MODTRAN®5.2 Radiative Transfer Model and Applications to HysplRI

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    Full Spectral Signature Simulation Models for Chemical Releases

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- Technical
  - Vincent J. Realmuto

    Jet Propulsion Laboratory

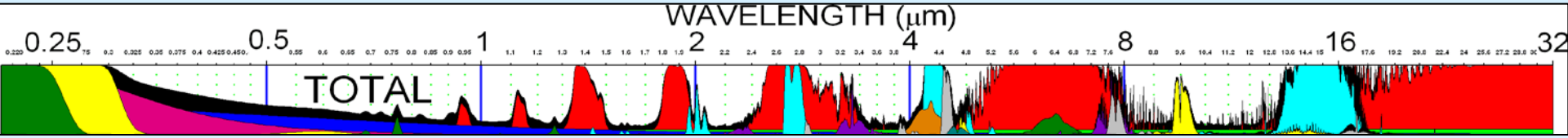
Presentation Outline

- MODTRAN Overview

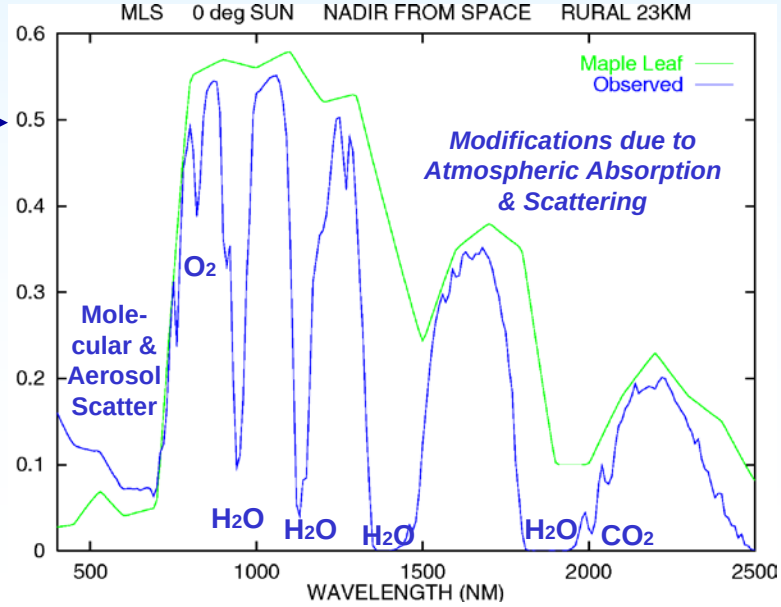
- A Localized Chemical Cloud Option

MODTRAN5
- General Description -

- Overview
  - 0.2 cm^{-1} IR/Vis/UV Transm., Rad. & Fluxes from 0.1 cm^{-1} Band Model

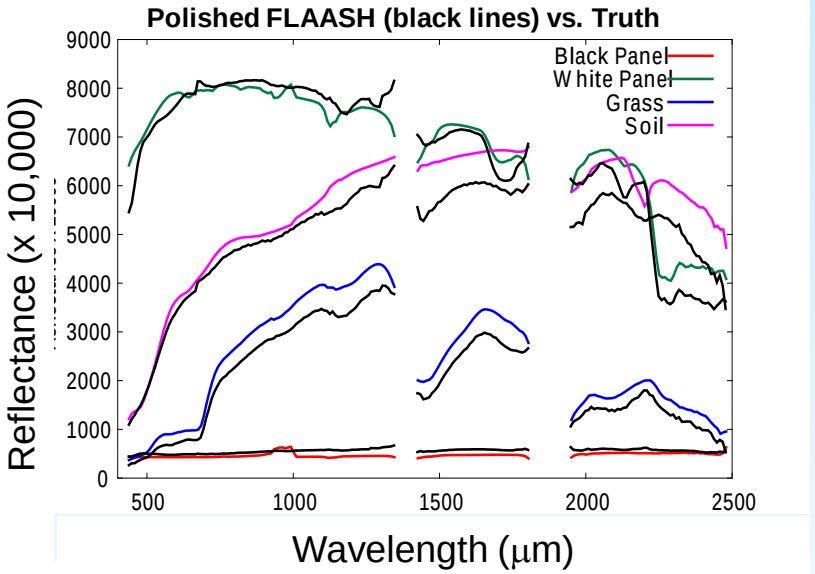


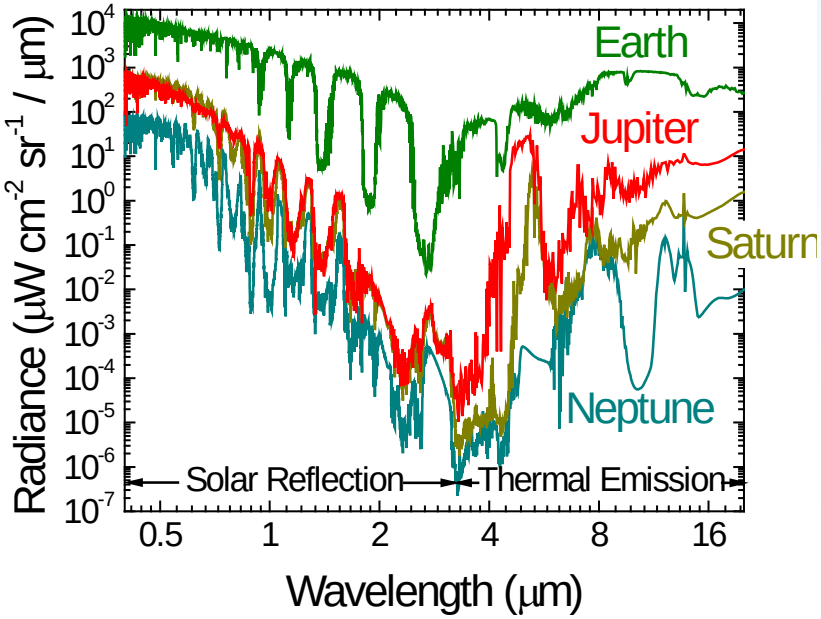
  - Stratified (1D) Molecular / Aerosol / Cloud Atmosphere
  - 2-Stream and DISORT Solar and Thermal Scattering
  - Spherical Refractive Geometry
- Many Applications Pertinent to HyspIRI
  - Sensor Design
  - Atmospheric Correction →
  - Measurement / Data Analyses
  - Scene Simulation
  - Algorithm Development
  - Today's focus:
    - *Localized chemical clouds*



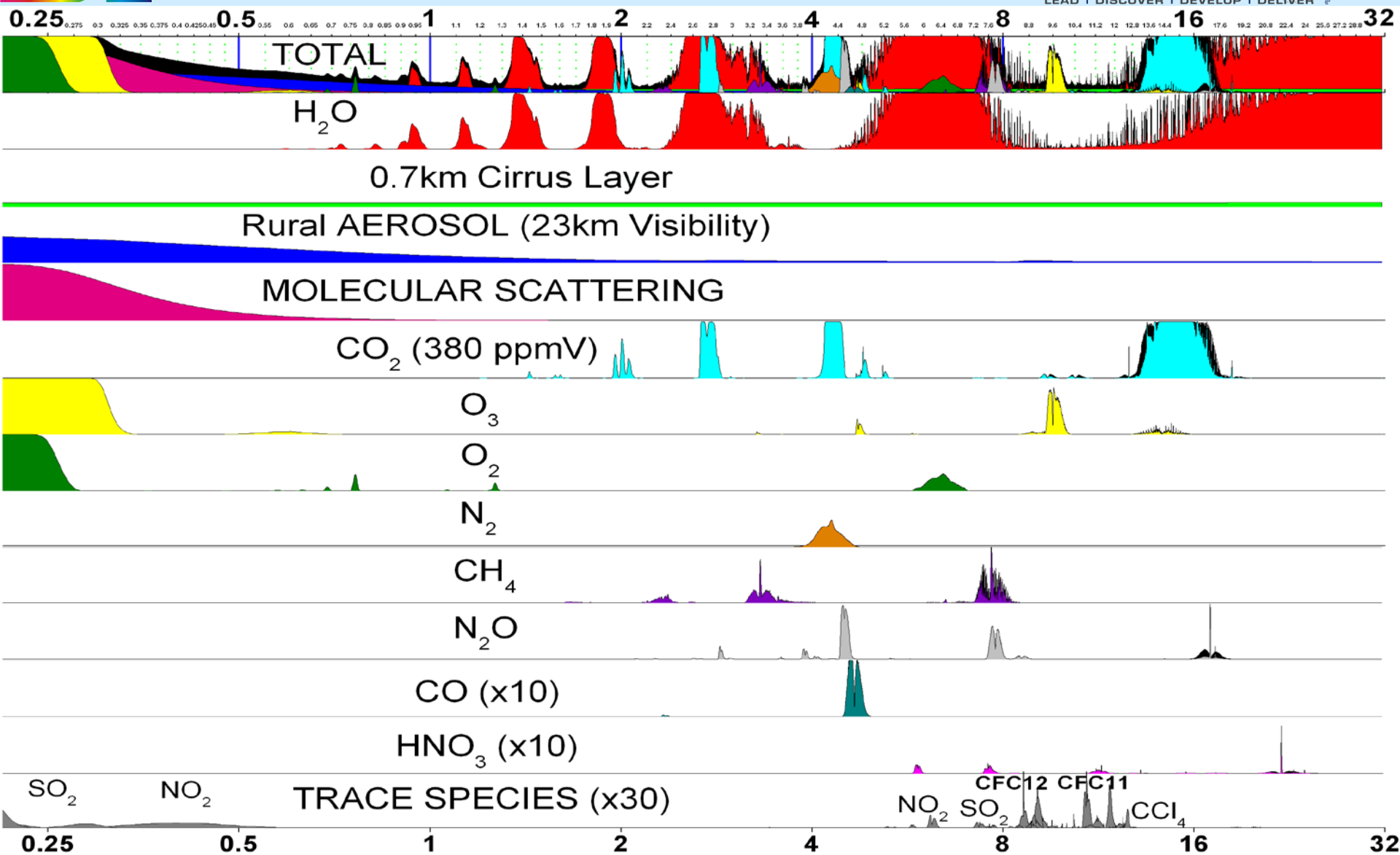
Sample MODTRAN Applications

- **FLAASH: *Fast Line-of-sight Atmospheric Analysis of Spectral Hypercubes***
  - **MODTRAN**-based atmospheric correction
  - SSI is lead developer with AFRL, NGA, NASA and SITAC collaboration & support
  - Retrieves scene visibility and pixel water vapor using 2-band methods
  - Compensates for atmospheric scattering (including adjacency effect) and absorption
  - Includes automated wavelength calibration, spectral polishing
- **PLANETS: *PLANETary Spectroscopy***
  - SSI planetary radiation transfer algorithm based on **MODTRAN5** band model
  - Validated against Jupiter, Saturn, Neptune and exoplanet spectra
    - Microwave through UV
    - Extended temperature range (5- 600K)
    - Planetary aerosol models
    - H_2-H_2, H_2-He, H_2-CH_4 and CH_4-CH_4 collision induced continua (CIA)





MODTRAN®5 Overview
Absorbance = 1 – Transmittance



What's New
- Selected Upgrades -

	MODTRAN®4	MODTRAN®5.2.0.0 / 5.2.1.0
Band Model		
Spectral Resolutions	1.0, 5.0, 15.0 cm^{-1}	… + 0.1 cm^{-1}
Voigt Transmittance	Rogers-Williams interpolation	Exact expansion
HITRAN Data	Circa 2003	2008 with 2009 H_2O Update
Constituents	First 12 HITRAN molecules	39 HITRAN2008 molecules + Auxiliary Species Option
Inputs / Outputs		
Profile Scaling Input	CO_2, H_2O, O_3	All built-in molecular profiles
Spectral Data	Direct Transmittance, Flux, (Ir)Radiance, Cooling Rates	… + Diffuse Transmittances, Spherical Albedo
Spectral Channel (chn) File	Frequency, Wavelength, Transmittance, (Ir)Radiance	… + Component Transmittances, Component (Ir)Radiances, Brightness Temperature, Surface Directional Emissivity, Top-Of-Atmosphere Solar Irradiance
General		
Configuration Control	No	SVN w/ Configuration Control Board

HyspIRI Remote Sensing of Volcanic Plumes - Vincent J. Realmuto

TQ1: How can we help predict and mitigate earthquake and volcanic hazards through the detection of transient thermal phenomena?

Do volcanoes signal impending eruptions through changes in surface temperature and gas emission rates and are such changes unique to specific types of eruptions? **[DS 227]**

→ **Map SO_2 Content of Plumes**

What are the characteristic dispersal patterns and residence times for volcanic ash clouds and how long do such clouds remain a threat to aviation? **[DS 224]**

→ **Detect Plumes and Track Positions over Time**

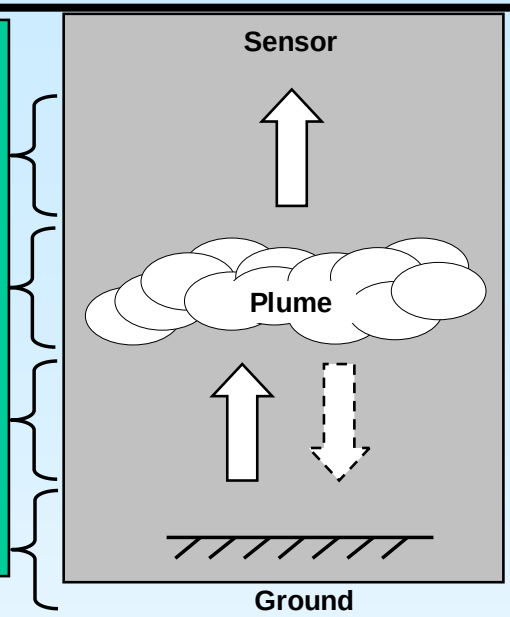
3-Slab Radiative Transfer Model

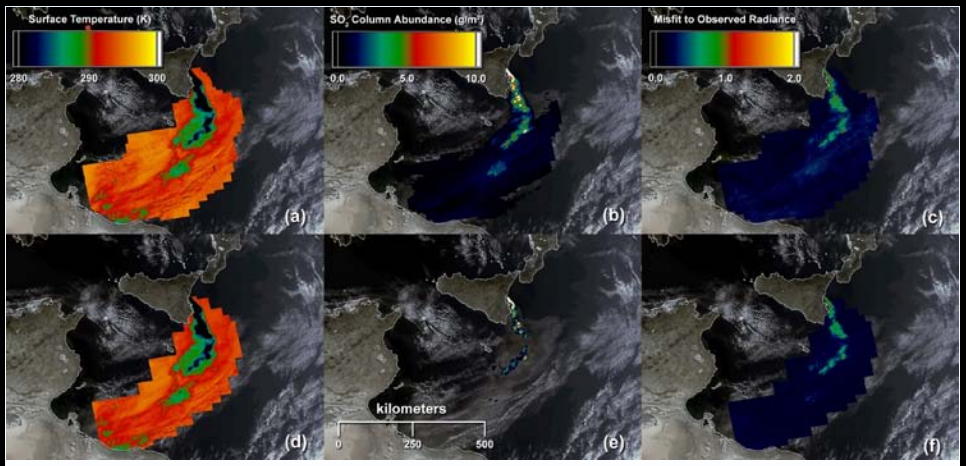
Slab 2 Radiance = $\varepsilon_3(\lambda, x_3)\, B(\lambda, T_3) + \tau_3(\lambda, x_3)$[Plume Radiance]

Plume Radiance = $\varepsilon_2(\lambda, x_2)\, B(\lambda, T_2) + \tau_2(\lambda, x_2)$[Slab 1 Radiance]

Slab 1 Radiance = $\varepsilon_1(\lambda, x_1)\, B(\lambda, T_1) + \tau_1(\lambda, x_1)$[Ground Radiance]

Ground Radiance = $\varepsilon_o(\lambda, x_o)\, B(\lambda, T_o) + [1 - \varepsilon_o(\lambda, x_o)]\, \varepsilon_1(\lambda, x_1)\, B(\lambda, T_1)$





MODIS-Based SO_2 Retrievals: 28 October 2002

Comparison of Retrievals with 5-Band (Top Row) and 4-Band (Bottom Row) Surface Temperatures

Improved Sensitivity to Low Concentrations of SO_2

Increased Influence of Water Vapor on SO_2 Estimates – Requires Better Descriptions of Atm. Water Vapor (NCEP Reanalysis or AIRS L2?)

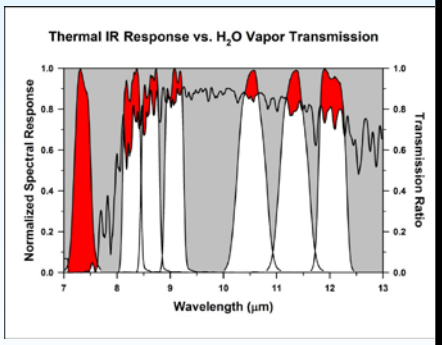
Summary Remarks

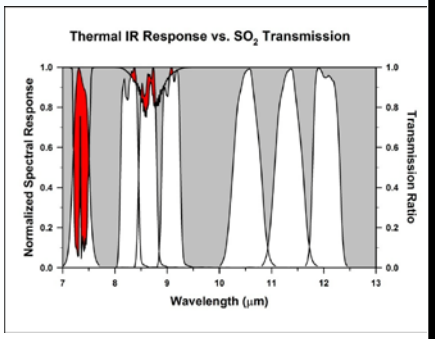
Inferior HyspIRI Results in Combined Retrieval are Counter-Intuitive
- HyspIRI Should Have More Leverage due to Higher Spectral Resolution
- More Analysis Necessary to Verify that Current Results are Repeatable

Success of H_2O Retrievals Bodes Well for Land Surface Products

In Practice, the Retrievals w/ 7.3 μm Channel have Been Problematic
- Technique Applied to MODIS and AIRS Data
- Too Much Variability in (Actual) Conditions within a Pixel? Need Increased Spatial Res?
- Restrict Application to Plumes at Altitudes >> 5 km?

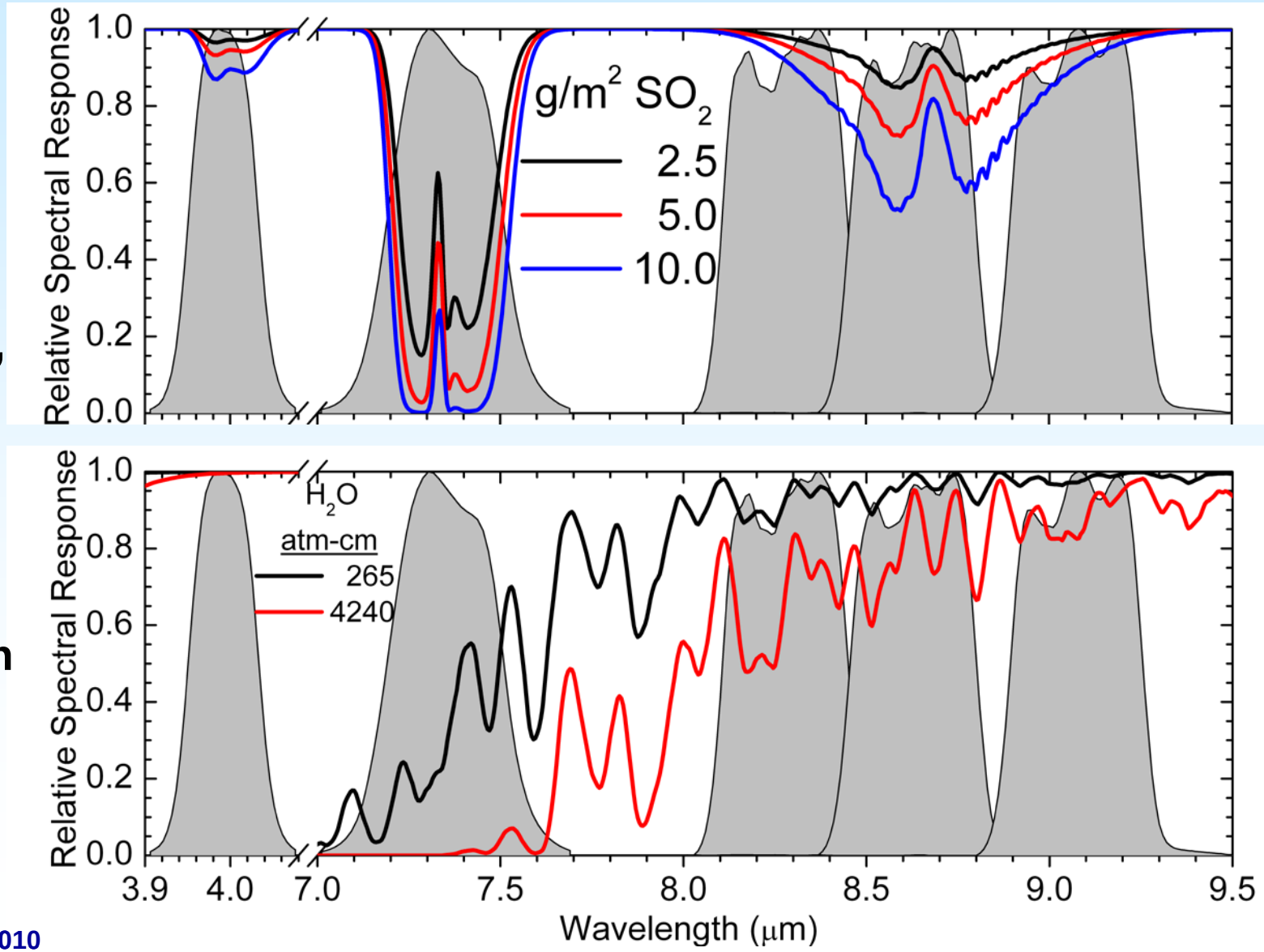
Need Channels that will not Saturate in the Presence of H_2O and SO_2
- Additional Channel Between 7.5 and 8 μm(?)
- Shift the Positions of Bands 2 and 3 to Narrow the Intervening Gap





HyspIRI Channels with SO_2 Absorption

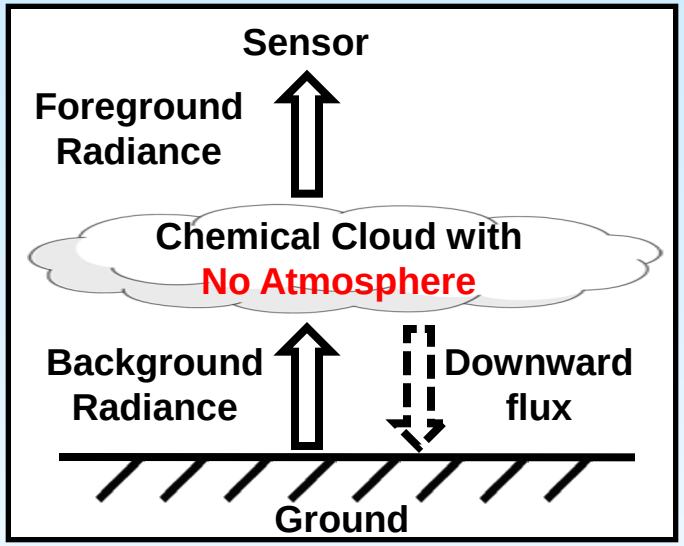
The 4μm channel, which is unaffected by H_2O absorption, contains a weak SO_2 band, and the solar scatter contribution to the radiance is significant



Modeling Chemical Clouds with MODTRAN
- Traditional Approaches -

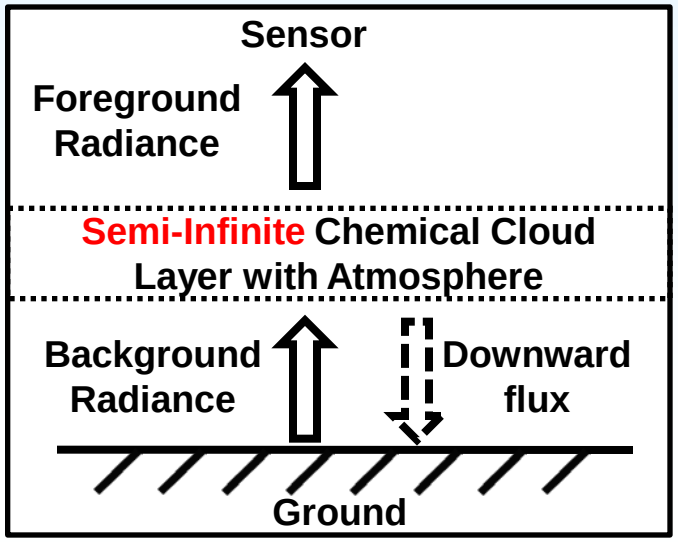
1. Model chemical cloud externally

- MODTRAN cloud-free radiances
- Offline chemical cloud transmittances and source radiances
- Neglect finite cloud thickness, i.e., that the cloud and atmosphere actually coexist
- Sufficiently accurate for many applications



2. Embed cloud layer into atmosphere

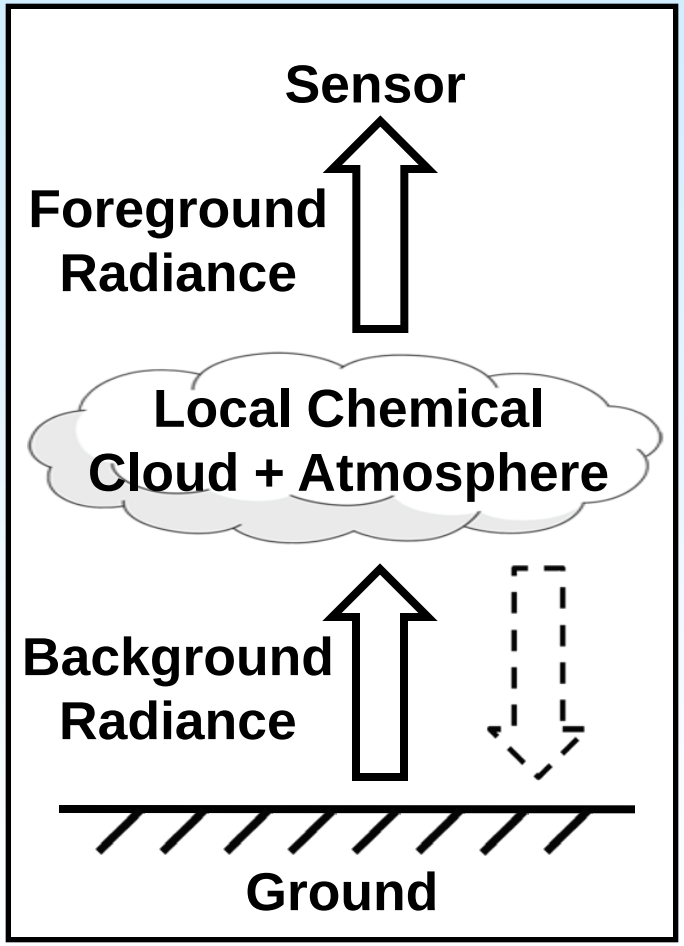
- Cumbersome to implement
- Chemical cloud modeled as semi-infinite
  - Adversely affects flux and scattered radiance calculations
- Transition region temperature gradients can cause failure of spherical refraction



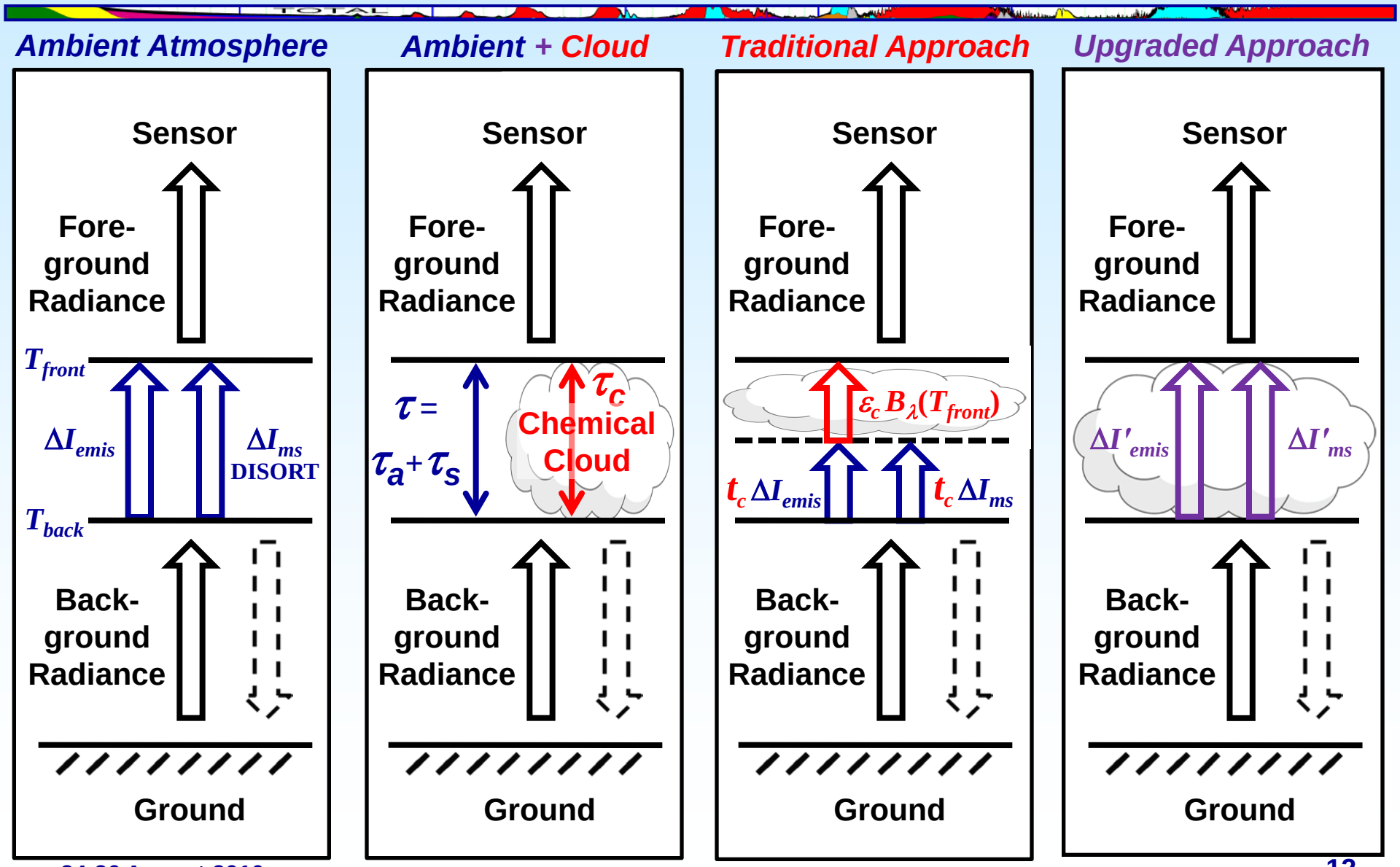
Modeling Chemical Clouds using MODTRAN
- New Local Cloud Approach -

3. Introduce a MODTRAN "*local*" chemical cloud option

- Band model data for 100's of molecules
- User-friendly cloud specification
- Line-of-sight (LOS) & solar geometries computed with cloud-free atmosphere to eliminate refractive path failures
- Radiative Transfer
  - ***Tailored treatment of chemical cloud single scatter solar radiation***
  - ***DISORT diffuse (scattered) radiance field determined from ambient atmosphere***
  - ***Chemical cloud absorption included in LOS scattered, $\Delta I'_{ms}$, and emitted, $\Delta I'_{emis}$, segment radiance calculations***
- Output cloud-free, cloud + atmosphere & contrast spectral signatures

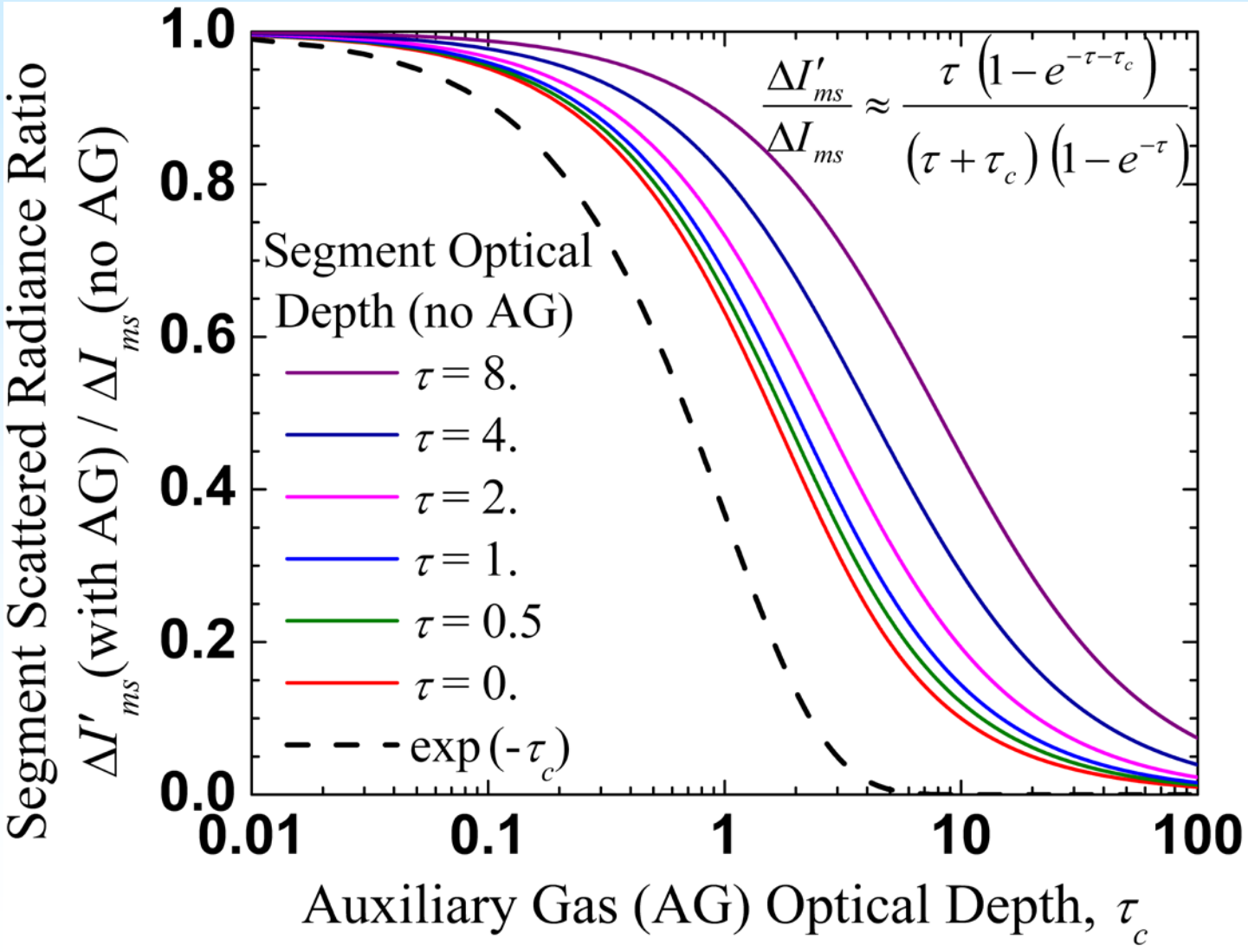


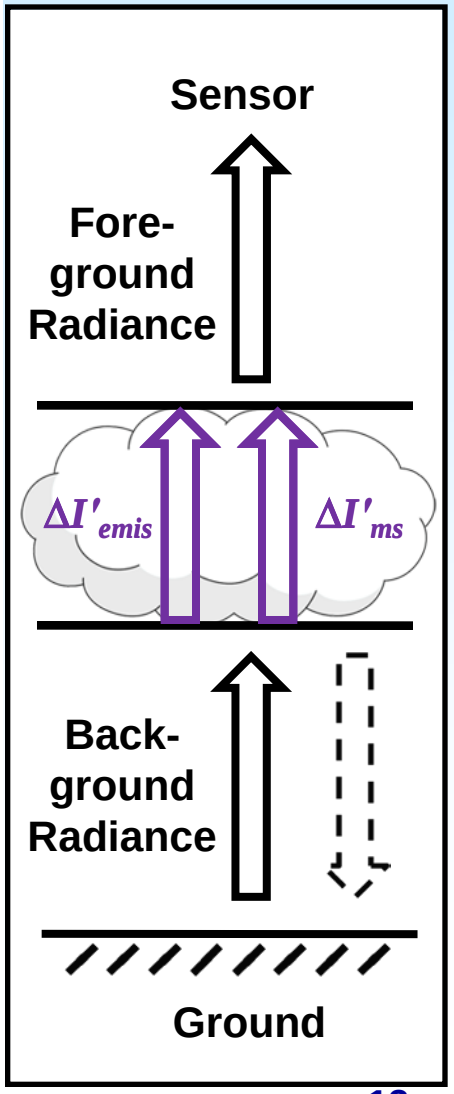
Single Layer Cloud Illustrations



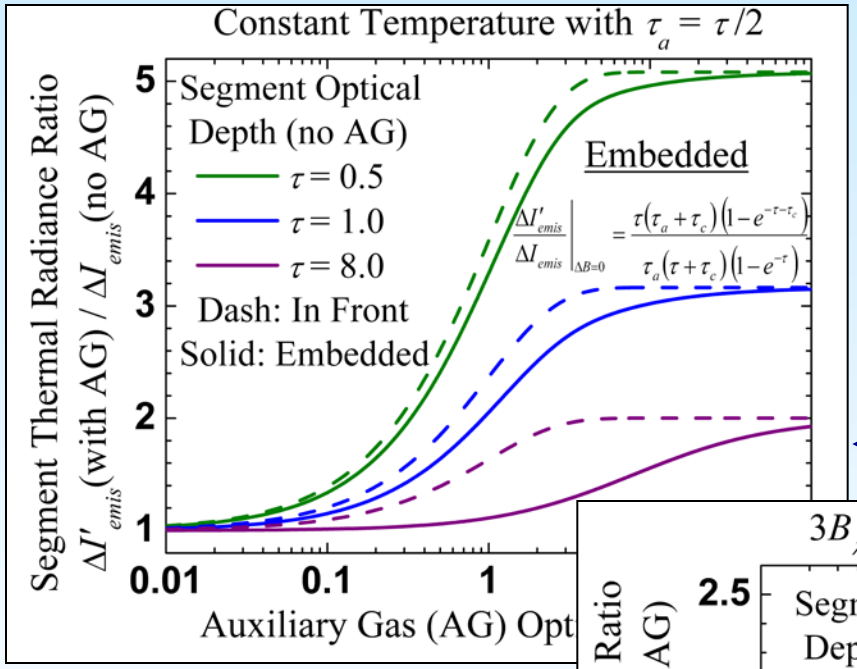
Chemical Cloud Effect on Segment Scattered Radiance

Upgraded Approach





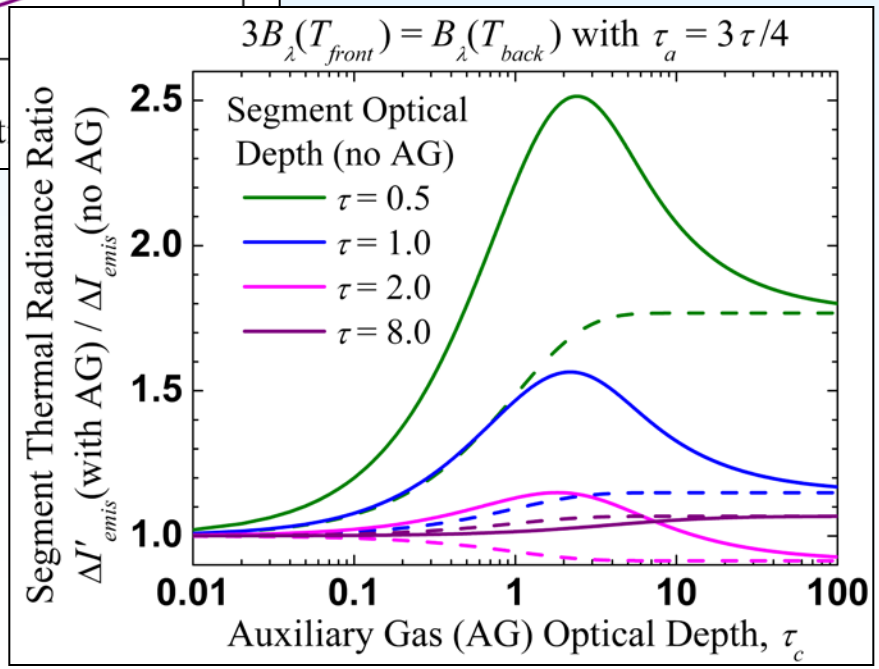
Chemical Cloud Effect on Segment Emitted Radiance



Utilize Linear-in-τ:

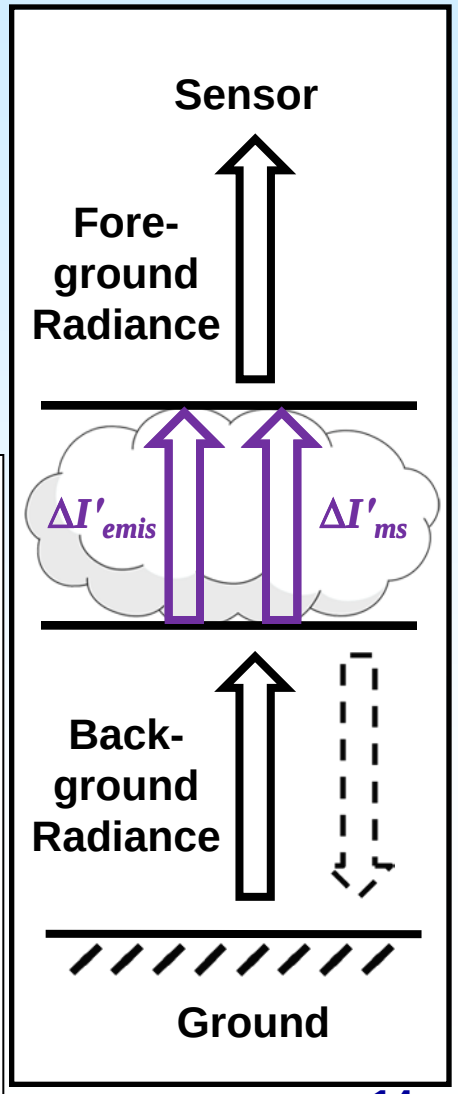
Linear variation of Planck emission with path absorption optical depth

← Isothermal Segment



Planck Emission increasing with Optical Depth, τ

Upgraded Approach



Summary

- **MODTRAN®5.2 has been available since June 2009**
  - **The model provides major enhancements over MODTRAN4**
  - **Can serve as an important tool for NASA and HyspIRI program**
- **MODTRAN is designed for broad range of applications**
  - **Code developers (SSI / AFRL) provide support as needed**
  - **Presentation focused on modeling of local chemical cloud**
    - **New option includes radiative coupling of atmosphere + cloud**
      - **Being developed for DOE**
      - **Work in progress: MODTRAN upgrade will be complete by 30sep2010**
    - **Designed to provide user-friendly inputs, an extensive chemical database, and state-of-the-art radiative transfer**
    - **Year 2 will focus on verification (MCScene and DIRSIG 3D modeling) and validation (measurement comparisons)**

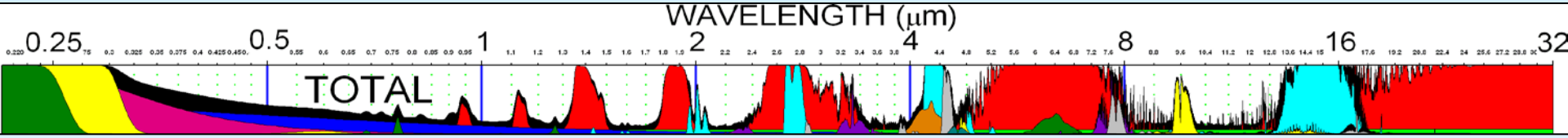
MODTRAN5 Distribution

- MODTRAN®5.2 is available for license at **www.modtran.org**
  - Developed, maintained and validated by SSI and AFRL
  - Distributed for SSI by Ontar Corporation
  - Government Use 'price' covers code distribution, maintenance and limited customer support costs
- An End User License Agreement (EULA) is required
  - States license terms of use, limits on re-distribution (3 users at a single site)
  - A single copy EULA can be accepted electronically during online purchase
  - Many organization legal departments require review and minor modifications
- Customized license agreements can be developed with SSI for
  - Site licenses (>7 user group at a single location),
  - Enterprise/embedded code licenses,
  - Contractor operated Government facilities licenses,
  - University and State government agency licenses,
  - Educational classroom use licenses,
  - Etc.

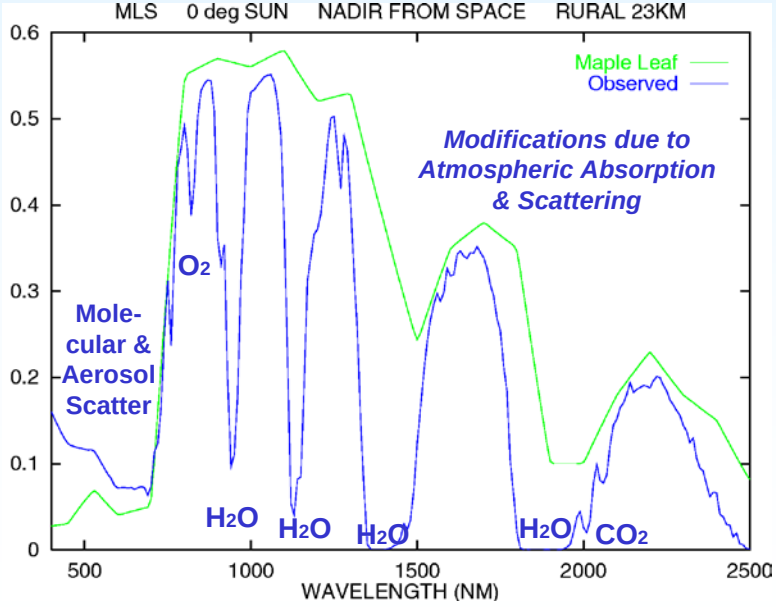
Back ups

MODTRAN5 Overview
- General Description -

- IR / Vis / UV Transmittances, Radiances and Fluxes
  - Up to 0.2 cm^{-1} Spectral Resolution from 0.1 cm^{-1} Band Model



- Stratified Molecular / Aerosol / Cloud Atmosphere
  - Built-in, Auxiliary & User-Specified Molecules and Particulates
- 2-Stream and DISORT Solar and Thermal Scattering
  - Diffuse Transmittance and Spherical Albedo for Atmosphere Correction →
- Spherical Refractive Geometry
- Spectral Convolution & Filtering
- Many Applications Pertinent to HyspIRI
  - Sensor Design, Atmospheric Correction, Measurement / Data Analyses, Scene Simulation, Algorithm Development, …
  - Today's focus: Localized chemical clouds



What's New

	MODTRAN®4	MODTRAN®5.2.0.0 / 5.2.1.0
Band Model		
Spectral Resolutions	1.0, 5.0, 15.0 cm^{-1}	… **+** 0.1 cm^{-1}
Voigt Transmittance	Rogers-Williams interpolation	Exact expansion
Line Tail Model	Constant within spectral bin	Spectra fit to Padé Approximants
Line Center Model	One (S/d, 1/d) pair	… **or** Two (S/d, 1/d) pairs
HITRAN Data	Circa 2003	2008 with 2009 H_2O Update
Constituents	First 12 HITRAN molecules	39 HITRAN2008 molecules **+** Auxiliary Species Option
Temperature Range	180K to 305K	180K to 330K
Correlated-*k* Algorithm		
Number of *k*'s	33 (slow) or 17 (medium)	… **w/** Adaptive Reduction to 4 or 1
Convergence	Rare Failures	No Failures (to date)
DISORT Scattering		
Max Streams No.	16	32 or Increase Parameter MI
Solar Zenith	Most Angles < 90°	Any Angles < 90°

What's New

	MODTRAN®4	MODTRAN®5.2.0.0 / 5.2.1.0
Inputs		
Temperature Profile	Model Atmosphere, User Defined	… **or** Model Atm. Perturbation
Water Profile	Model Atm. Density, User Defined	… **or** Model Atm. Relative Humidity
Profile Scaling	CO_2, H_2O, O_3	All built-in molecular profiles
Outputs		
Format	ASCII	… **or** Binary
Spectral Data	Direct Transmittance, Flux, (Ir)Radiance, Cooling Rates	… **+** Diffuse Transmittances, Spherical Albedo
Radiance Modes	Thermal only, Thermal and Solar	… **+** Solar Only
Primary (tp6) Output File	General Information, Spectral Data, and In-Band Cooling Rates	… **or** General Information Only **or** File Not Generated
Spectral Data (tp7,7sc) Files	Frequency, Wavelength, Component Transmittances, Component (Ir)Radiance	… **+** Brightness Temperature, Surface Directional Emissivity, Top-Of-Atmosphere Solar Irradiance
Spectral Channel (chn) File	Frequency, Wavelength, Transmittance, (Ir)Radiance	… **+** Component Transmittances, Component (Ir)Radiances, Brightness Temperature, Surface Directional Emissivity, Top-Of-Atmosphere Solar Irradiance

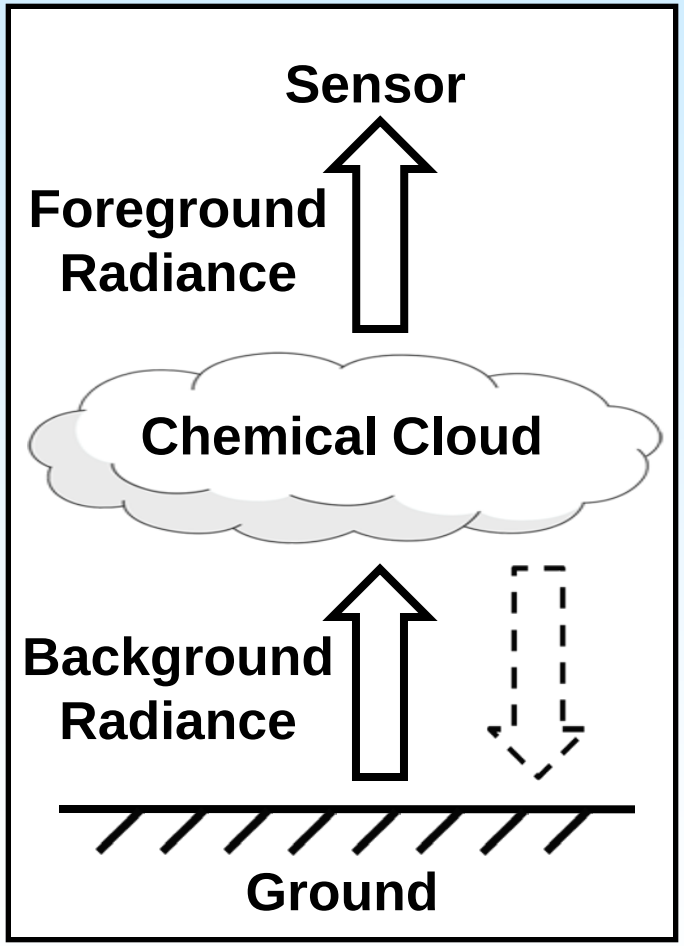
What's New

	MODTRAN®4	MODTRAN®5.2.0.0 / 5.2.1.0
Optical Data		
Molecular Cross-Sections	13 CFC species	… + O_2O_2 Visible Absorbance + Auxiliary Species Option
User Defined Aerosols	Spectral Tables (no data checking)	Spectral Tables (with data checking) or Angstrom Law Inputs
Cloud	Built in Model Clouds	… + Mie Water/Ice Data Table
Surface Reflectance	Spectral Albedo, Spectral BRDF	… w/ Surface liquid water
Geometry		
Refraction	Based on Band Central Frequency	… or User-Defined Frequency
General		
Configuration Control	No	SVN w/ Configuration Control Board
Multiple Runs	Repeat Run from Single Input File	… + Multiple Input File Capability
Test Cases	27 sample inputs	58 sample inputs
Bug Fixes (See Readme)		

Modeling Chemical Clouds using MODTRAN

1. Model chemical cloud externally

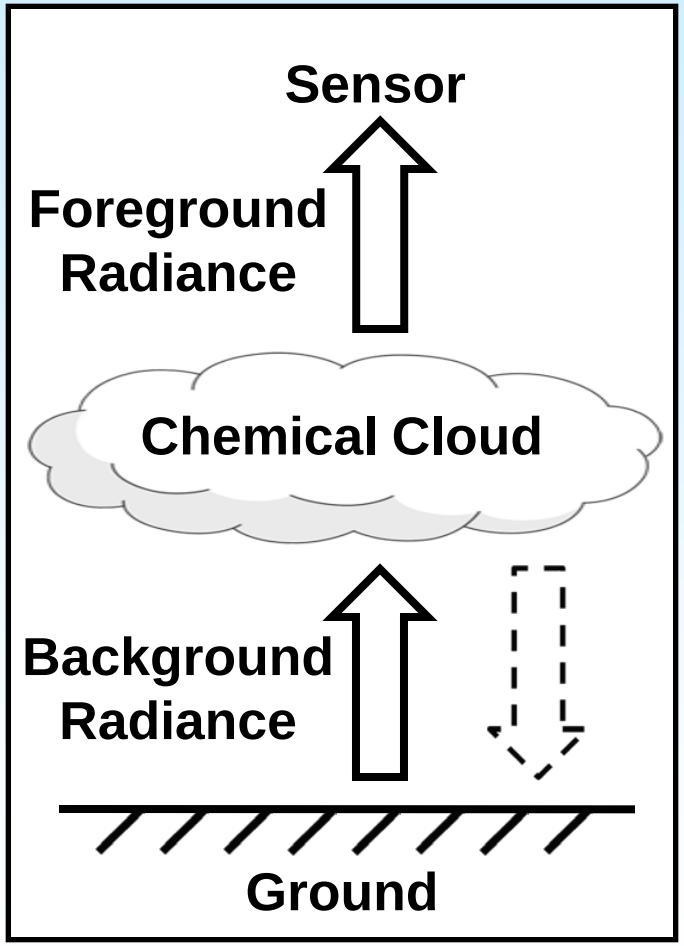
- Cumbersome and Labor Intensive
  - Run MODTRAN to compute foreground + background and foreground radiances
  - Compute chemical cloud transmittance and source radiance offline
  - Spectrally combine components
- Neglects mixing of chemical cloud and atmosphere
  - Approximate treatment of radiative spectral correlations
  - Approximate treatment of emission and scattering radiance components
- Sufficiently Accurate for many applications



Modeling Chemical Clouds using MODTRAN

2. Embed chemical cloud stratified layers into atmosphere

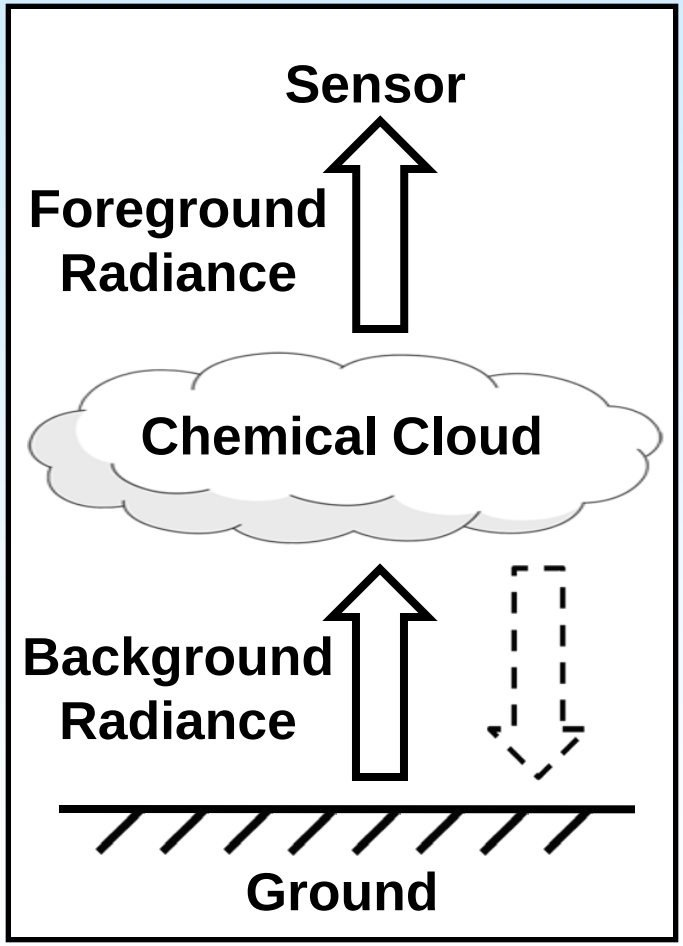
- Cumbersome to implement
  - Relaying often necessary for each LOS
  - Difficult to scale column densities
- Chemical cloud modeled as semi-infinite
  - Unintended perturbation of scattered radiance calculations
  - Unintended perturbation of vertical flux calculations
- Large vertical temperature gradients can arise within the chemical cloud to ambient atmosphere transition regions
  - *Spherical refraction geometry algorithm can fail*!



Modeling Chemical Clouds using MODTRAN

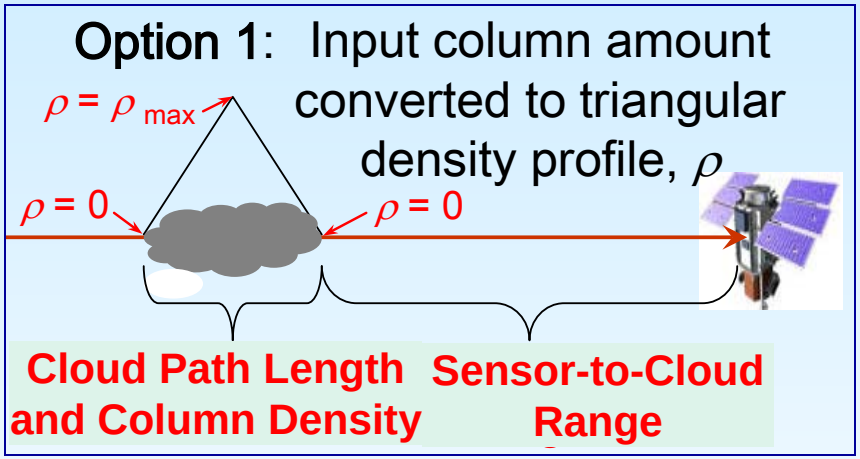
3. Introduce a MODTRAN "*local*" chemical cloud option

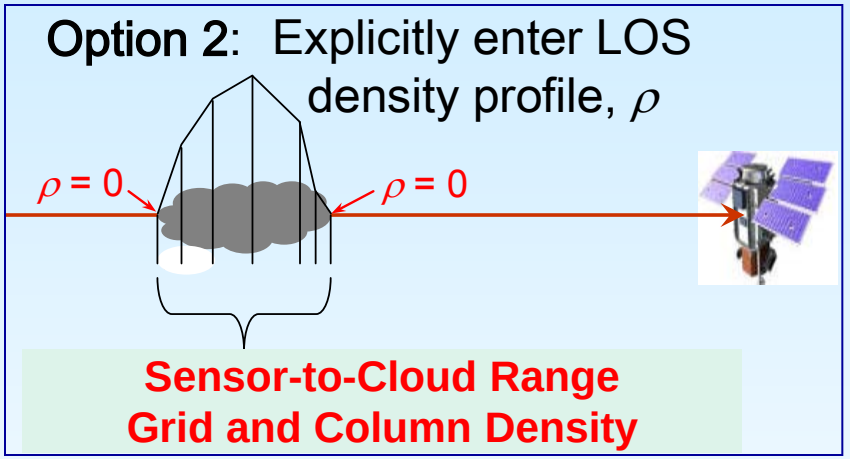
- Band model data for 100's of molecules
- User-friendly cloud specification
- Path geometry without chemical cloud
  - Eliminates refractive algorithm failures
  - Insures contrast signature paths match
- Radiative Transfer
  - Single scatter solar illumination paths attenuated by chemical cloud only for altitude levels containing cloud
  - ***Chemical cloud excluded from DISORT scattered radiance field calculation***
  - **Chemical cloud absorption effects on line-of-sight (LOS) radiance are modeled**
  - Output of cloud-free, cloud + atmosphere and contrast spectral signatures



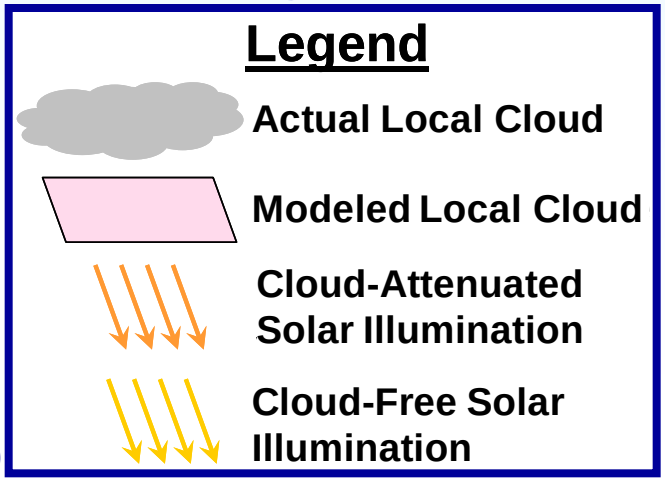
MODTRAN Local Chemical Cloud Option

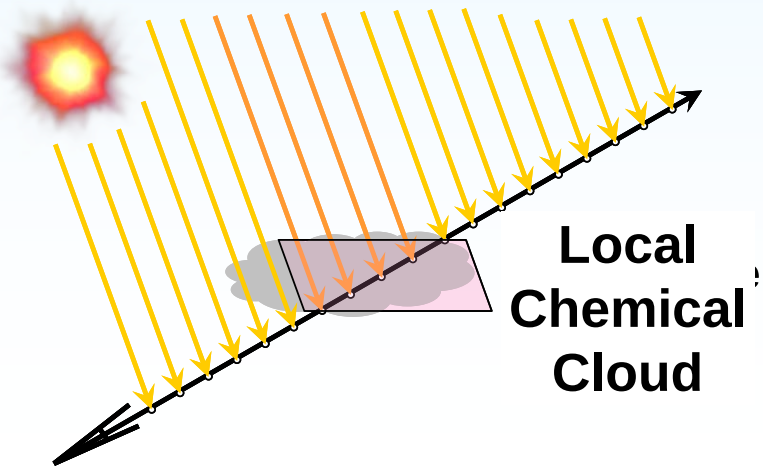
User-friendly chemical cloud specification



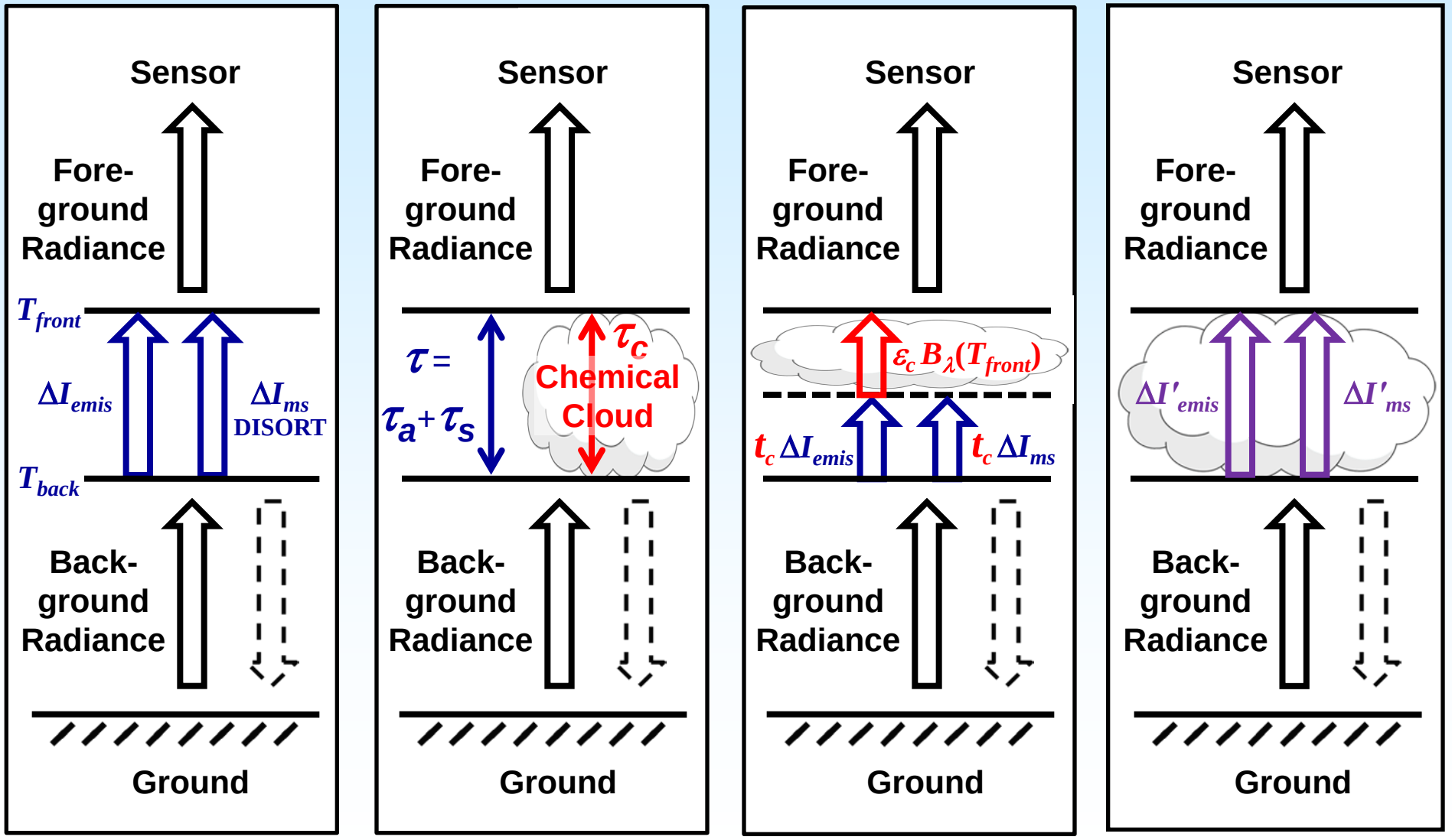


Single scatter solar illumination paths attenuated by chemical cloud only for altitude levels containing cloud



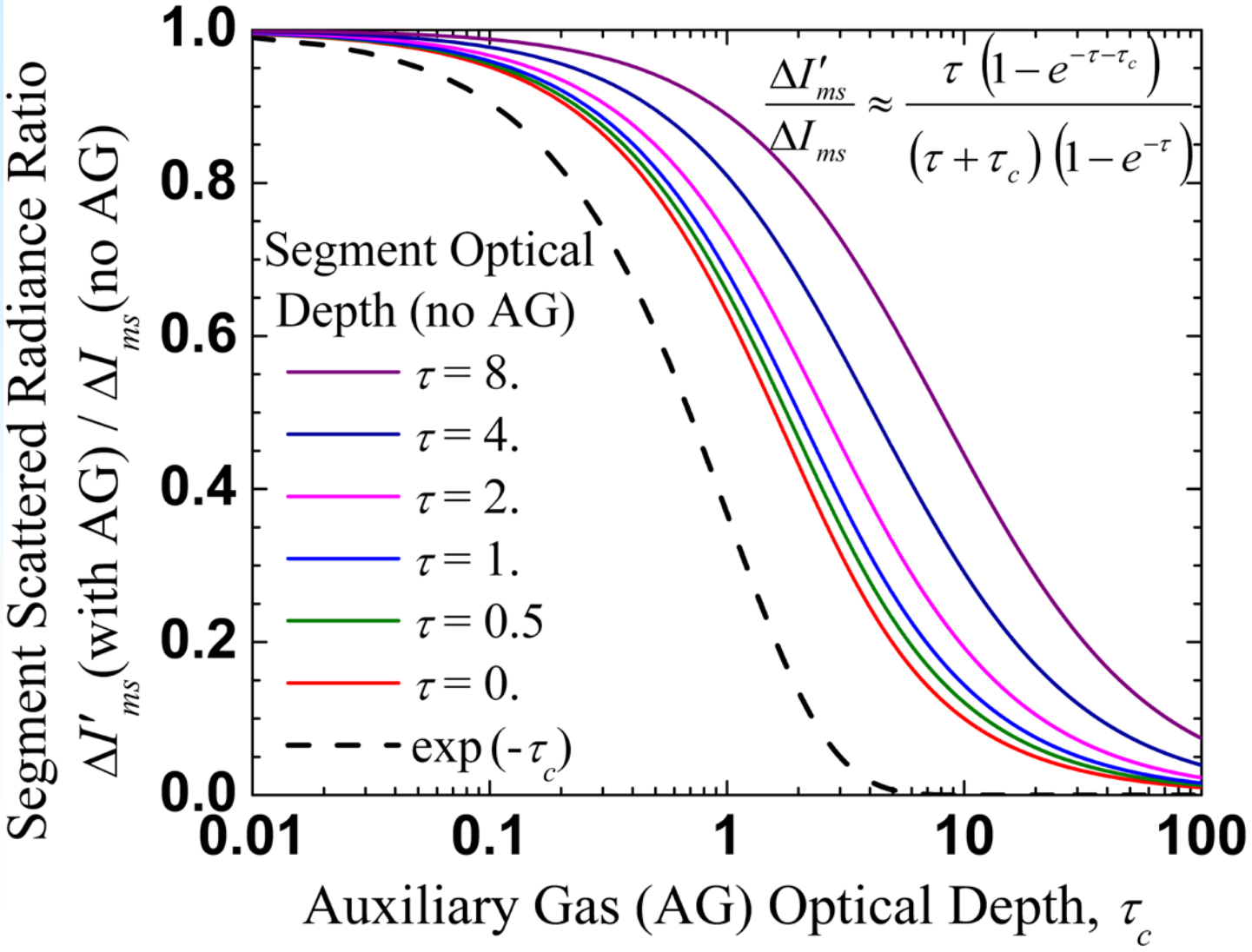


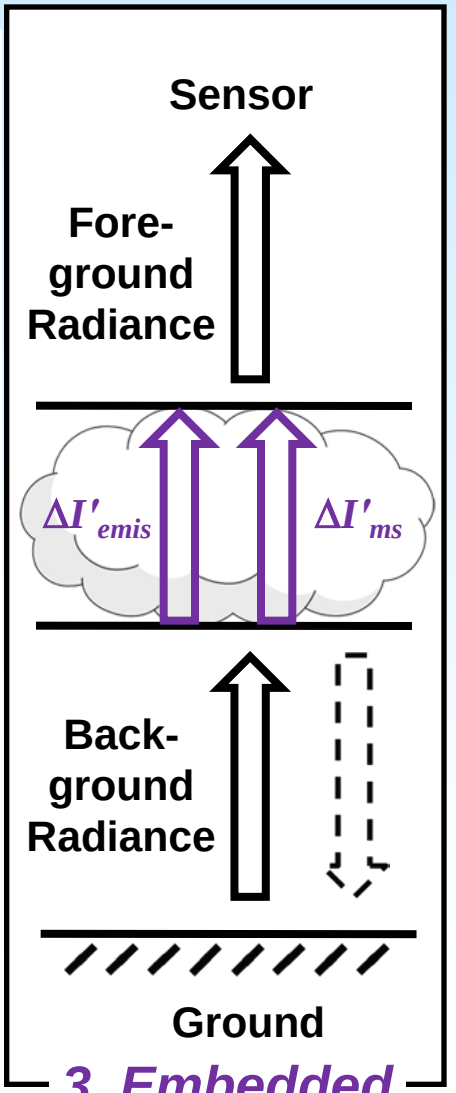
Single Layer Cloud Illustrations



No Cloud **1. External Cloud** **3. Local Cloud**

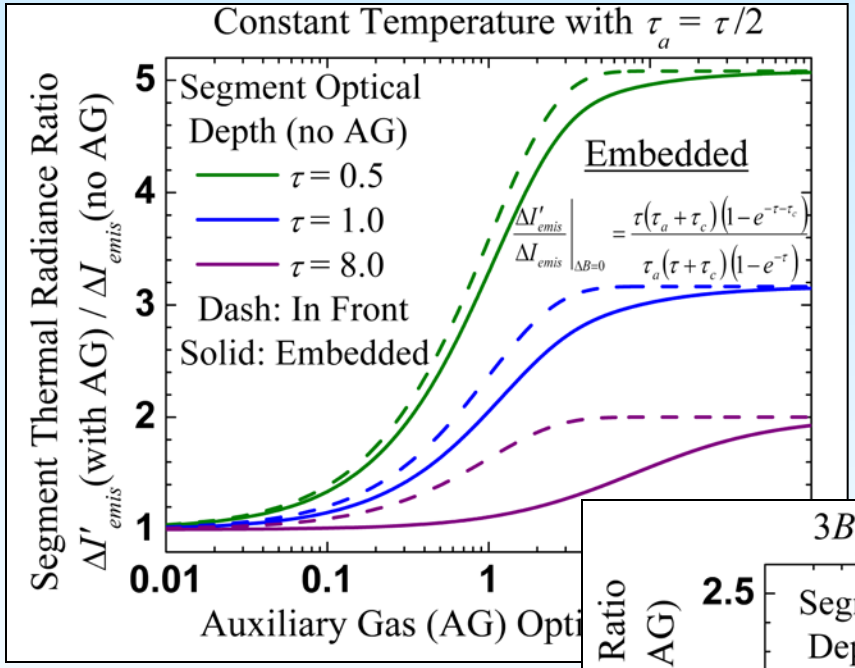
Chemical Cloud Effect on Segment Scattered Radiance





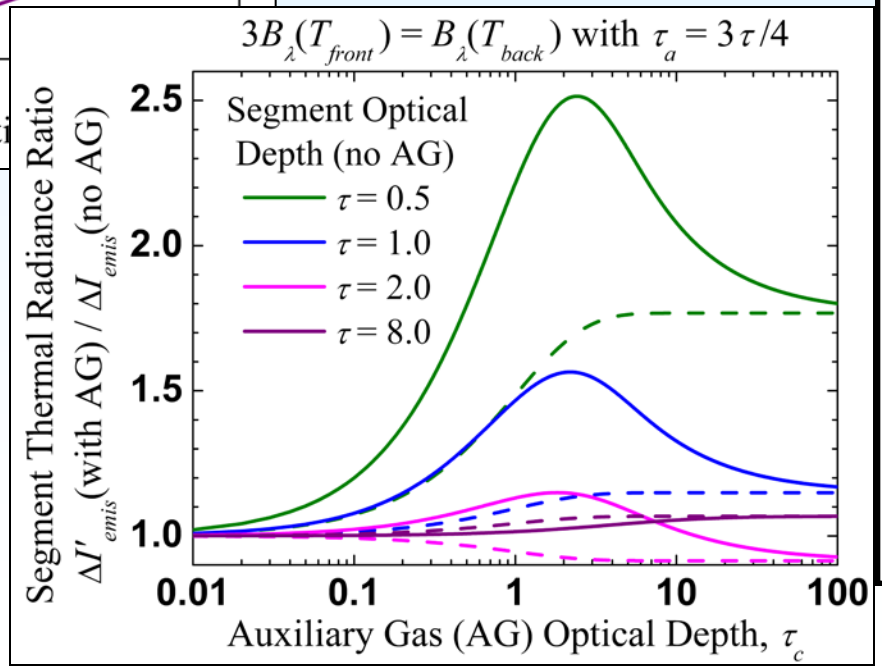
3. Embedded Local Cloud

Chemical Cloud Effect on Segment Emitted Radiance

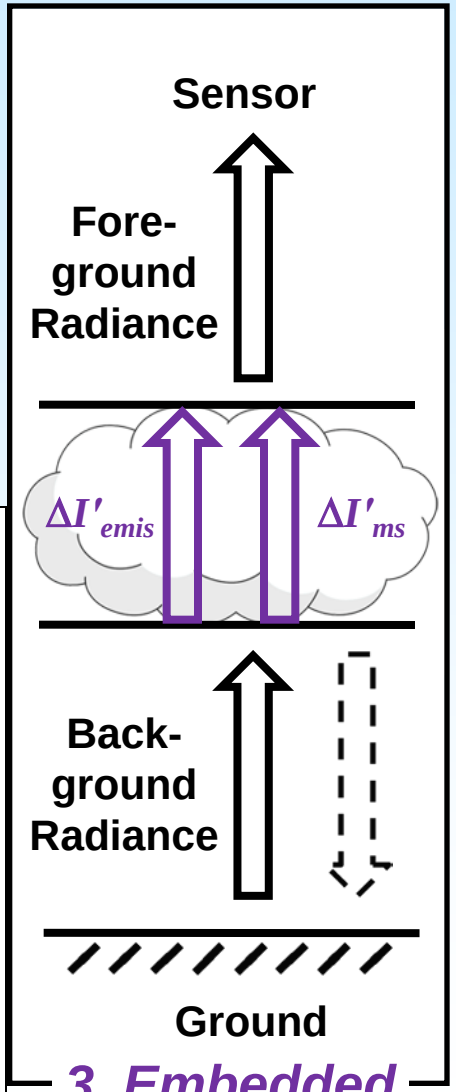


Utilizing Linear-in-τ Approach

Isothermal Segment



Planck Emission Increasing with Optical Depth, τ



3. Embedded Local Cloud