Relevance of Radiative Transfer Model in Physical Inversion

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Outline of the Presentation

1. Requirements on radiative transfer model for physical inversion
2. Overview of radiative transfer calculation in inhomogeneous atmosphere
3. Calculation of Analytical Jacobians
4. Transformation of variables using EOFs before physical inversion
5. Overview of how to model channel radiances
6. Application of OSS forward model to CrIS and NAST-I instruments
7. Conclusions

What is an idea Fast Radiative Transfer Model for Physical Inversion

$$R = F(x) + \varepsilon \qquad \delta R = K \delta x$$

- **Accurate**
  - Idea if the accuracy relative to LBL is controllable
- **Physical parameterization**
  - Accuracy and physical parameterization is closely coupled
  - Use least non-physical assumption
- **Fast**
  - Modern computer technology can accommodate large model parameters
  - ILS (SFR) convolution should be done during the training
- **Perform RT calculation monochromatically**
  - Calculates Jacobian efficiently
  - Calculates downwelling radiances efficiently
  - Be able to handle multiple scattering
- **Treat Planck function and surface properties properly**
  - Be able to model non-localized instrument line shape function efficiently
- **Train the forward model under variety of conditions**
  - Be able to handle variable observation altitude for aircraft instrument

Radiative Transfer Equation for Infrared Spectral Region

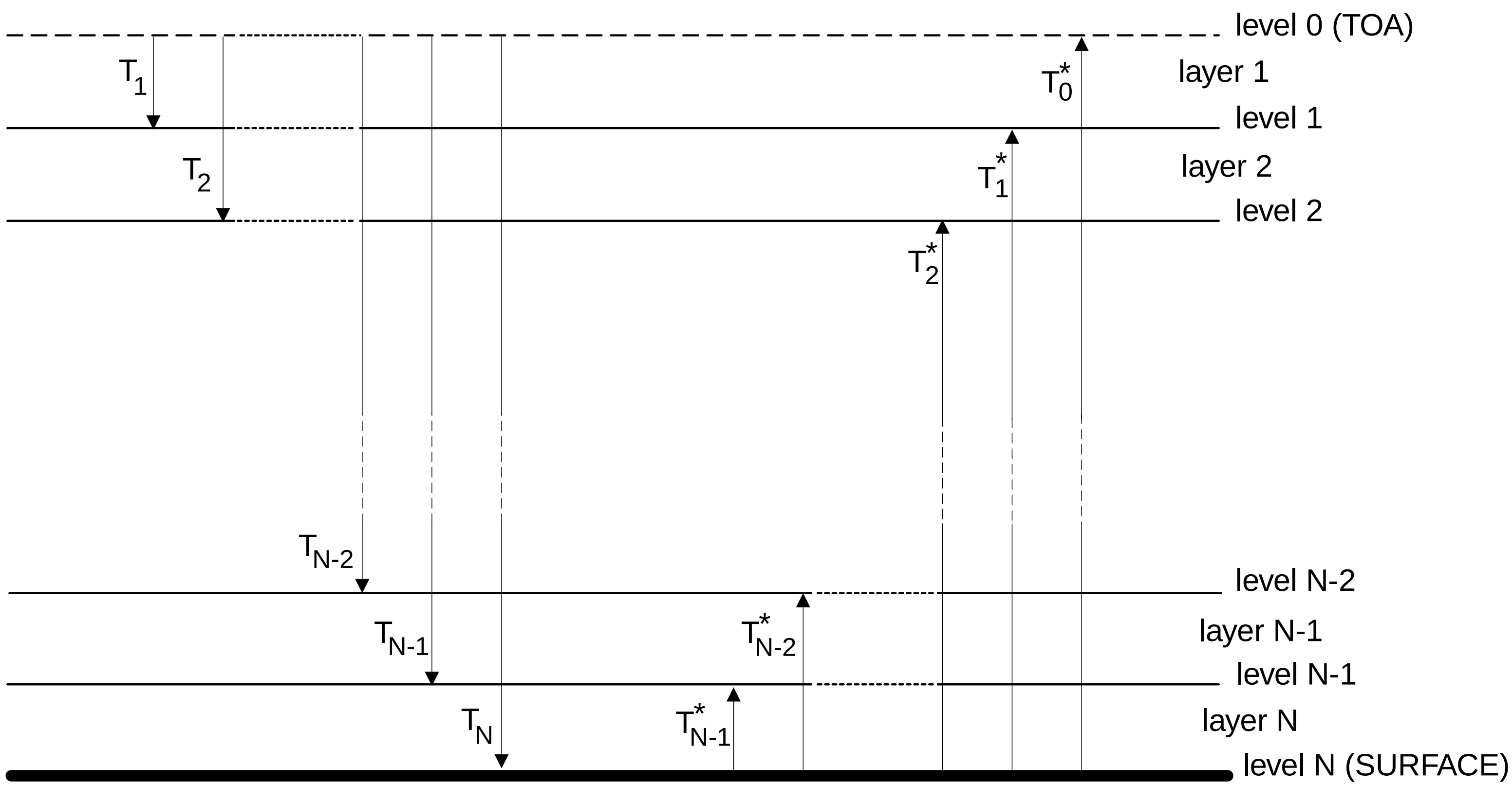
$$R_\nu \cong \varepsilon_\nu B_\nu(\Theta_s) T_{s,\nu} + \int_{p_s}^{0} B_\nu(\Theta(p)) \frac{\partial T_\nu(p,\theta_u)}{\partial p} dp$$

$$+ (1-\varepsilon_\nu) T_{s,\nu} \int_{0}^{p_s} B_\nu(\Theta(p)) \frac{\partial T_\nu^*(p,\theta_d)}{\partial p} dp + \rho_\nu T_{s,\nu} T_\nu(p_s, \theta_{sun}) F_{0,\nu} \cos\theta_{sun}$$

- **The first term is the surface emission**
- **The second term is the upwelling thermal emssion**
- **The third term is the reflected downwelling radiation**
- **The last term is the reflected solar radiation**

Defining Atmospheric Layering

- **Schematic for atmospheric layer convention**



Recursive Radiative Transfer Calculations

$$R_\nu = \sum_{i=1}^{N} (T_{\nu,i-1} - T_{\nu,i}) B_{\nu,i}^{+} + \varepsilon_{\nu s} T_{\nu,N} B_{\nu,s}^{+} + (1-\varepsilon_{\nu s}) T_{\nu,N} \sum_{i=1}^{N} (T_{\nu,i}^{*} - T_{\nu,i-1}^{*}) B_{\nu,i}^{-}$$
$$+ \rho_s T_{\nu,N} T_{sun}(p_s, \theta_{sun}) F_{0,\nu} \cos\theta_{sun}$$

If we define: $T_{\nu,l}^{'} = (1-\varepsilon_{\nu s}) T_{\nu,N} T_{\nu,l}^{*}$

$$R_\nu = B_{\nu,i}^{+} \sum_{i=1}^{N} (T_{\nu,i}^{'} - T_{\nu,i-1}^{'}) + \varepsilon_{\nu s} T_{\nu,N} B_{\nu,s}^{+} + B_{\nu,i}^{-} \sum_{i=N}^{1} (T_{\nu,i-1} - T_{\nu,i})$$
$$+ \rho_s T_{\nu,N} T_{sun}(p_s, \theta_{sun}) F_{0,\nu} \cos\theta_{sun}$$

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Calculation of Analytical Jacobians

$$\tau_l^0 = \tau_{fix}(\bar{p}_l,\Theta_l) + [k_{H2O}(\bar{p}_l,\Theta_l) + k_{H2O}^{self}(q_{H2O},\Theta_l)\omega_{H2O}]\omega_{H2O} + k_{O3}(\bar{p}_l,\Theta_l)\omega_{O3} + \ldots\ldots$$

$$T_l = \exp\left(-\sum_{i=1}^{l}\tau_i^0 \sec\theta_{obs}\right)$$

$$T_l^* = \exp\left(-\sum_{i=l+1}^{N}\tau_i^0 \sec\theta_d\right)$$

$$\frac{\partial R}{\partial X_l} = \frac{\partial R}{\partial \tau_l^0}\frac{\partial \tau_l^0}{\partial X_l} + \frac{\partial R}{\partial B_l}\frac{\partial B_l}{\partial X_l}$$

$$\frac{\partial T_i}{\partial \tau_l^0} = \begin{cases} -T_i \sec\theta_{obs} & i \ge l \\ 0 & i < l \end{cases}$$

$$\frac{\partial T_i^*}{\partial \tau_l^0} = \begin{cases} -T_i^* \sec\theta_d & i < l \\ 0 & i \ge l \end{cases}$$

$$\frac{\partial R}{\partial X_l} = -\frac{\partial \tau_l^0}{\partial X_l}\left\{\left[-T_l B_l^+ + \sum_{i=l+1}^{N}(T_{i-1}-T_i)B_i^+ + T_N\varepsilon_s B_s^+ + \sum_{i=1}^{N}(T_i^{'}-T_{i-1}^{'})B_i^-\right]\sec\theta_{obs}\right.$$
$$\left. + \left[-(1-\varepsilon_s)T_N T_{l-1}^* B_l^- + \sum_{i=1}^{l-1}(T_i^{'}-T_{i-1}^{'})B_i^-\right]\sec\theta_d - R_{sol}(\sec\theta_{obs} + \sec\theta_{sun})\right\}$$
$$+ \frac{\partial B_l^+}{\partial X_l}(T_{l-1}-T_l) + \frac{\partial B_l^-}{\partial X_l}(T_l^{'}-T_{l-1}^{'})$$

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Calculation of Jacobians

$$\frac{\partial R}{\partial \Theta_l} = \frac{\partial R}{\partial \tau_l^0}\frac{\partial \tau_l^0}{\partial \Theta_l} + \frac{\partial R}{\partial \overline{B}}\frac{\partial \overline{B}}{\partial \Theta_l} \cong \frac{\partial \overline{B}_l}{\partial \Theta_l}(T_{l-1} - T_l) + \left[\frac{\partial R}{\partial \Theta_l}\right]_d$$

δτ/δΘ can be calculated from the lookup table easily

$$\frac{\partial R}{\partial \overline{B}}\frac{\partial \overline{B}}{\partial \Theta_l} = \frac{\partial \overline{B}_l}{\partial \Theta_l}(T_{l-1} - T_l) + \frac{\partial \overline{B}_l}{\partial \Theta_l}(T_l^{'} - T_{l-1}^{'})$$

$$\frac{\partial R}{\partial \omega_l^m} = \frac{\partial R}{\partial \tau_l^0} \times k_l^m, \quad m = 1,\ldots,M$$

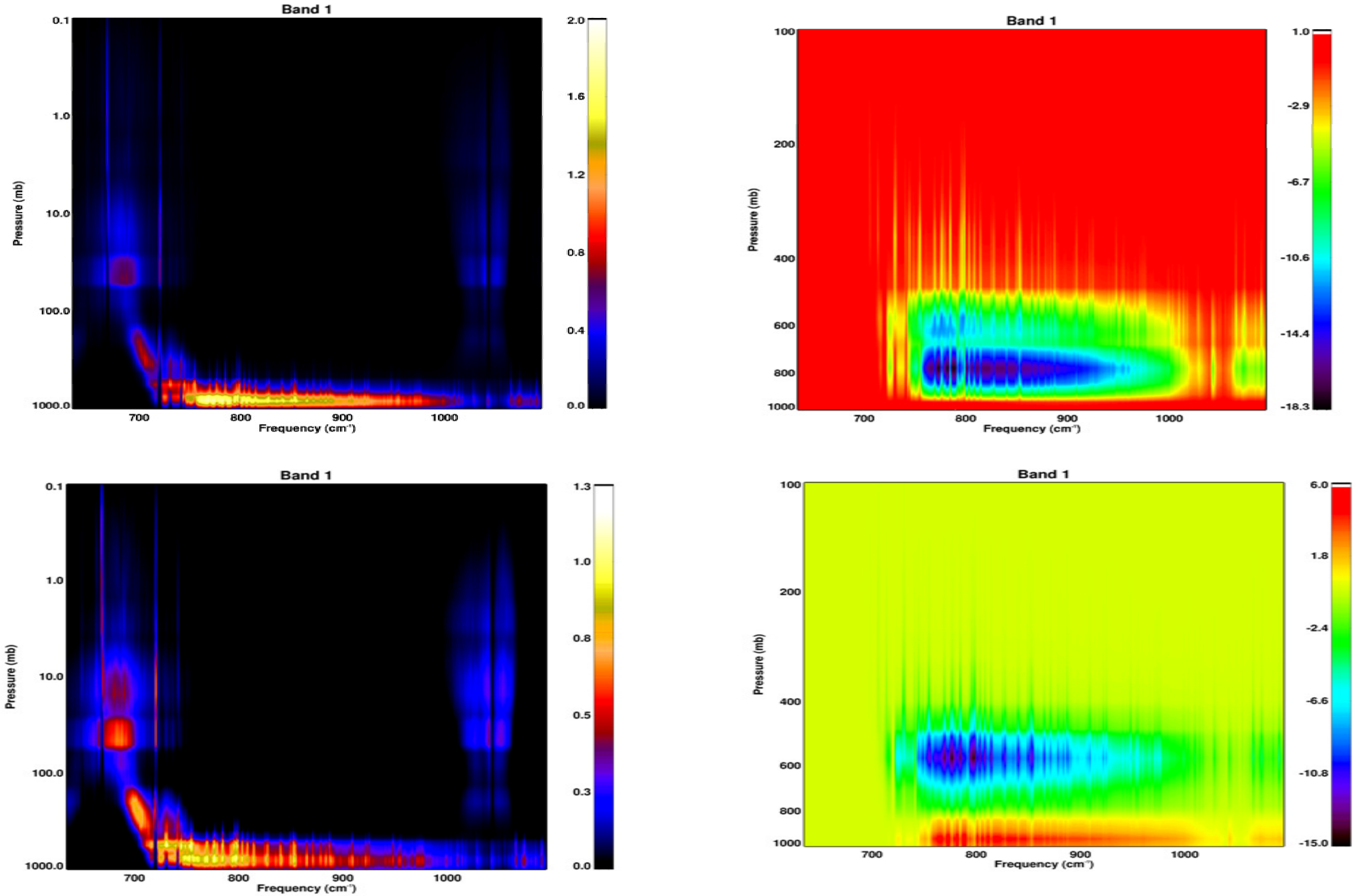
$$\frac{\partial R}{\partial \tau_l^0} = (-\Sigma_l^+ + \overline{B}_l T_l)\sec\theta_{obs} + \left[\frac{\partial R}{\partial \tau_l^0}\right]_d + \frac{\delta R_{sol}}{\partial \tau_l^0}$$

$$\frac{\partial R}{\partial \Theta_s} = T_N \varepsilon_s \frac{\partial B_s}{\partial \Theta_s}$$

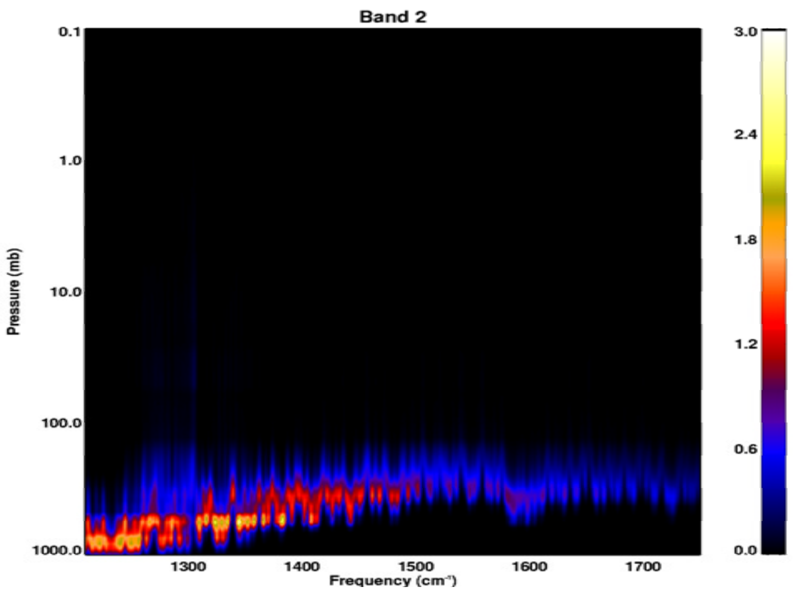
$$\frac{\partial R}{\partial \varepsilon_s} = T_N B_s - \Sigma_N^- / (1 - \varepsilon_s)$$

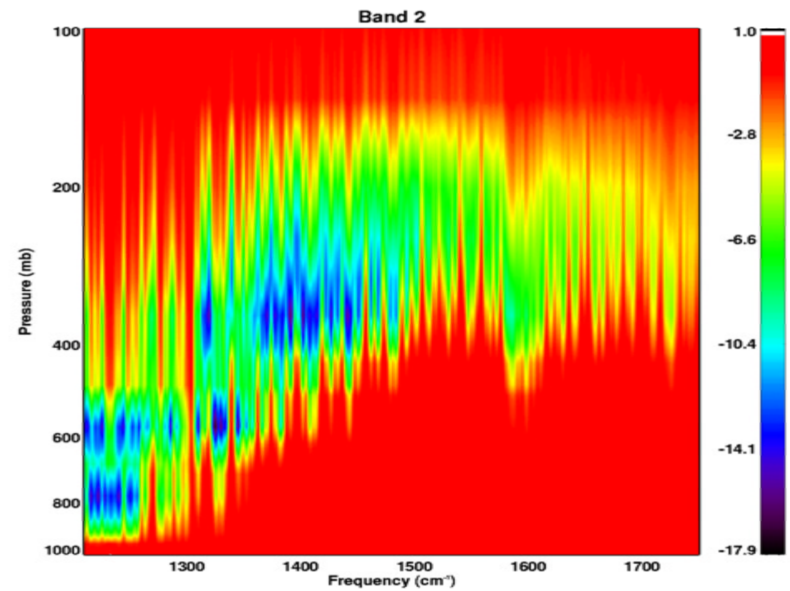
$$\frac{\partial R}{\partial \rho_s} = T_N F_0 \cos\theta_{sun} \exp\left(-\sum_l \tau_l^0 \sec\theta_{sun}\right) = R_{sol} / \rho_s$$

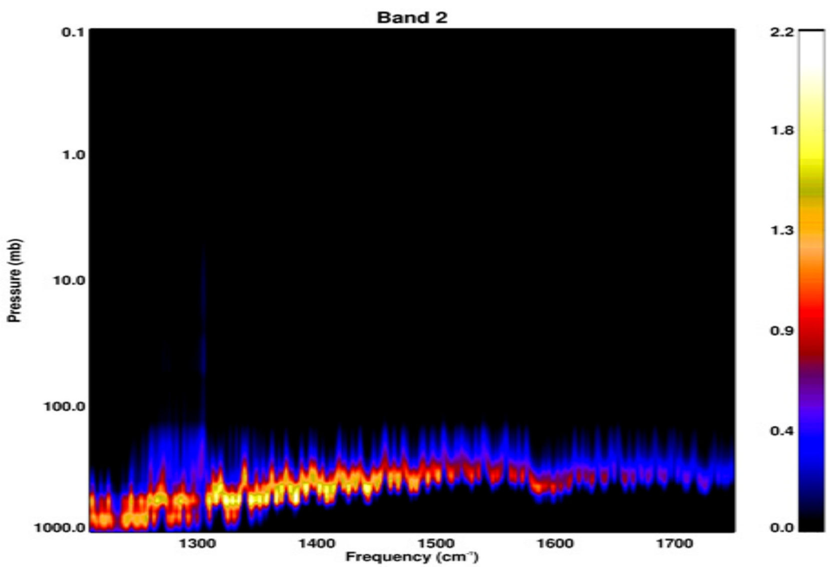
Temperature and Moisture Jacobians

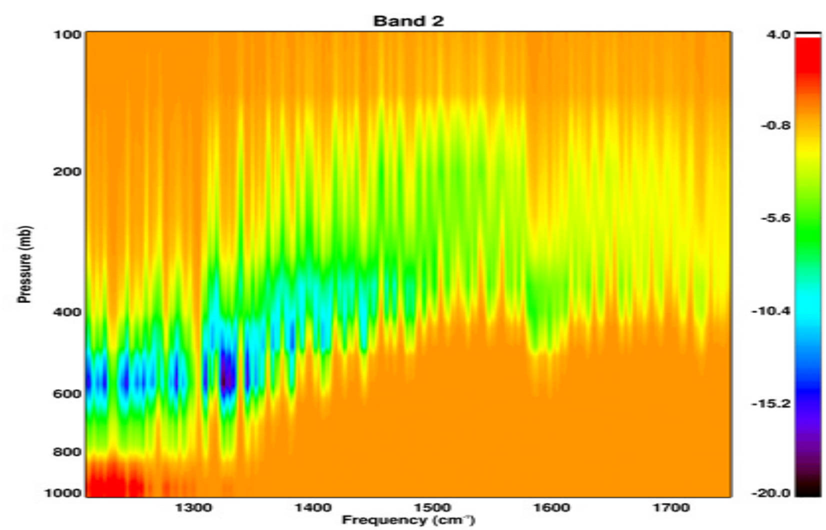


Temperature and Moisture Jacobians









Transformation of variables

- **The layer derivative can be converted to level derivative by:**

$$\frac{\partial R}{\partial X_{lev}} = \frac{\partial R}{\partial X_{lay}^{above}} \frac{\partial X_{lay}^{above}}{\partial X_{lev}} + \frac{\partial R}{\partial X_{lay}^{below}} \frac{\partial X_{lay}^{below}}{\partial X_{lev}}$$

- **The truncted EOF (U) obtained from background covariance can be used compress *ΔX* and *K:***

$$\Delta\tilde{x} = U^T \Delta x$$
$$\tilde{K}_i = K_i U$$

$$\Lambda = U^T S_x U$$

$$\Delta\tilde{x}_{i+1} = (\tilde{K}_i^T S_y^{-1} \tilde{K}_i + \Lambda)^{-1} \tilde{K}_i^T S_y^{-1} (y_0 - y_i + \tilde{K}_i \Delta\tilde{x}_i)$$

- **If the full correlation of noise covariance S_y can be compressed using truncated EOF obtained from PCA of radiance spectra**
  - **The inversion of the transformed matrix will be more efficient**

Difficulties of Modeling Channel Radiances or Transmittance

$$R_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu - \nu')R(\nu)d\nu' \qquad T_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu - \nu')T(\nu)d\nu'$$

- **where Φ is normalized ILS (SFR)**
- **LBL calculation of monochromatic layer transmittances or TOA radiances is very time consuming**
- **Convolving monochromatic radiances or transmittances with ILS (SRF) is also time consuming**
- **The Beer's Law is no longer valid**
  - **It's difficult to handle inhomogeneous path and multiple gases**

$$\int_{\Delta\nu} \phi(\nu)T_{gas1}T_{gas2}d\Delta\nu' \neq \int_{\Delta\nu} \phi(\nu)T_{gas1}d\Delta\nu' \int_{\Delta\nu} \phi(\nu)T_{gas2}d\Delta\nu'$$

$$\int_{\Delta\nu} \phi(\nu)T_{layer1}T_{layer2}d\Delta\nu' \neq \int_{\Delta\nu} \phi(\nu)T_{layer1}d\Delta\nu' \int_{\Delta\nu} \phi(\nu)T_{layer2}d\Delta\nu'$$

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Comparison of Different Fast RT Model

Model Type	Characterisitic	Limitations
Band Model	Simple parameterization Fast Curtis Godson approximation can be used to handle inhomogeneous atmos.	Limited accuracy Not accurate to extend to multiple gases
Neural net	Simple Fast	Jacobian calculations? Non-physical parameterization
Correlated k Distributions (CKD)	Monochromatic (g-v mapping) Level to level k correlation is approximate Overlapping gases treatment is approximate	Not perfect for inhomogeneous path and overlapping gases
Exponential Sum Fitting Transmissions (ESFT)	Monochromatic (select few k terms or v points) Level to level k correlation is approximate (methods exist to handle it) Overlapping gases treatment is approximate	Standard method is perfect for inhomogeneous path and overlapping gases
Optran, RTTOV ,SARTA,Gastropd ….	Polychromatic Smart way to treat overlapping gases Teat inhomogeneous path	Effective layer optical depth depends on layer above it
Optimal Spectral Sampling (OSS)	Monochromatic Treat inhomogeneous path and overlapping gases well Parameterization is physical	Very good treatment of inhomogeneous path and overlapping gases

Overview of Different Fast RT Models

- **K distribution (KD)**

$$T(\Delta v,\omega)=\int_{\Delta v}\phi(v-v')T(v,\omega)dv' \cong \sum_{i=1}^{N}\Delta g_i \exp[-k_i(g_i)\omega]$$

$$R(\Delta v,\omega)=\sum_{i=1}^{N}\Delta g_i \{B_i(\Theta,g)+[R_{0,i}-B_i(\Theta,g)]\exp[-k_i(g)\omega]$$

$$\sum_{i=1}^{N}\Delta g_i = 1$$

Δg_i and k_i obtained by grouping k(v)

- **Correlated-K distribution (CKD)**
  - **Correlation between the spectral shape and positions is different layers is approximate**
    - **KD made for a set of T,P, independently**
    - **Methods exist to correct this approximation**
      - Use same g-v mapping for all layers (e.g Mlayer et al….)
      - Reference layer add-subtract method (e.g. Oinas, Edward ….)

Overview of Different Fast RT Models

Correlated-K distribution (Continued)

- **Treatment of overlapping gases is approximate**
  - **Assume gases are uncorrelated:**

$$T(\Delta v,\omega_1,\omega_2) = \int_{\Delta v} \phi(v-v')T(v,\omega_1)T(v,\omega_2)dv'$$

$$\cong T(\Delta v,\omega_1)T(\Delta v,\omega_2) = \sum_{i=1}^{N} \Delta g_{1,i} \exp[-k_{1,i}(g_{1,i})\omega_1] \sum_{j=1}^{M} \Delta g_{2,j} \exp[-k_{2,j}(g_{2,j})\omega_2]$$

  - **Introduce ω_i (or functions of $\omega_{i,}$ i=gas1, gas2….) as additional factor when generating k**

    k(g,p,T,ω)

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Overview of Different Fast RT Models

- **Exponential Sum Fitting of Transmissions (ESFT)**

$$T(\Delta v,\omega) = \int_{\Delta v} \phi(v - v')T(v,\omega)dv' \cong \sum_{i=1}^{N} w_i \exp[-k_i(v_i)\omega]$$

$$R(\Delta v,\omega) = \sum_{i=1}^{N} w\{B_i(\Theta,v) + [R_{0,i} - B_i(\Theta,v)]\exp[-k_i(g)\omega]$$

$$\sum_{i=1}^{N} w_i = 1$$

  - **w_i and the spectral location of k_i obtained by a selection/regression process**
- **Treatment of inhomogeneous atmosphere**
  - **Use w_i and ν_i obtained for a reference layer and scale exponential term with appropriate function of P and T**
  - **Include all layers in the regression and selection process (Armbruster and fisher 1996)**

$$T_L^{TOA}(\Delta v, p_L, \omega) \cong \sum_{i=1}^{N} w_i(v_i)\exp[-\sum_{l=1}^{L} k_i(v_i, p_l)\omega(p_l)]$$

Overview of Different Fast RT Models

- ESFT (continued)
  - Treatment of mixing gases
    - Similar to CKD (assume uncorrelated)

$$T(\Delta v, \omega_1, \omega_2) = \int_{\Delta v} \phi(v - v')[\overline{T_1} + \delta T_1(v, \omega_1)][\overline{T_2} + \delta T_2(v, \omega_2)]dv'$$

$$= \overline{T_1}\,\overline{T_2} + \sum_{i=1}^{N} w_i \delta T_{1,i}(v, \omega_1) \delta T_{2,i}(v, \omega_2)$$

$$\overline{T_1}\,\overline{T_2} = \int_{\Delta v} \phi(v - v') T_1(v, \omega_1) dv' \int_{\Delta v} \phi(v - v') T_2(v, \omega_2) dv'$$

    - Equivalent extinction (Ritter and Geleyn, Edwards…)
    - Additional interpolation variable as a function of ω_i (or functions of $\omega_{i,}$ i=gas1, gas2….)
    - Frequency sampling method or radiance sampling method (Sneden et al. 1975, Tjemkes and Schmetz, 1997)

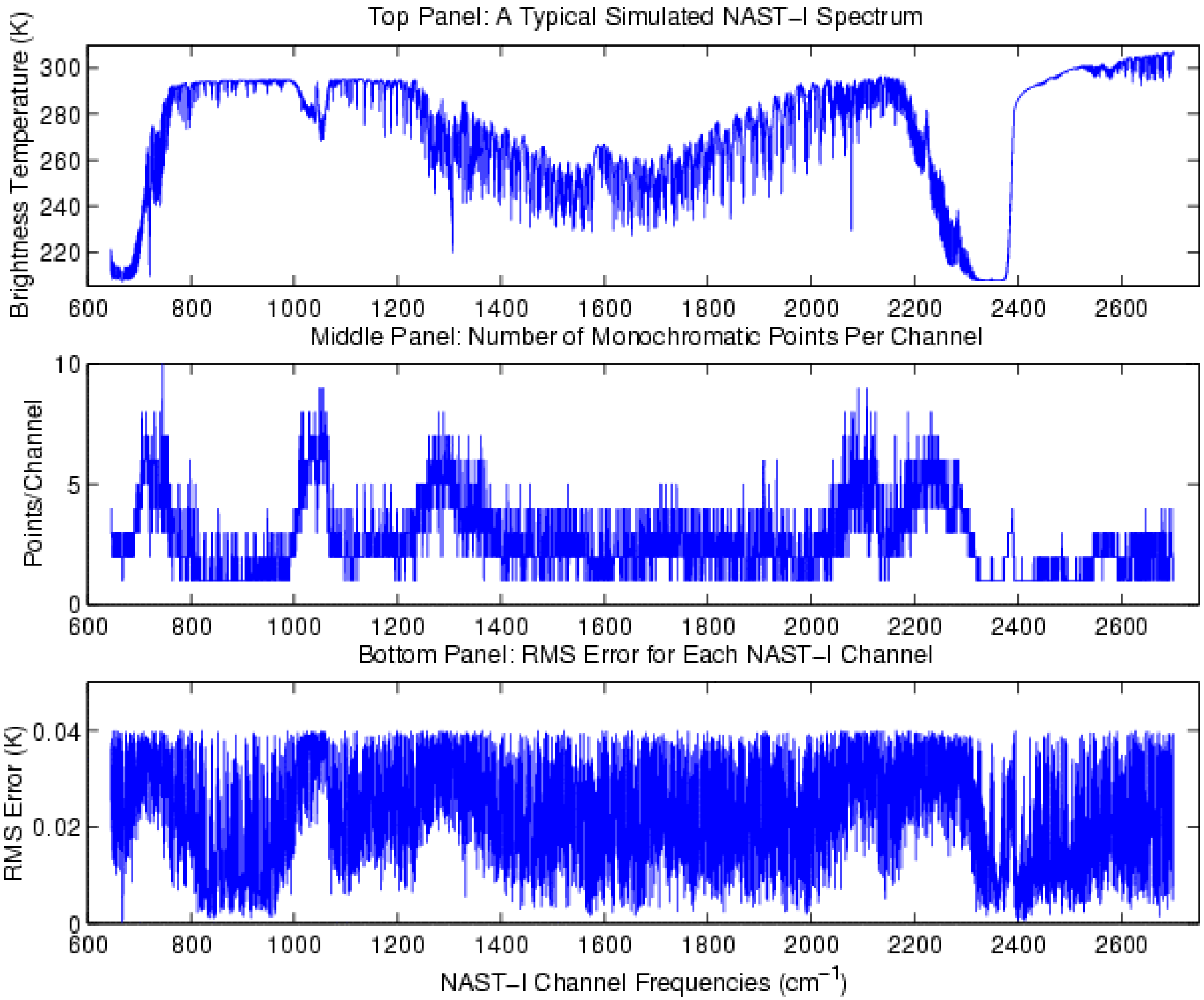
Overview of the OSS forward model

- **Optimal Spectral Sampling (OSS) approximates channel radiances (or transmittances) according to:**

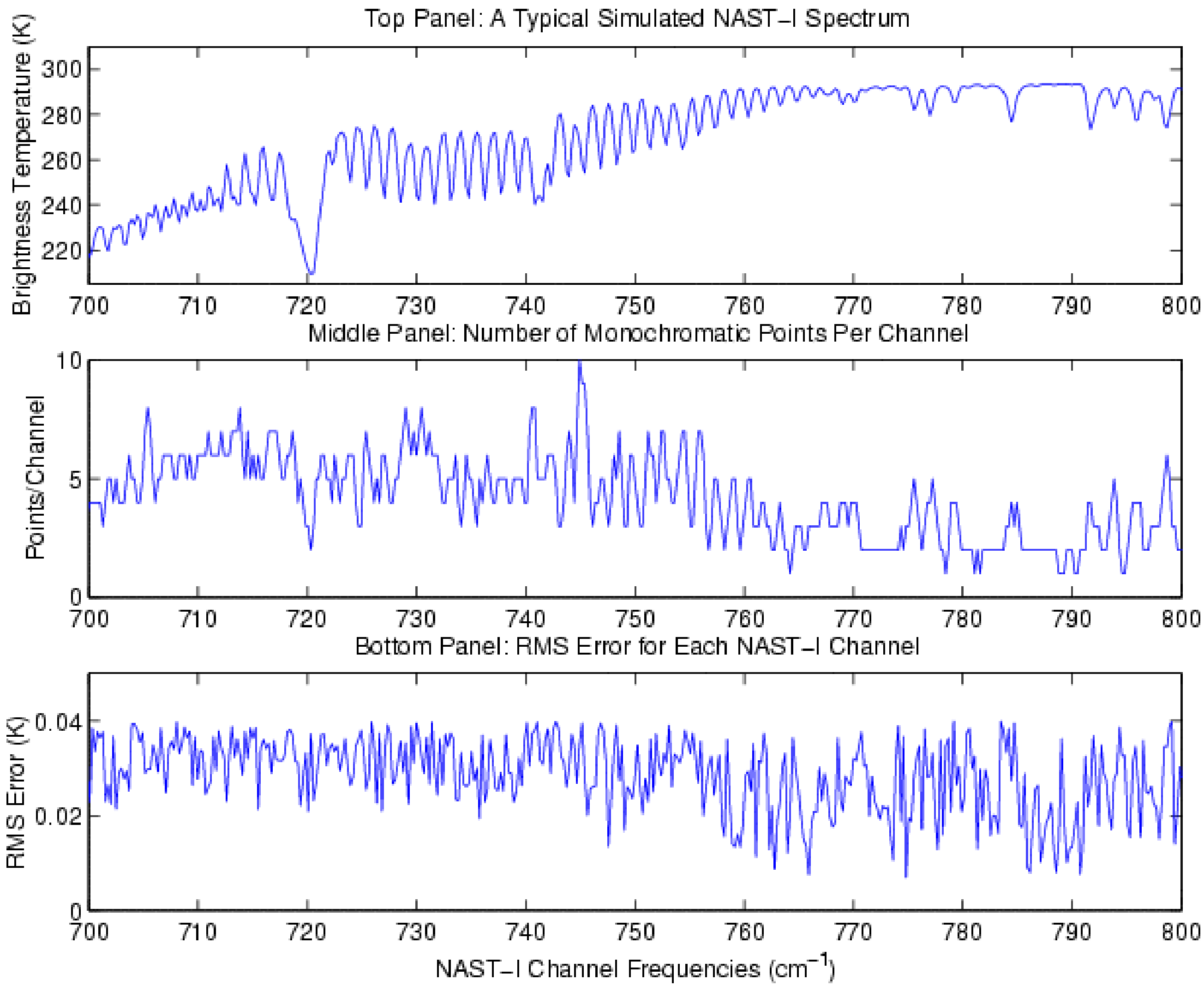
$$R_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu - \nu^{'}) R(\nu \quad) d\nu' = \sum_i w_i R_{\nu_i} + \varepsilon$$

- **Channel radiances are a linear combination of monochromatic radiances at pre-selected frequencies**
- **Spectral locations/weighting coefficients are obtained through a selection/regression process**
- **The computational gain is more than 3 orders of magnitude relative to the line-by-line calculations**
- **RT is done monochromatically**
  - **Monochromatic lookup table is used to calculate the transmittance for various gases and different atmospheric layers (no approximates need to be made)**
  - **Calculates Jacobian analytically (very efficient)**
  - **Treats reflected radiance accurately**
  - **Can be easily coupled with multiple scattering codes**

Application of OSS to NAST-I



Expanded View of the RMS of the Forward Model

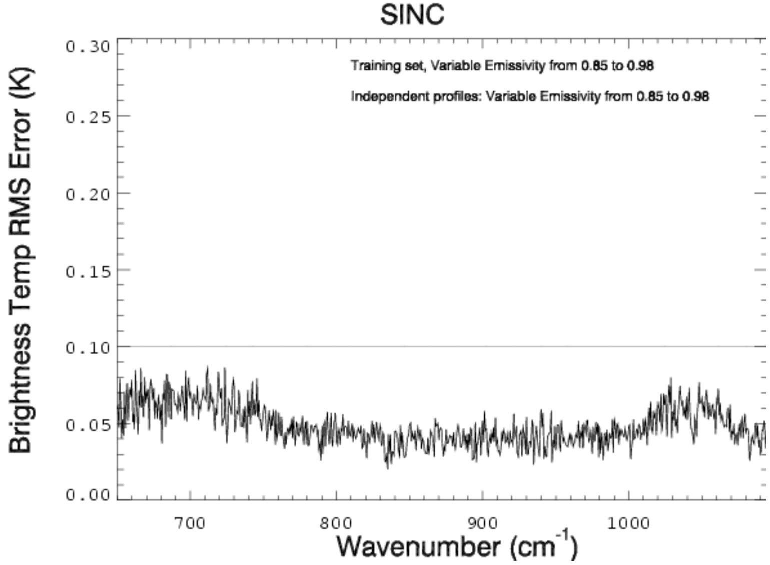


Number of Points Per Channel

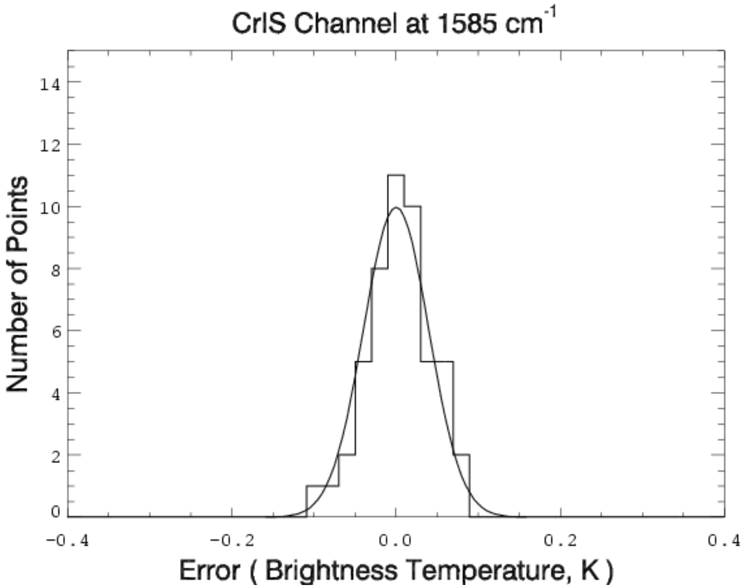
- **Average of 2.59 monochromatic spectral calculations are needed for each NAST-I channel**

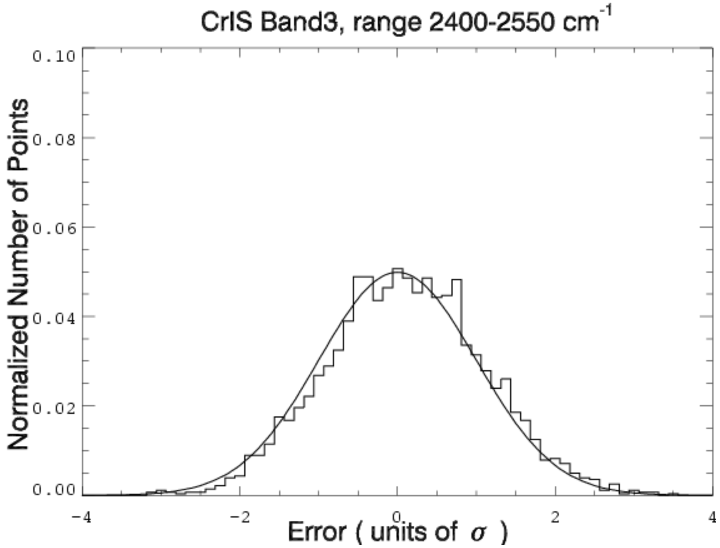
NAST-I Spectral Band	Number of Channels	Number of Monochromatic Points	Average Points per Channel
LWIR	2718	7464	2.75
MWIR	2946	7283	2.47
SWIR	2968	7569	2.55

Validation of OSS Forward Model Accuracy

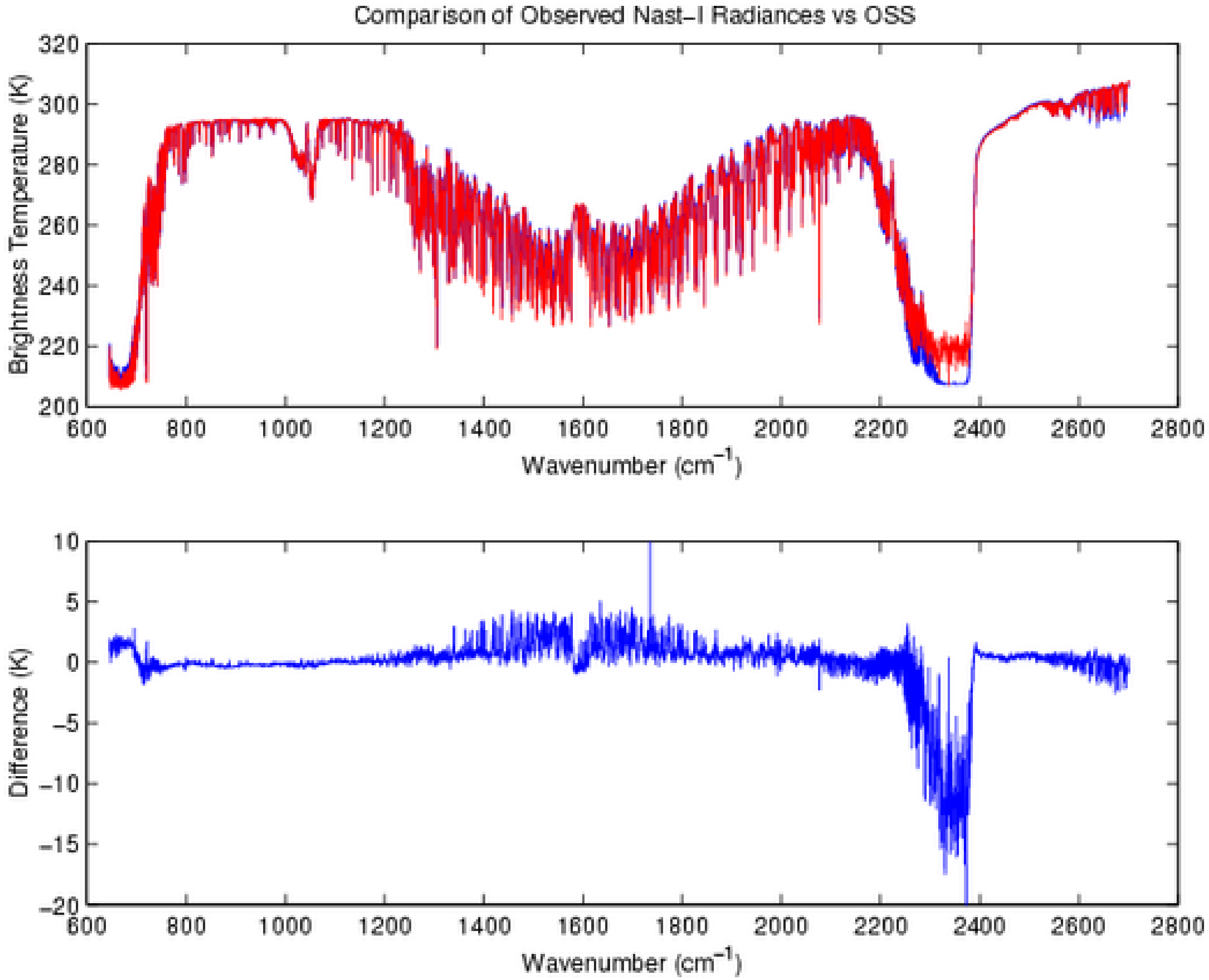


- The radiance errors derived from independent profile set follow a Gauss distribution

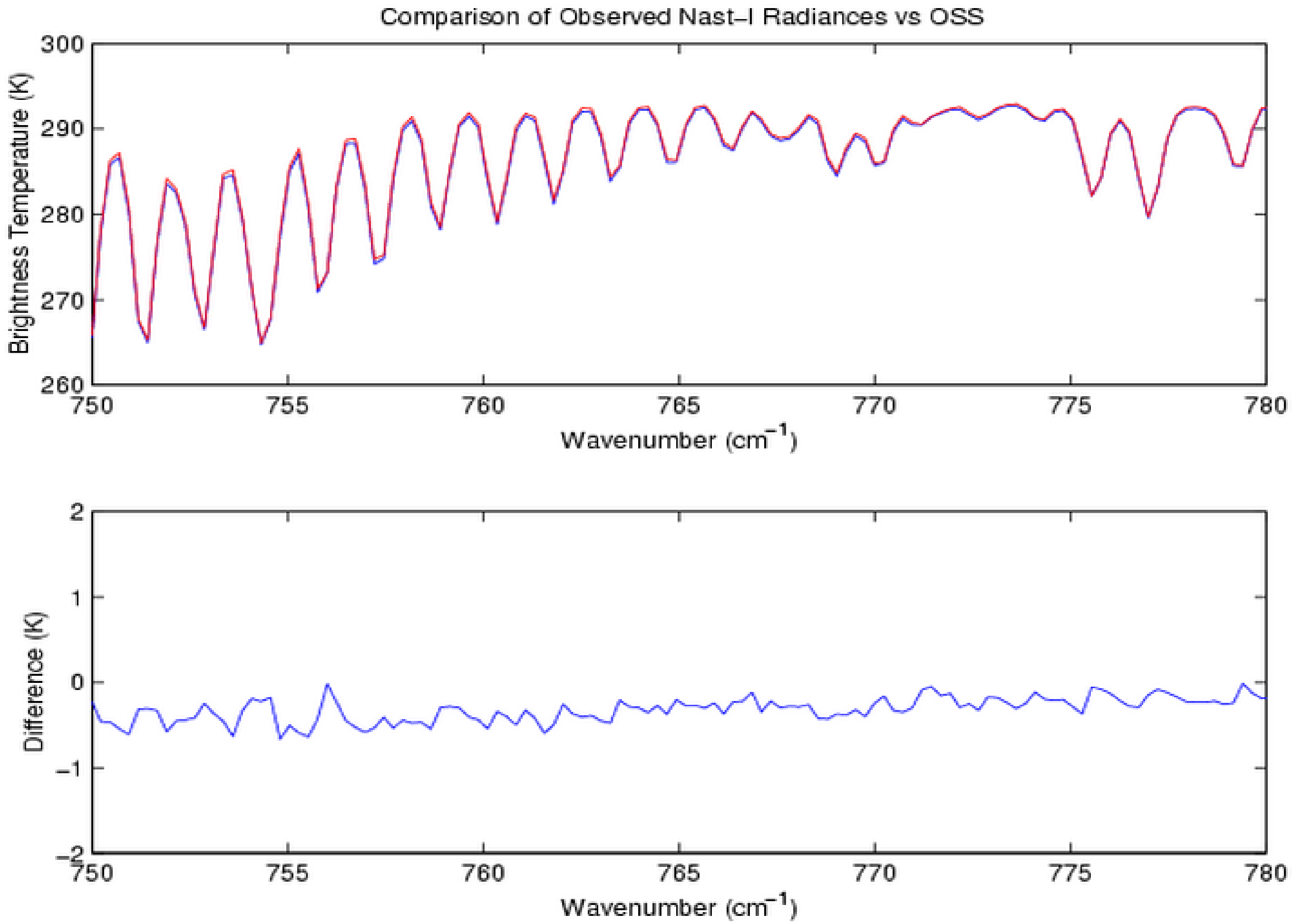




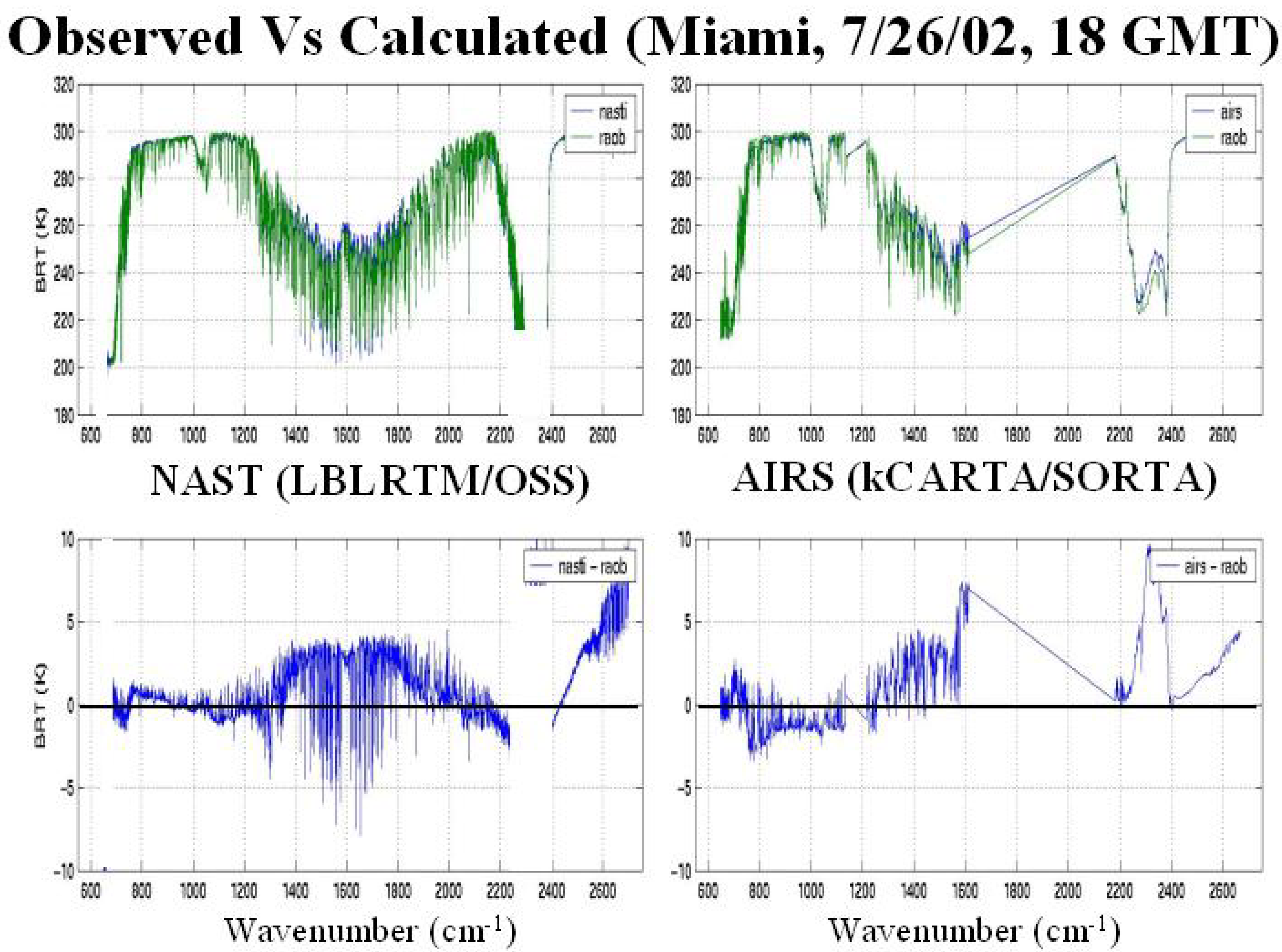
Observed and Modeled NAST-I Radiances for 7/14/01 CLAM Campaign



Expanded View of the Observed and Calculated NAST-I Radiances



Observed vs. Calculated NAST Radiance for Crystal-Face AIRS Underflight



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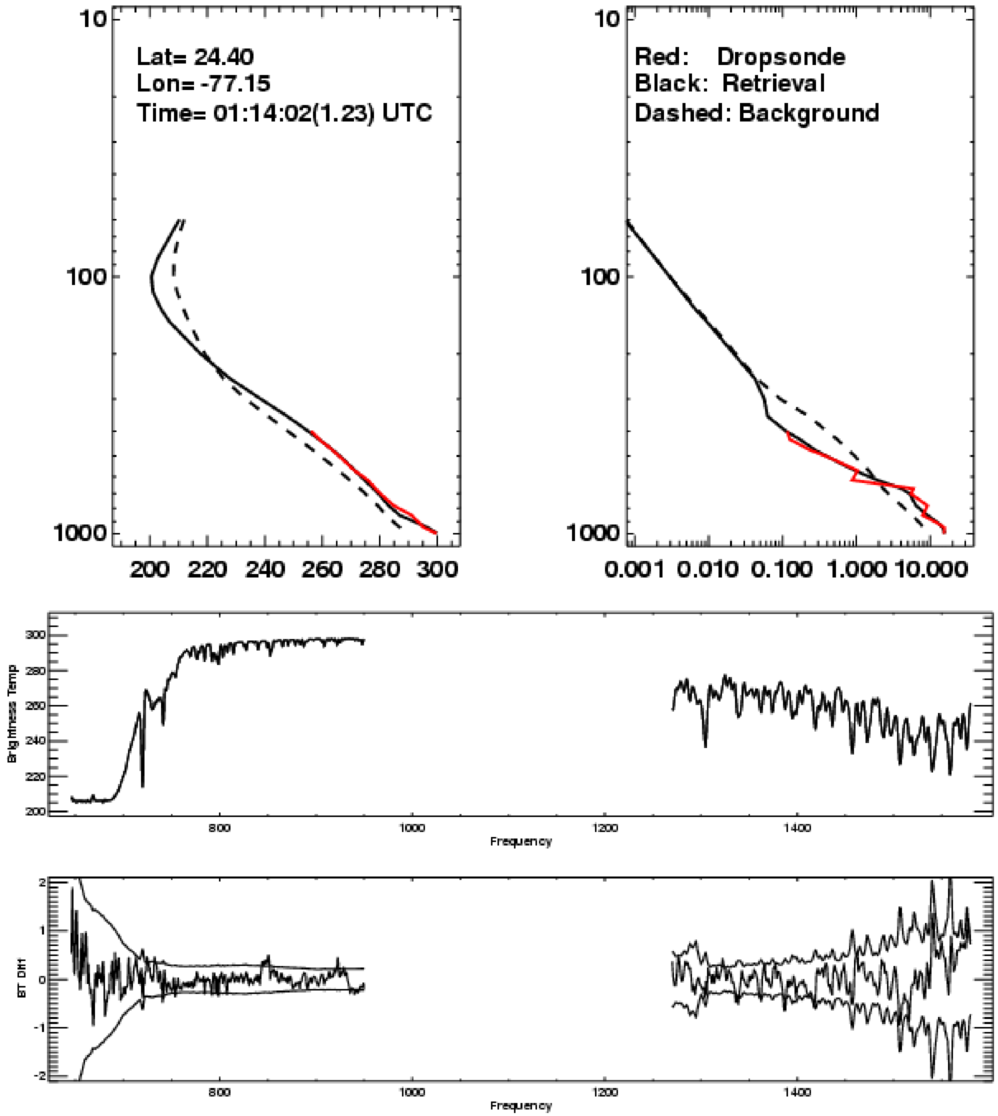
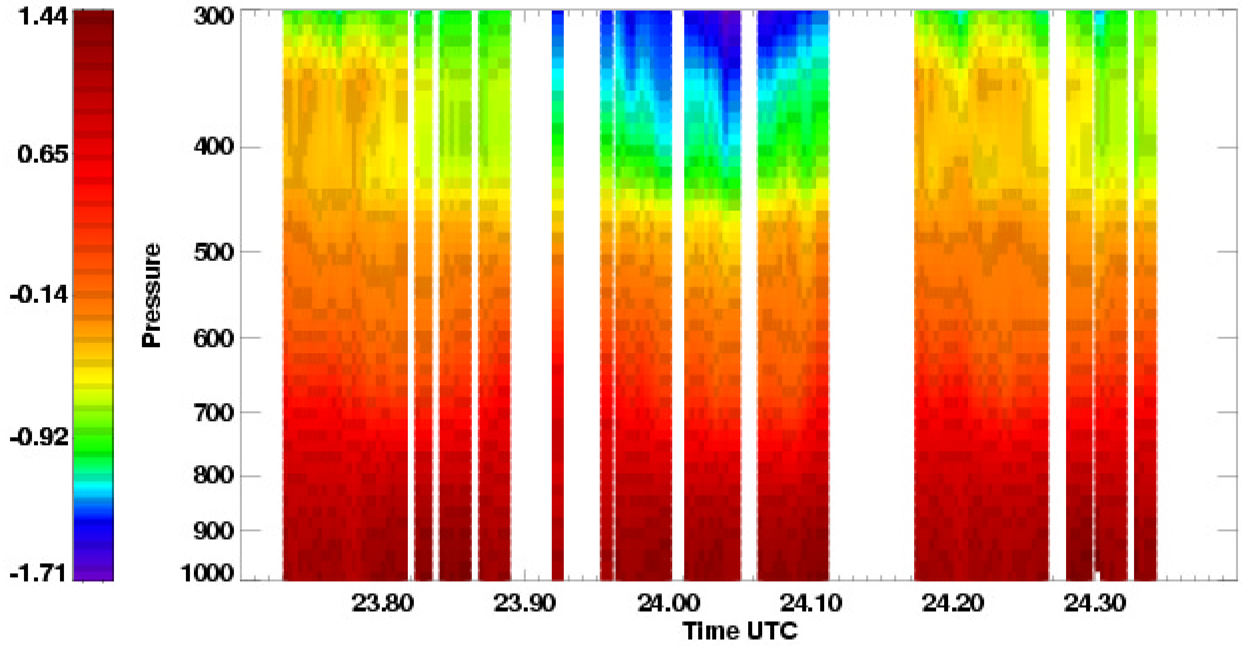
Retrieved Profiles For the CAMEXIII Campaign Near Andros Island

CrIS Retrieval Algorithm was used



Retrieved Temperature Profiles from NAST-I Instrument



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Conclusions

- Jacobian provides sensitivity of radiance with respect to the retrieved parameters
  - Recursive RT calculation gives insights
  - Most terms needed for the radiances calculation can be used for Jacobian calculation (time saving)
- Transformation of variable accelerate inversion process
  - It also provides stability to the inversion
- The fast radiative transfer model is best done at monochromatic frequencies
  - Physical parameterization
  - Efficient in calculating Jabcobian matrix needed for inversion
  - Can include multiple scattering calculations
- It's best to train all atmospheric layers and all major gases simultaneous
- OSS model has been developed to model NAST-I radiances and was incorporated into NASA's retrieval algorithm
- OSS has been used to simulate the CrIS EDR retrieval performance and the retrieval algorithm has been validated using NAST-I data