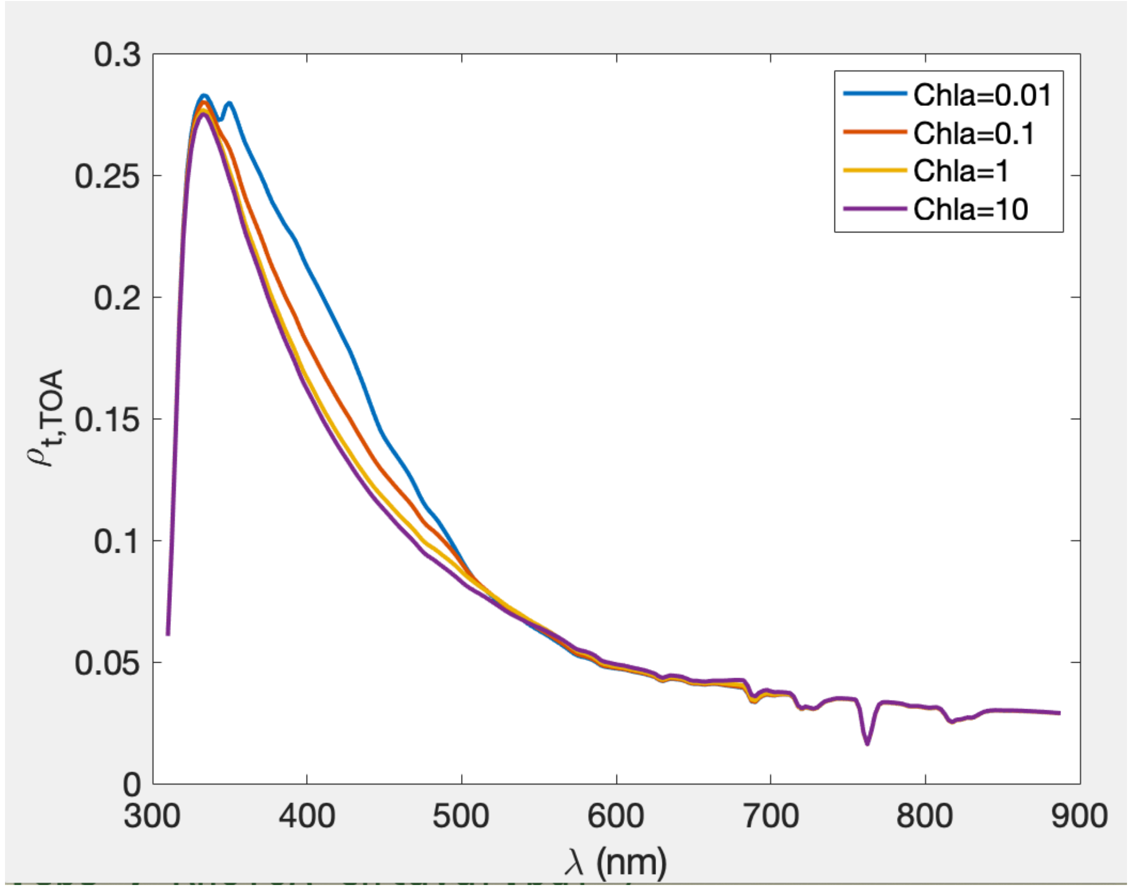
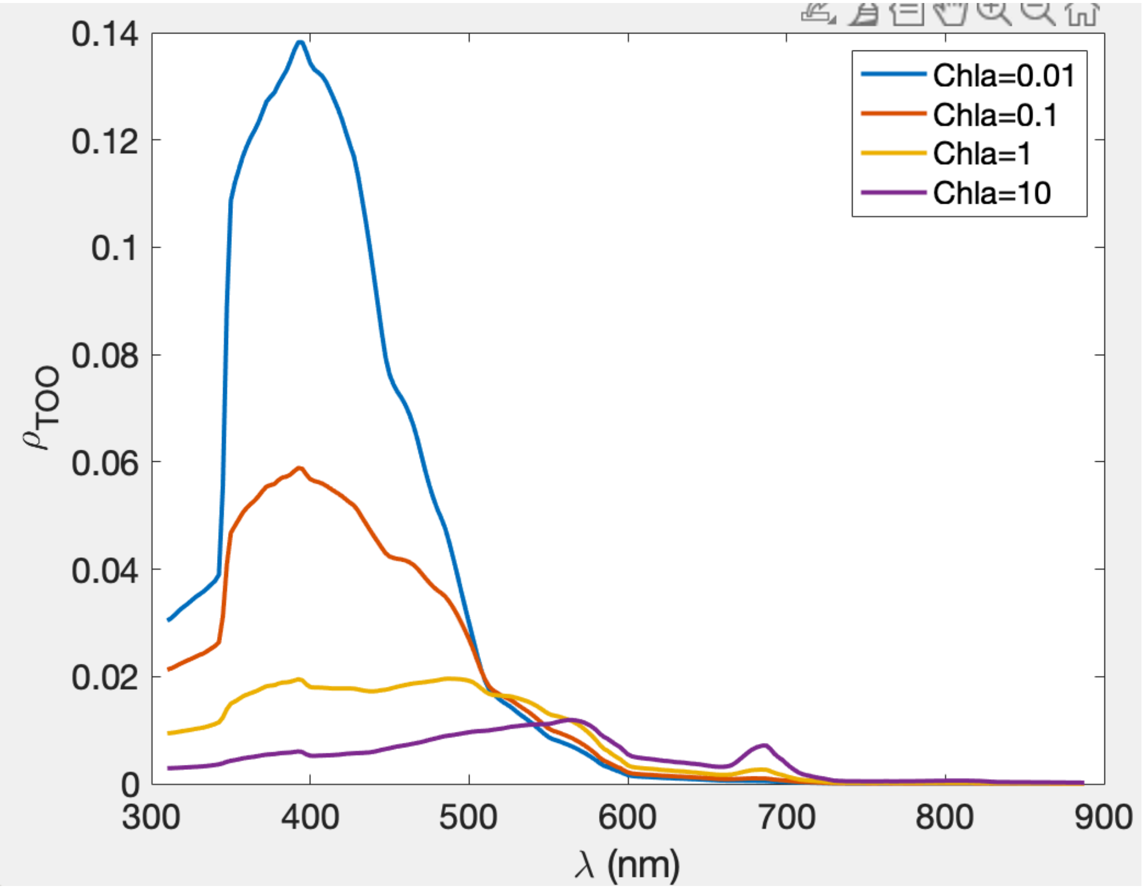
OCI Relative Spectral Response function





Application I: TOA Reflectance Example



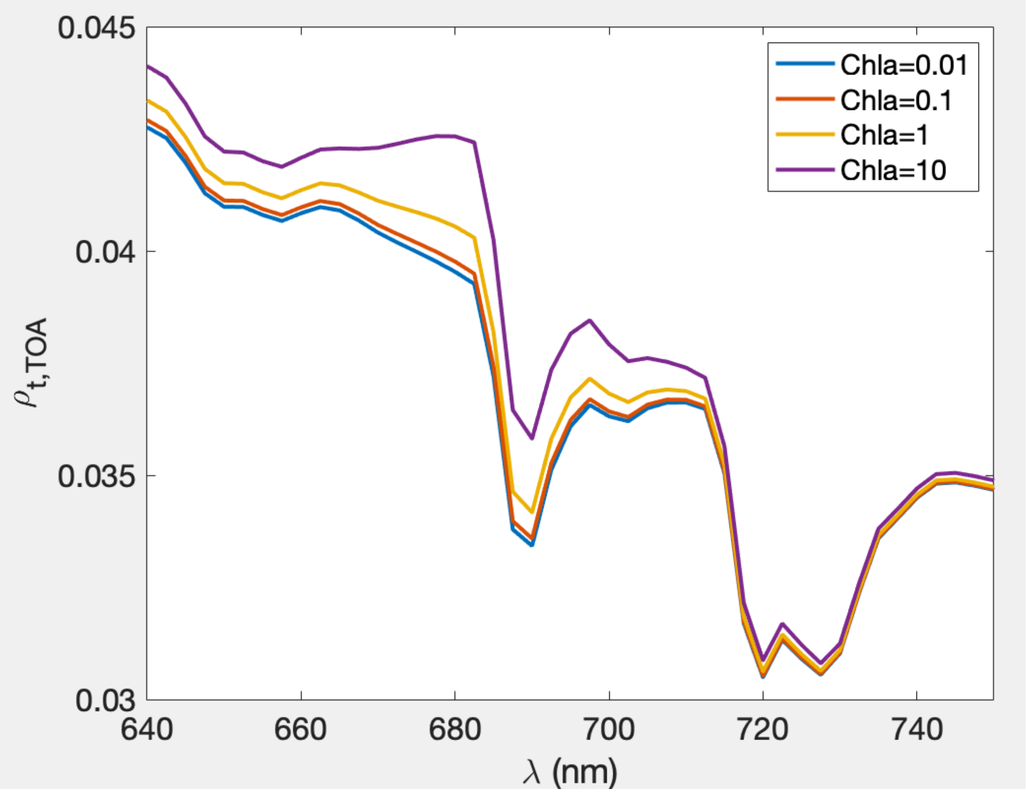


Atmosphere:
$\tau_{a,550\ nm}$=0.1
Aerosol model: Ahmad et al, 2010
Fine-mode volume fraction: 20%
Relative humidity: 80%
Gas absorption: H_2O, Ozone, CO2, CH4, O2, NO2.

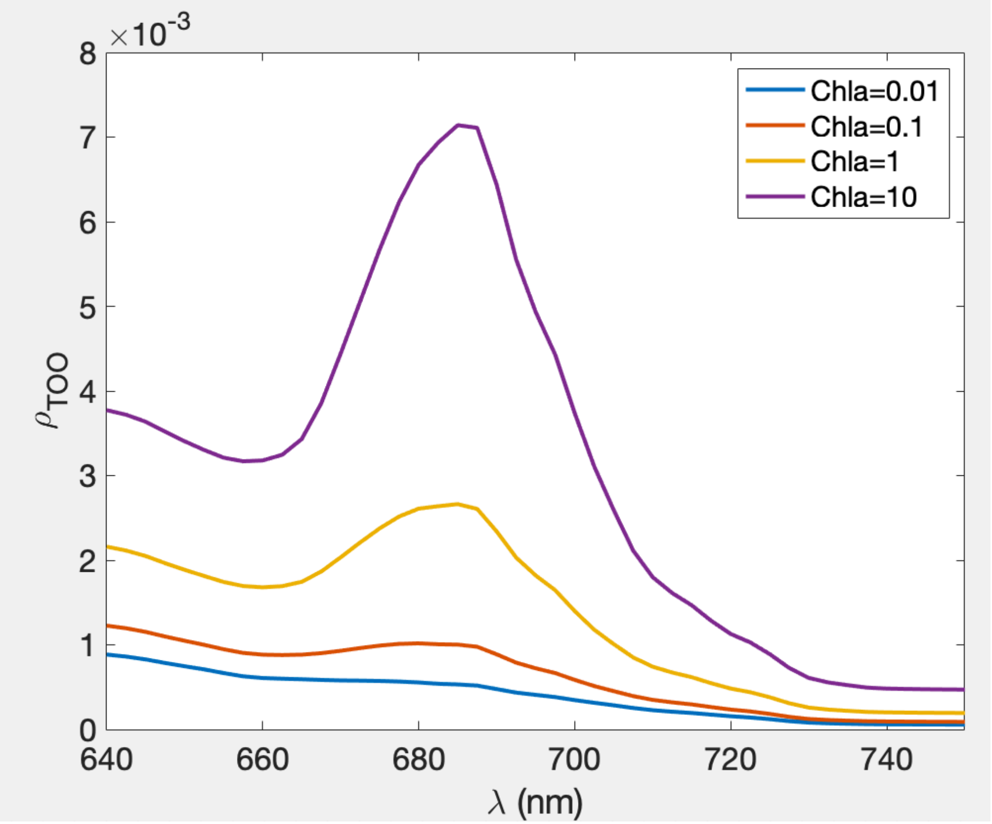
Ocean water model:
pure sea water,
phytoplankton covariant particle,
CDOM

Solar zenith angle: 30 degree.

Application II: Chlorophyll a Fluorescence …

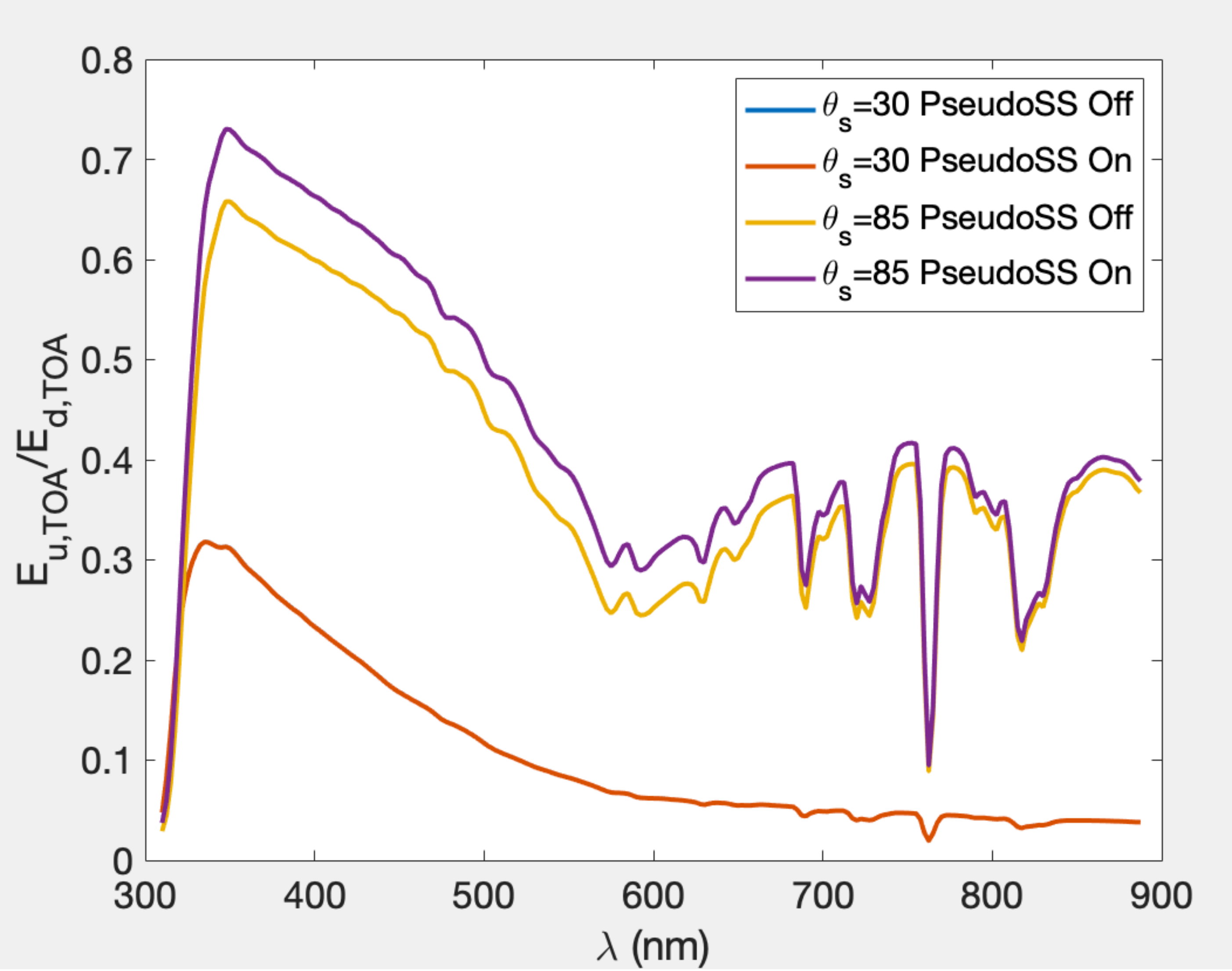


Solar zenith angle: 30 degree.
$\tau_{a,550\ nm}$=0.1, Aerosol model: Marinetime
Gas absorption: (H2O, CO2, CH4, O2, O3, NO2)



Ocean water model:
pure sea water,
phytoplankton covariant particle,
CDOM

Application III: Modeling Pseudo-Spherical Shell Effects



Progress so far:

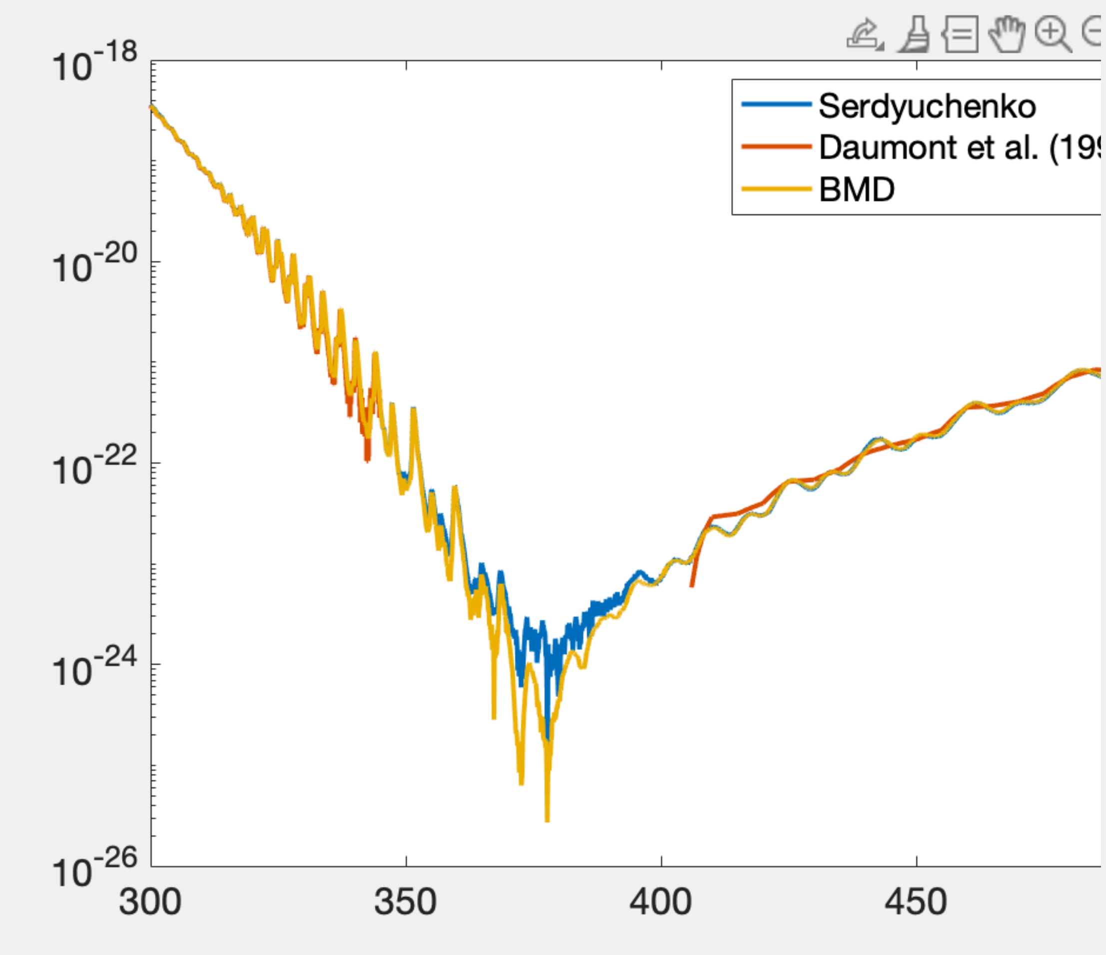
- Fitting ozone absorption cross section measurement (Serdyuchenko 2013) in terms of quadratic relations of temperature in Celsius degree. The wavelength range covers all the PACE wavelength.
- Implementation of the new ozone absorption file in the simulator.
- Flexible input controls to the simulator, including aerosol models, ocean bio-optical models, surface pressure rescaling, water vapor and column ozone assignment, etc.
- Delivered the first version of the PACE simulator to the PACE project team.
- On-going effort:
  - Integrating non-spherical dust scattering models in the simulator
  - Collaborating with Meng Gao, Nima Pahlevan in developing inversion algorithms for atmosphere and ocean.

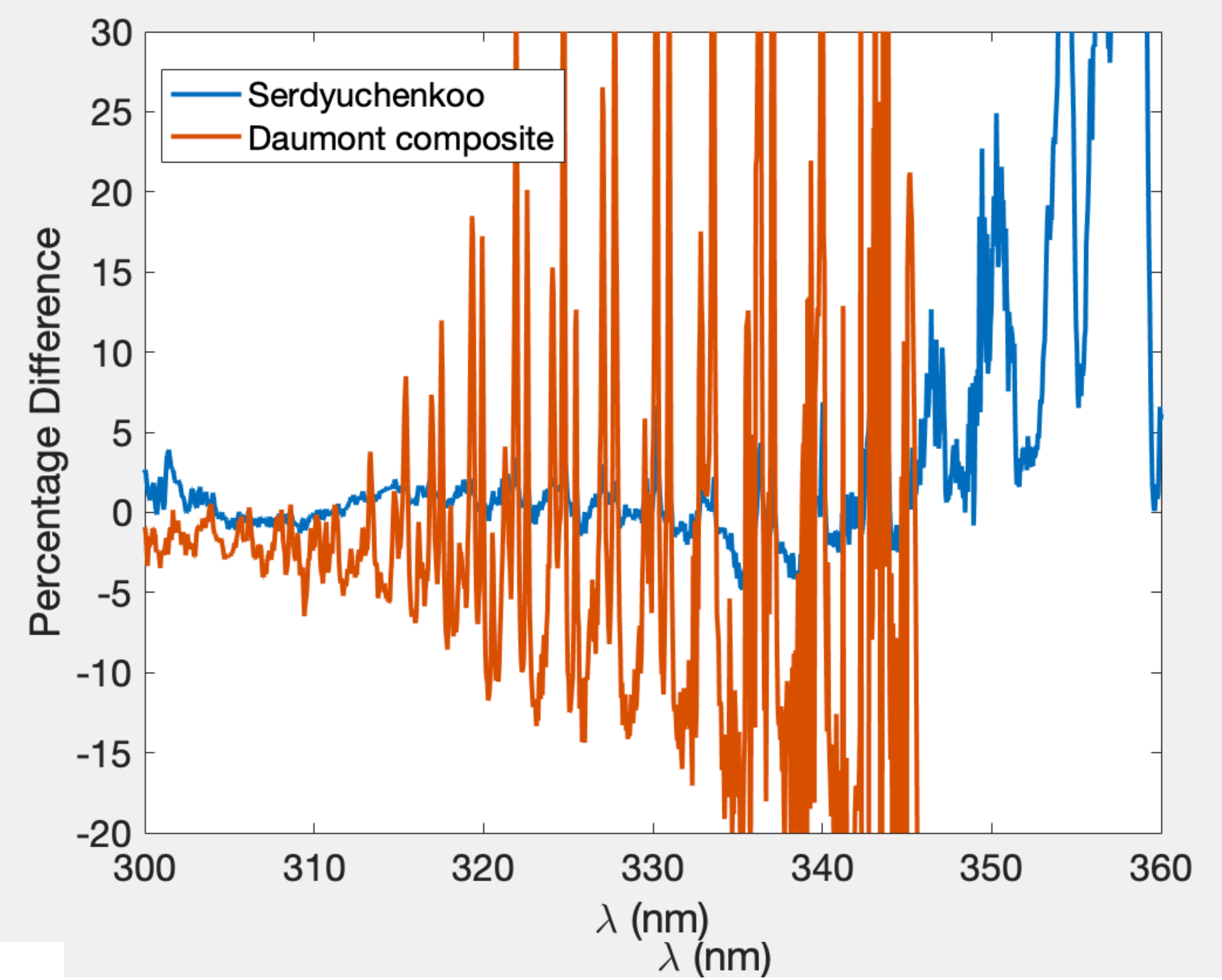
Summary and future plans

- We have developed a PACE simulator based on rigorous vector radiative transfer model.
- The philosophy of this model is to preserve/simulate all physics processes as much as possible, including: multiple scattering, gas absorption, flexible RSR, pseudospherical shell, atmosphere and ocean coupling, and inelastic scattering in ocean.
- The simulator will be used for sensitivity study of a number of environmental parameters, including clouds, aerosols, hydrosols, etc.
- Synthetic dataset will be generated and provided to the science team if desired.

Synthetic Dataset Setting

1. SET 1. Use the standard ocean color aerosol (Zia) models, and assumes case 1 ocean waters (everything determined by the chlorophyll a value). The parameters to be varied would be aerosol optical depth, sun-viewing geometry, and chlorophyll a values. The atmosphere will be the US 76 standard. The motivation of this set is to check the consistency of the hyper spectral version of the atmospheric correction algorithms, with everything well defined.
2. SET 2. Use the standard aerosol model, but adopt a more complex ocean water model. I would adopt Meng Gao's 7 parameter model, which would provide enough ocean water BRDF variability in the UV and NIR. This is to test the algorithm in cases of coastal waters.
3. SET 3. Use some absorbing aerosol models and the 7 parameter ocean models to further examine the ability of the atmospheric algorithm for these very complex cases. This would be connecting to what we discussed in a separate email trend to assess the performance of the atmospheric correction in these extreme cases.
4. SET 4. If gas absorption correction is a concern, I can do SET 1 + different gas concentration, which includes different Ozone and water vapor amount.


Serdyuchenko
Daumont et al. (199
BMD
10^-18
10^-20
10^-22
10^-24
10^-26
300
350
400
450


Serdyuchenkoo
Daumont composite
Percentage Difference
30
25
20
15
10
5
0
-5
-10
-15
-20
300
310
320
330
340
350
360
λ (nm)
λ (nm)

Publication Related to PACE:

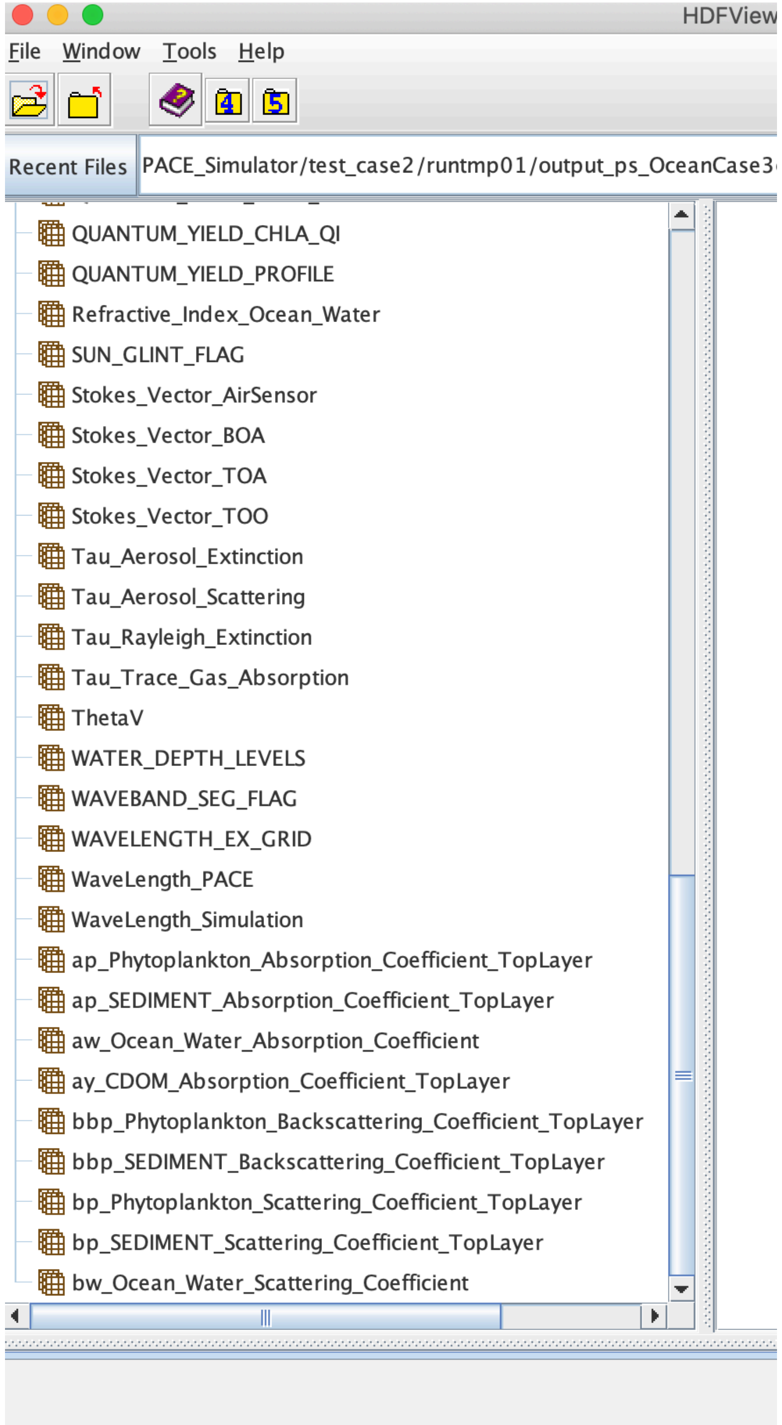
- M. Gao, P. Zhai, B. Franz, Y. Hu, K. Knobelspiesse, P. J. Werdell, A. Ibrahim, B. Cairns, and A. Chase, “Inversion of multiangular polarimetric measurements over open and coastal ocean waters: a joint retrieval algorithm for aerosol and water-leaving radiance properties”, Atmos. Meas. Tech., 12, 3921-3941, https://doi.org/10.5194/amt-12-3921-2019, 2019.
- P. Zhai, E. Boss, B. Franz, P. J. Werdell, and Y. Hu, Radiative Transfer Modeling of Phytoplankton Fluorescence Quenching Processes. Remote Sens. 10, 1309 (2018).
- M. Gao, P. Zhai, B. Franz, Y. Hu, K. Knobelspiesse, P. J. Werdell, A. Ibrahim, F. Xu, and B. Cairns, "Retrieval of aerosol properties and water-leaving reflectance from multi-angular polarimetric measurements over coastal waters," Opt. Express 26, 8968-8989 (2018).Top of Form
- L. Mukherjee, P. Zhai, Y. Hu, D. Winker, “Single scattering properties of non-spherical hydrosols modeled by spheroids,” Optics Express, 26, A124-A135 (2018).
- P. Zhai, K. Knobelspiesse, A. Ibrahim, B. Franz, Y. Hu, M. Gao, R. Frouin, “Water-leaving contribution to polarized radiation field over ocean,” Opt. Express, 25, A689-A708 (2017).
- L. Mukherjee, P. Zhai, Y. Hu, D. Winker, “Equivalence of internal and external mixture schemes of single scattering properties in vector radiative transfer,” Appl. Opt., 56(14), 4105-4112.
- P. Zhai, Y. Hu, D. M. Winker, B. Franz, J. Werdell, E. Boss, “Inelastic vector radiative transfer solution in ocean waters.,” Opt. Express, 25, A223-A239 (2017).
- P. Zhai, Y. Hu, D. M. Winker, B. Franz, E. Boss, “Contribution of Raman scattering to polarized radiation field in ocean waters,” Optics Express, **23**(18), 23582-23596 (2015).

Roles of Radiative Transfer in Remote Sensing Theory

- Explore the physical processes of light transport/propagation in turbid media.
- Perform sensitivity Study for different microphysical parameters.
- Build Look-Up Tables for aerosol or cloud reflectance.
- Act as a forward model for non-linear least squares fitting algorithms.
- Test operational retrieval algorithm.

Data Format

- H5 format
- Currently reports a large number of parameters, including the Stokes parameters at TOA at all OCI, HARP, SPEXone Channels; gas absorption optical depth averaged within the channels; Aerosol models and optical depth; hydrosol parameters; etc.
- Will add more if needed.



PACE_Simulator/test_case2/runtmp01/output_ps_OceanCase3

- QUANTUM_YIELD_CHLA_QI
- QUANTUM_YIELD_PROFILE
- Refractive_Index_Ocean_Water
- SUN_GLINT_FLAG
- Stokes_Vector_AirSensor
- Stokes_Vector_BOA
- Stokes_Vector_TOA
- Stokes_Vector_TOO
- Tau_Aerosol_Extinction
- Tau_Aerosol_Scattering
- Tau_Rayleigh_Extinction
- Tau_Trace_Gas_Absorption
- ThetaV
- WATER_DEPTH_LEVELS
- WAVEBAND_SEG_FLAG
- WAVELENGTH_EX_GRID
- WaveLength_PACE
- WaveLength_Simulation
- ap_Phytoplankton_Absorption_Coefficient_TopLayer
- ap_SEDIMENT_Absorption_Coefficient_TopLayer
- aw_Ocean_Water_Absorption_Coefficient
- ay_CDOM_Absorption_Coefficient_TopLayer
- bbp_Phytoplankton_Backscattering_Coefficient_TopLayer
- bbp_SEDIMENT_Backscattering_Coefficient_TopLayer
- bp_Phytoplankton_Scattering_Coefficient_TopLayer
- bp_SEDIMENT_Scattering_Coefficient_TopLayer
- bw_Ocean_Water_Scattering_Coefficient