



INFRA-RED SOUNDERS

Part 1: Basic Theoretical Considerations

Joel Susskind

NASA GSFC

**Workshop on Applications of Remotely Sensed Observations in Data
Assimilation**

August 7, 2007

Atmospheric Sounders

Measure upwelling thermal radiance in a number of spectral channels

Most channels are in opaque spectral regions that do not see the surface

15 μm and 4.2 μm CO_2 bands, 6.7 μm H_2O band, 9.6 μm O_3 band, etc.

(667 cm^{-1}) (2350 cm^{-1}) (1600 cm^{-1}) (1040 cm^{-1})

Provide information about atmospheric temperature and constituent profiles

Channels are characterized by central frequency ν_i and band pass $\Delta\nu_i$

Fields of view (FOV's) are roughly 15 km at nadir

IR and microwave sounders are complementary and often fly together

Recent and Scheduled Future IR Sounders

HIRS2

1979-present TIROS-N - NOAA 18

NOAA operational polar orbiting IR sounder, accompanied by MSU/AMSU

19 channel filter wheel IR radiometer $667 \text{ cm}^{-1} - 2750 \text{ cm}^{-1}$ ($15 \text{ }\mu\text{m} - 3.6 \text{ }\mu\text{m}$)

$\nu_i / \Delta\nu_i \approx 100$ $\Delta\nu_i$ goes from $10 \text{ cm}^{-1} - 25 \text{ cm}^{-1}$

Spatial resolution $\approx 15 \text{ km}$ at nadir from 824 orbit

AIRS

Launched on Eos Aqua in May 2002

2360 channel grating detector array spectrometer $650 \text{ cm}^{-1} - 2665 \text{ cm}^{-1}$

$\nu_i / \Delta\nu_i \approx 1200$ $\Delta\nu_i$ goes from $0.5 \text{ cm}^{-1} - 2.2 \text{ cm}^{-1}$

Spatial resolution $\approx 13 \text{ km}$ at nadir from 705 km orbit

IASI

Launched on Metop 2 in October 2006

8461 channel interferometer $645 \text{ cm}^{-1} - 2760 \text{ cm}^{-1}$

$\Delta\nu_i = 0.5 \text{ cm}^{-1}$

Spatial resolution $\approx 12 \text{ km}$ at nadir - not contiguous

CrIS

Scheduled to fly on NPP and NPOESS

Interferometer - similar spectral characteristics to AIRS

Monochromatic Radiative Transfer Equation

Clear Sky - assuming Local Thermodynamic Equilibrium (LTE)

$$R_{v,CLR} = \varepsilon_v B_v(T_s) \tau_v(p_s) + \int B_v [T(p)] \left(\frac{d\tau_v}{dl np} \right) dl np + \rho_v H_v \tau'_v(p_s) + (1 - \varepsilon_v) R_v \downarrow \tau_v(p_s)$$

Emitted by surface Emitted by atmosphere Reflected sunlight Reflected thermal

$$\tau_v(p), \frac{d\tau_v}{dl np} \text{ depend on constituent profile} \quad \tau_v(p) = e^{-\int_0^p \sum_l k_{v,l}(p) c_l(p) dp}$$

Unknowns

- ε_v spectral surface emissivity
- ρ_v spectral surface bi-directional reflectance
- T_s surface skin temperature
- $T(p)$ temperature profile
- $q(p)$ water vapor profile
- $O_3(p)$ ozone profile
- $CO(p)$ carbon monoxide profile
- $CH_4(p)$ methane profile
- $CO_2(p)$ carbon dioxide profile

Partial Cloud Cover

$$R_v = \left(1 - \sum_j \alpha_j \right) R_{v,CLR} + \sum_j \alpha_j R_{v,CLD,j} \quad j \text{ cloud types}$$

α_j is fractional cloud cover of cloud type j

Monochromatic Weighting Functions

$$W_{\nu}(p) = \frac{d\tau_{\nu}}{dl np}$$

$$\int \left(\frac{d\tau_{\nu}}{dl np} \right) dl np = \int d\tau = 1 - \tau_{\nu}(p_S)$$

If $k(p)$, $c(p)$ are constant and one gas is absorbing

$$\tau_{\nu}(p) = e^{-k_{\nu}cp}$$

$$\frac{d\tau_{\nu}}{dl np} = k_{\nu}cp e^{-k_{\nu}cp} = x_{\nu} e^{-x_{\nu}}$$

Maximum value = .37 when $x = 1$, occurs at $p_{\nu} = \frac{1}{k_{\nu}c}$

A narrower weighting function means information comes from a thinner slice of the atmosphere

If k increases with p , weighting function is narrower (line wing)

If k decreases with p , weighting function is broader (line center)

If k increases with T , and T increases with p , $W(p)$ is narrower

If c increases with p , $W(p)$ is narrower – water vapor lines

Radiative Transfer for Channel i

$$R_i = \int R_\nu f_i(\nu) d\nu / \int f_i(\nu) d\nu$$

$f_i(\nu)$ = spectral response function of channel i

$\Delta\nu_i$ = half-width of channel i

If $\Delta\nu_i$ is narrow and there is LTE

$$R_i \approx \varepsilon_i B_i(T_s) \tau_i(p_s) + \int B_i [T(p)] W_i(p) dl np + \rho_i H_i \tau_i'(p_s) + (1 - \varepsilon_i) R_i \downarrow \tau_i(p_s)$$

where $\tau_i(p) = \int \tau_\nu(p) f_i(\nu) d\nu / \int f_i(\nu) d\nu$

$$W_i(p) = \int W_\nu(p) f_i(\nu) d\nu / \int f_i(\nu) d\nu$$

$$B_i(T) = B_{\nu_i}(T)$$

etc.

Brightness Temperature Θ_i

The brightness temperature Θ_i of channel i with radiance R_i is the temperature of a black-body that would emit R_i at frequency ν_i

$$\Theta_i = B_{\nu_i}^{-1}(R_i)$$

$$B_\nu(T) \approx \nu^3 \left(e^{1.439\nu/T} - 1 \right)^{-1} \text{ when } \nu \text{ is in cm}^{-1}$$

In microwave region, $\nu \approx 1 \text{ cm}^{-1}$

$$B_\nu(T) \approx \nu^2 T$$

$\Theta_{\text{mic}}(R_\nu)$ is set equal to T in calibration process

In IR, $e^{1.439\nu/T} \gg 1$

$$B_\nu(T) \approx \nu^3 e^{-1.439\nu/T}$$

$B_\nu(T)$ changes by 3 orders of magnitude between 650 cm^{-1} and 2660 cm^{-1} for same T

$$\Theta_i(R_i) \approx \nu_i \left[\ln \left(\frac{1.439\nu_i^3 + 1}{R_i} \right) \right]^{-1}$$

$\Theta_i(R_i)$ is on the order of T for all frequencies

Sensitivity of Opaque Channel Brightness Temperature to Atmospheric Temperature Changes

$$R_i [T(p) + \Delta T] - R_i [T(p)] = \int_0^1 (B_i [T(p) + \Delta T] - B_i [T(p)]) d\tau_i$$

In microwave region

$$B_i(T) = T$$

$$\Theta_i [T(p) + \Delta T] - \Theta_i [T(p)] = \Delta T$$

Equation holds in IR as well

A 1K change in $T(p)$ over the whole atmosphere results in a 1K change in Θ_i

Likewise, for a 1K change only within the non-zero part of $W_i(p)$

Advantages of High Spectral Resolution

High spectral resolution means absorption features due to single lines can be observed

Many channels are observed

AIRS has 2378 channels with $\nu / \Delta\nu \approx 1200$

Allows for selectivity of channels to be used

Best channels are primarily sensitive to absorption by a single species

“Fixed” gases - CO₂, N₂O - for temperature sounding

H₂O, O₃, CH₄, CO for constituent profiles

Window (relatively transparent) channels for surface parameters

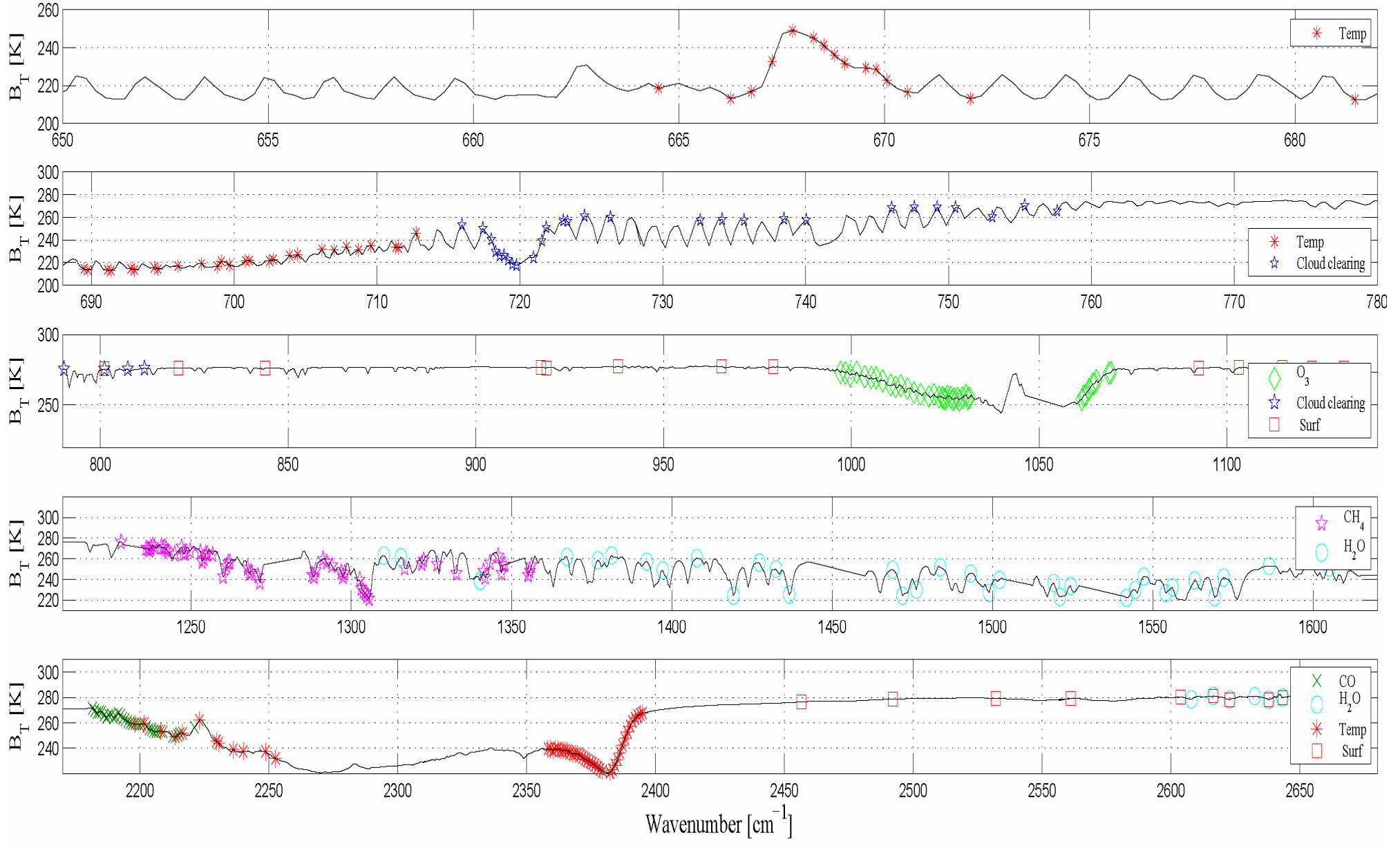
Best channels are usually in line wings or on line centers

Channels in line wings have sharp $W_i(p)$

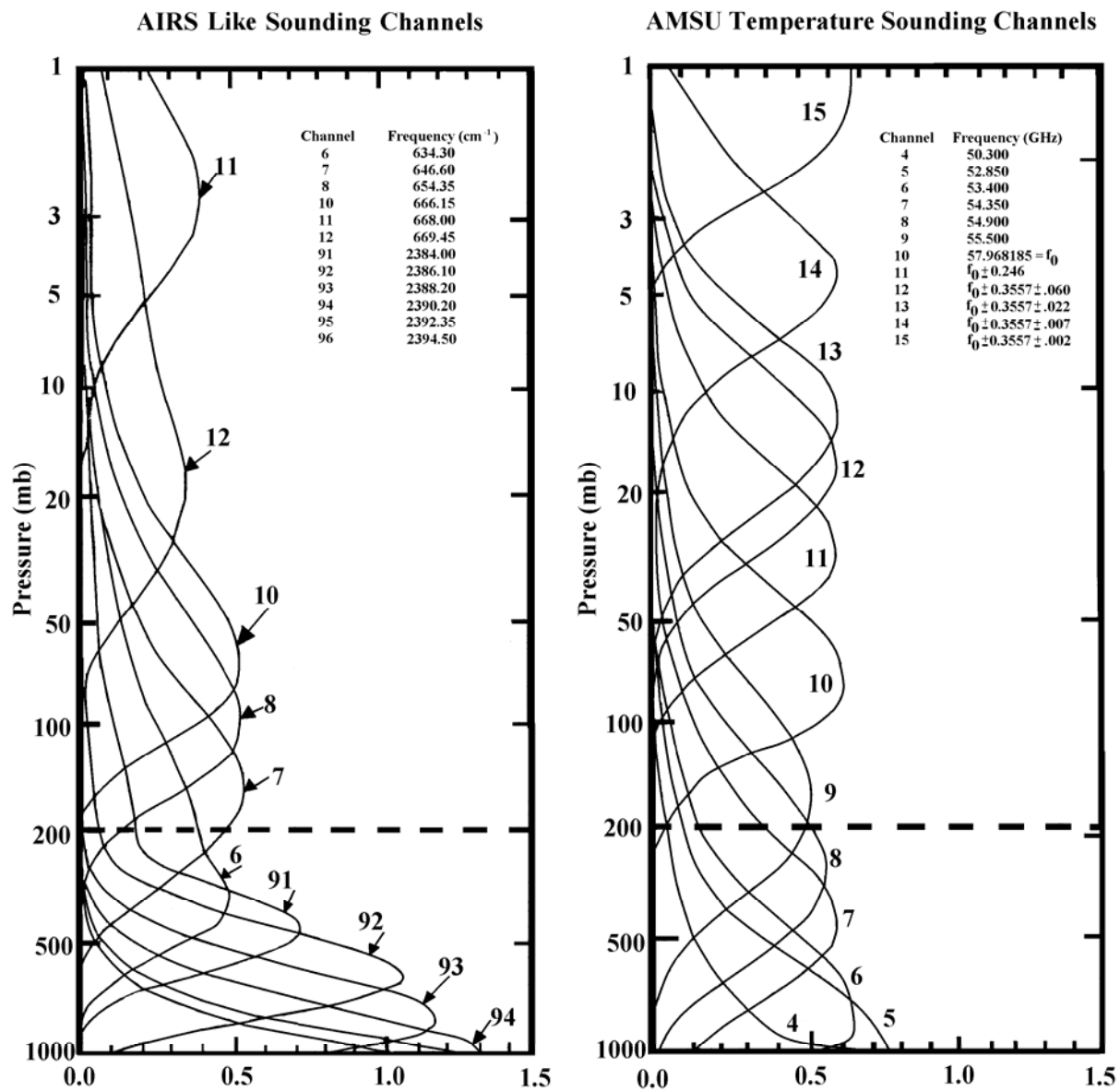
Channels on line centers are most sensitive to trace gas absorption

Channels with redundant information can be used together to reduce noise

Version 5.0 Channels



TEMPERATURE WEIGHTING FUNCTIONS



IR and Microwave Observations are Very Complementary

IR Strengths

- Best vertical resolution (accuracy) of $T(p)$ in mid-lower troposphere
- Water vapor profile information up to the tropopause
- Best information about surface skin temperature
- Trace gas profile information

IR Limitations

- Most channel observations are strongly affected by clouds

MW Strengths

- MW observations are not affected by most clouds
- MW observations help in accounting for effects of clouds on IR observations
 - Microwave soundings of $T(p)$, $q(p)$ can be produced in overcast conditions

MW Limitations

- Channels sensitive to lower troposphere are highly affected by variable surface emissivity

Approaches to Account for Clouds in the Field of View (FOV)

1) Avoid clouds

a) Do soundings in areas “thought to be clear” (about 5% of the time)

b) Assimilate only channel radiances “thought to be unaffected by clouds”

All stratospheric sounding channel radiances (15 μm channels we use for T(p))

Tropospheric sounding channel radiances that do not see down to cloud tops

1b) is the approach used operationally by ECMWF, NCEP

2) Include cloud radiative transfer model in radiance calculation

Needs detailed knowledge of cloud microphysical and geometric properties within FOV

Potentially useful for single layer thin cirrus clouds

3) Attempt to determine cloud cleared radiances \hat{R}_i from observations in adjacent fields of view

\hat{R}_i represents radiances sounder “would see” if no clouds were in the FOV

K cloud formations requires K+1 FOV's to obtain \hat{R}_i

We use approach 3) to analyze AIRS/AMSU data

\hat{R}_i , as well as T(p), q(p), are products, each with their own error estimates

Cloud Clearing with a Single Cloud Layer

If fields of view 1 and 2 are otherwise identical but have differing amounts of a single cloud type

$$R_{i,1} = (1 - \alpha_1)R_{i,CLR} + \alpha_1 R_{i,CLD}$$

$$R_{i,2} = (1 - \alpha_2)R_{i,CLR} + \alpha_2 R_{i,CLD}$$

then

$$R_{i,CLR} = R_{i,1} + \eta(R_{i,1} - R_{i,2}) \quad \text{where } \eta = \alpha_1 / (\alpha_2 - \alpha_1)$$

If we have an estimate of $R_{i,CLR}^0$ for channel i , can solve for η^0

$$\eta^0 = \frac{R_{i,CLR}^0 - R_{i,1}}{R_{i,1} - R_{i,2}}$$

and

$$\hat{R}_j^0 = R_{j,1} + \eta^0 (R_{j,1} - R_{j,2}) \quad \text{for all channels } j$$

\hat{R}_j^0 is used to derive soundings

Methodology to obtain η - Dual Frequency Cloud Clearing Principle

Start with initial state $T^0(p) = T(p) + \delta T(p)$ where $\delta T(p)$ is the error in $T^0(p)$ - say $\delta T(p) = 1K$

Compute $R_{i,CLR}^0$ from $T^0(p)$

$$\delta\eta_i = \eta_i^0 - \eta = \frac{R_{i,CLR}^0 - R_{i,CLR}}{R_{i,1} - R_{i,2}} \approx \frac{\delta R_{i,CLR}}{R_i} \approx \frac{[dB(\nu, T) / dT] \times \delta T}{B(\nu, T)}$$

$$\left[\frac{dB(\nu, T)}{dT} / B(\nu, T) \right] \approx \nu / T^2$$

For the same temperature profile error, $\delta\eta_i$ is proportional to ν_i

$\delta\eta$ computed from channel i at 730 cm^{-1} is $\left(\frac{730}{2390} \right)$ smaller than from channel i at 2390 cm^{-1}

A - If you use $15 \mu\text{m}$ channels for cloud clearing, and $4.2 \mu\text{m}$ channels to retrieve $T^1(p)$

$$T^1(p) - T(p) \approx 0.3 \left[T^0(p) - T(p) \right]$$

B - If you use $15 \mu\text{m}$ channels (or $4.2 \mu\text{m}$ channels) for both

$$T^1(p) - T(p) \approx T^0(p) - T(p) \text{ nothing is gained}$$

Therefore it is optimal to do A

Overview of AIRS Cloud Clearing Procedure

Uses radiances in 9 fields of view R_{ij} channel i , FOV j within AMSU A FOR

Allows for up to 8 cloud formations

\bar{R}_i = average radiance over 9 FOV's in a set of i cloud clearing channels

$$\hat{R}_i^n = \bar{R}_i + \sum_{j=1}^9 \eta_j^n (R_{i,j} - \bar{R}_i) = \bar{R}_i + \sum_{j=1}^9 \eta_j^n \Delta R_{i,j}$$

9 values of η_j determine \hat{R}_i for all channels

We compute expected values of $R_{i,CLR}^n$ from a surface and atmosphere state X^n to obtain η^n

$$\eta_j^n = \left(\Delta R' N^{-1} \Delta R \right)^{-1} \Delta R' N^{-1} \Delta R_{CLR,i}^n \quad N = \text{channel noise covariance matrix}$$

where

$$\Delta R_{CLR,i}^n = R_{i,CLR}^n - \bar{R}$$

\hat{R}_i^n should in principle produce an unbiased state X^{n+1} if X^n is unbiased

Using 15 μm channels to determine η and 4 μm channels to give $T(p)^{n+1}$ minimizes effect of bias in X^n

Statistical and Physical Retrievals

Statistical retrieval - regression

$T(p_j) = \bar{T}(p_j) + \sum_i M_{j,i} (R_i - \bar{R}_i)$ using channel set I_{reg} - most AIRS channels are used

Matrix M determined from training set, which contains $T^{\text{Truth}}(p_j)$, and colocated observations R_i

Find M such that $\bar{T}(p_j) + \sum M_{j,i} (R_i - \bar{R}_i)$ best matches $T^{\text{Truth}}(p_j)$

\bar{R}, \bar{T} are mean values over the truth ensemble

$\bar{R}_i, \bar{T}(p_j), M$ used once and for all

R_i can be observed radiances or cloud cleared radiances \hat{R}_i

Physical retrieval - iterative

$T^{n+1}(p_j) - T^n(p_j) = f \left[\hat{R}_i - R_{i,\text{CLR}} \left(T^n(p) \right) \right]$ - uses a select set of channels

Needs ability to compute $R_{i,\text{CLR}}^n$ very accurately given atmosphere and surface state

Solution minimizes the residual of \hat{R}_i and $R_{i,\text{CLR}}^n$

RMS residual of $\left(\hat{R}_i - R_{i,\text{CLR}}^n \right)$ is very important in generating error estimates and quality control

Note: $T(p)$ used as an example - can be for any set of variables X_j

Sequential Physical Retrieval System

Physical retrieval is done sequentially to make solution for the parameters in each step more linear

- Surface parameter retrieval

Solves for T_s, ϵ_v, ρ_v

Uses channels primarily sensitive to T_s, ϵ_v, ρ_v

- Temperature profile

Solves for $T(p)$ only

Uses channels primarily sensitive to $T(p)$, surface parameter

- Water vapor profile

Solves for $q(p)$ only

Uses channels sensitive to $q(p)$, surface parameters, $T(p)$

- O_3 profile

Solves for $O_3(p)$ only

Uses channels primarily sensitive to $O_3(p)$, surface parameters, $T(p)$, $q(p)$

In all cases values of parameters not solved for are fixed at current best estimate in computation of $R_{i,CLR}^n$

Uncertainty in parameters not solved for is included in channel noise covariance matrix for channels used

Also includes channel noise and cloud clearing noise

Overview of AIRS/AMSU Retrieval Methodology

Physically based system

Independent of GCM except for surface pressure - used to compute $R_{i,CLR}$

Uses cloud cleared radiances \hat{R}_i to produce solution

\hat{R}_i represents what AIRS would have seen in the absence of clouds

Basic steps

Initial cloud clearing produces \hat{R}_i^0

AIRS regression guess parameters based on cloud cleared radiances \hat{R}_i^0

Update cloud clearing using AIRS regression guess parameters: produces \hat{R}_i

Sequentially determine surface parameters, $T(p)$, $q(p)$, $O_3(p)$, $CO(p)$, $CH_4(p)$, using \hat{R}_i

Determine cloud parameters consistent with retrieved state and observed radiances

Generate error estimates and use for quality control

Goddard DAAC has been analyzing AIRS/AMSU data using AIRS Version 4 algorithm

AIRS Version 5 algorithm is now operational

Goddard DAAC began using Version 5 in July 2007

Go forward and reprocess old data at 12x rate

Significant Improvements in Version 5

Physical retrieval algorithm

Radiative transfer parameterization now accounts for Non-Local Thermodynamic Equilibrium

Allows for use of all shortwave temperature sounding channels in physical retrieval

Most longwave temperature profile channels used for cloud clearing

Shortwave temperature sounding channels used for temperature profile

This is optimal for soundings under partial cloud cover

Error estimates

New methodology developed to provide accurate case by case error estimates

Error estimates used directly for quality control

Each accepted sounding flagged good down to characteristic pressure p_{good}

Accurate case by case error estimates improves utility of data for data assimilation

Can be products or \hat{R}_i

“AIRS Only” retrieval system (Version 5 AO)

Developed as back-up system if AMSU A fails

Performs extremely well with new error estimate quality control

V5 Retrieval Steps

- 1 Cloudy regression using AIRS **and AMSU** observations produces X^0
- 2 \hat{R}_i^0 computed using X^0
- 3 Generate X^{reg} using \hat{R}_i^0 , $X^{\text{reg}} = X^1$
- 4 \hat{R}_i^1 computed using X^1
- 5 Physical retrieval gives X^2
Uses \hat{R}_i^1 **and AMSU observations**. Starts with X^1
- 6 \hat{R}_i^2 computed using X^2
- 7 Physical retrieval - uses \hat{R}_i^2 **and AMSU observations**. Gives solution X^3
- 8 Generate error estimates and use for quality control

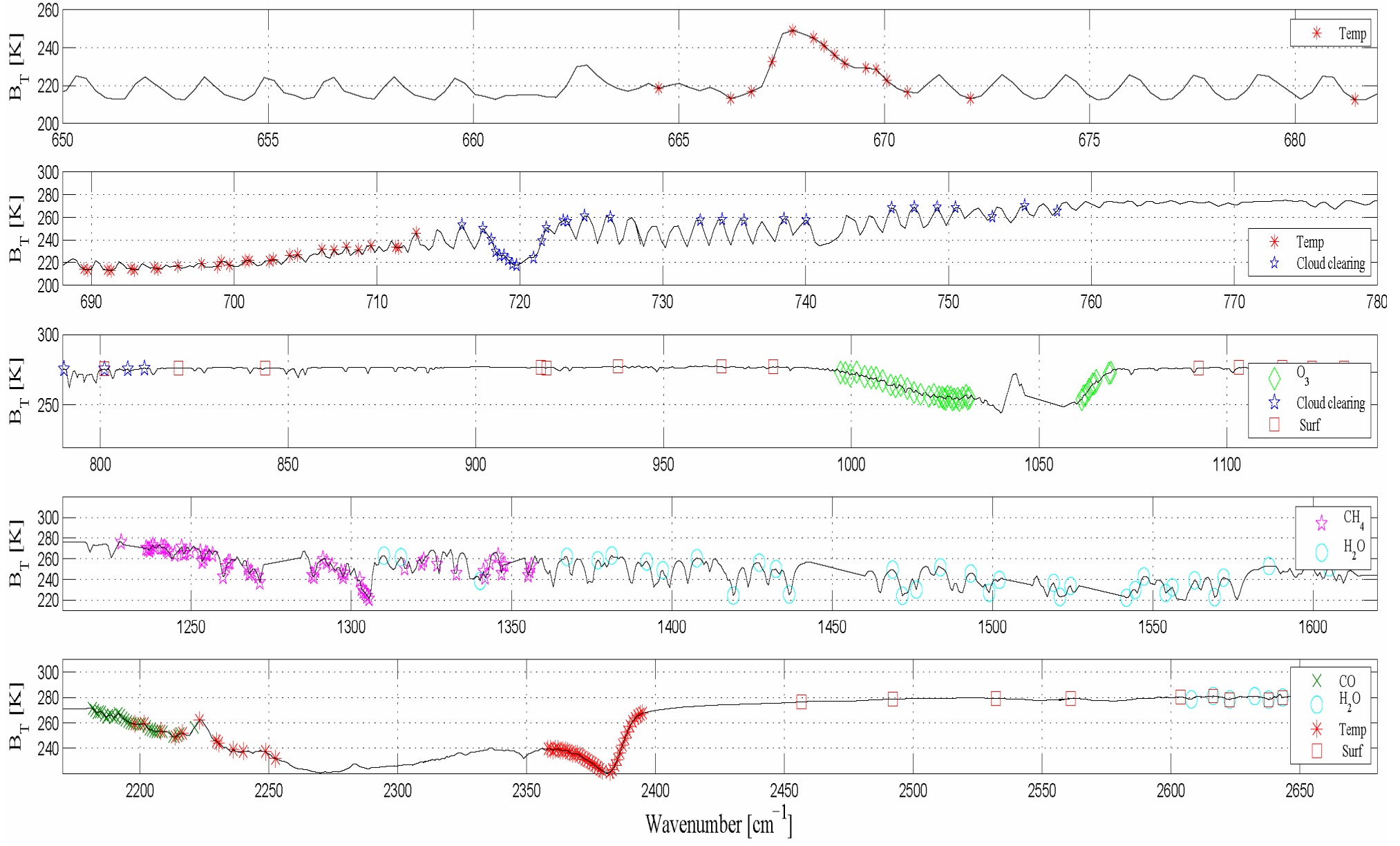
Cloudy regression (Step 1) and regression (Step 3) use most AIRS channels

Physical retrieval and cloud clearing steps use selected AIRS channels

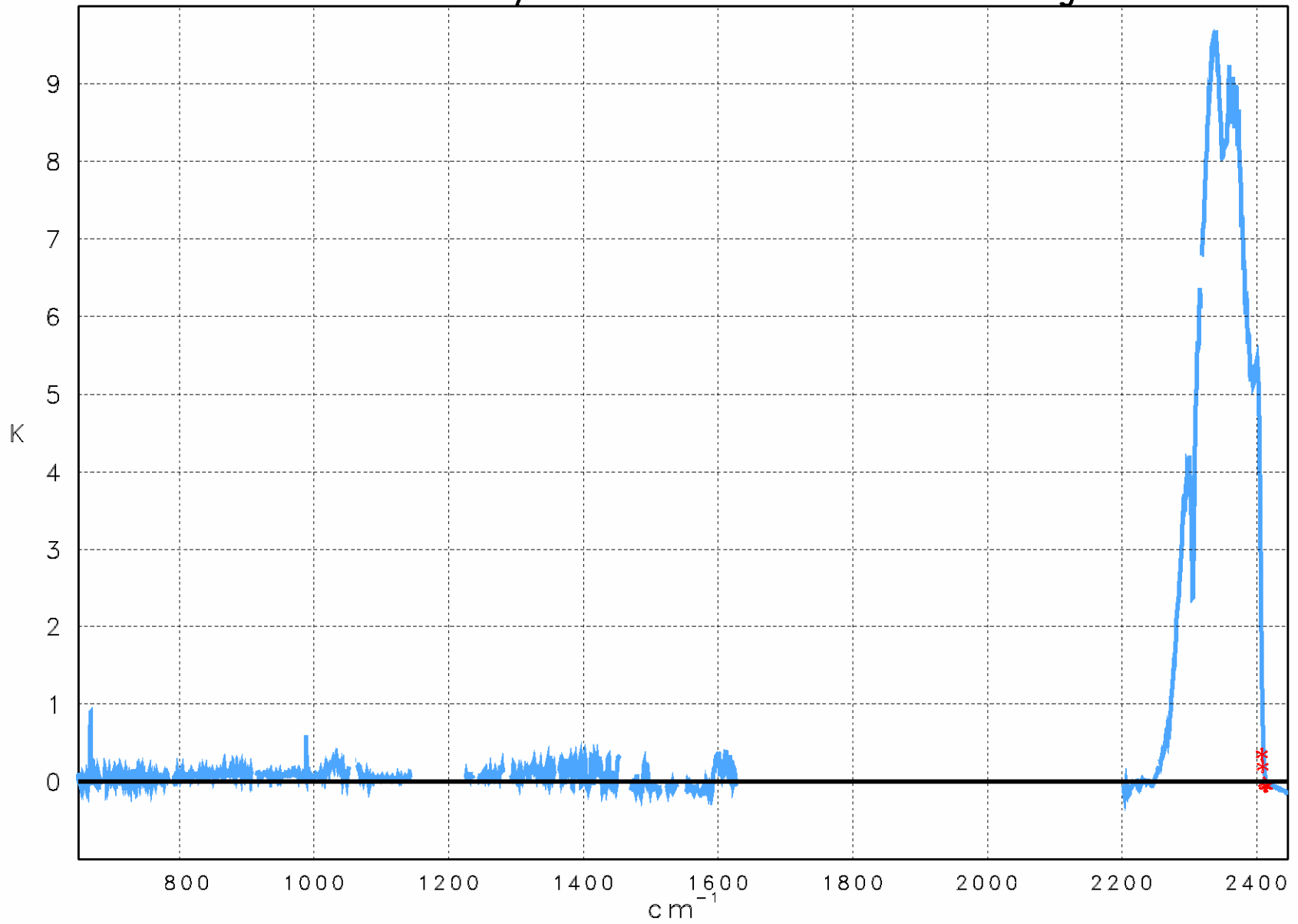
Version 5 AO does not include AMSU channels in regression or physical retrieval

Version 5 AO does not include AMSU related tests in error estimates

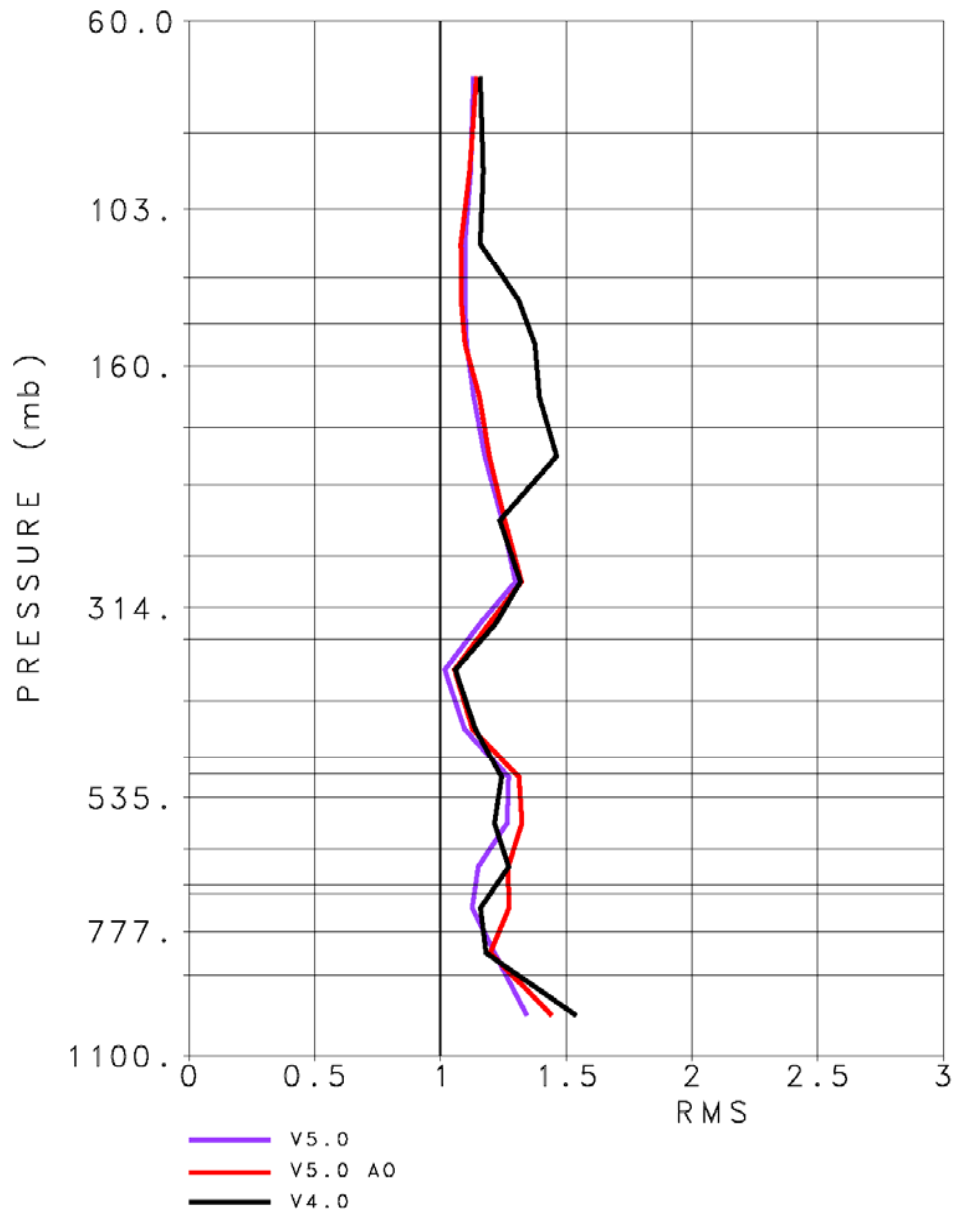
Version 5.0 Channels



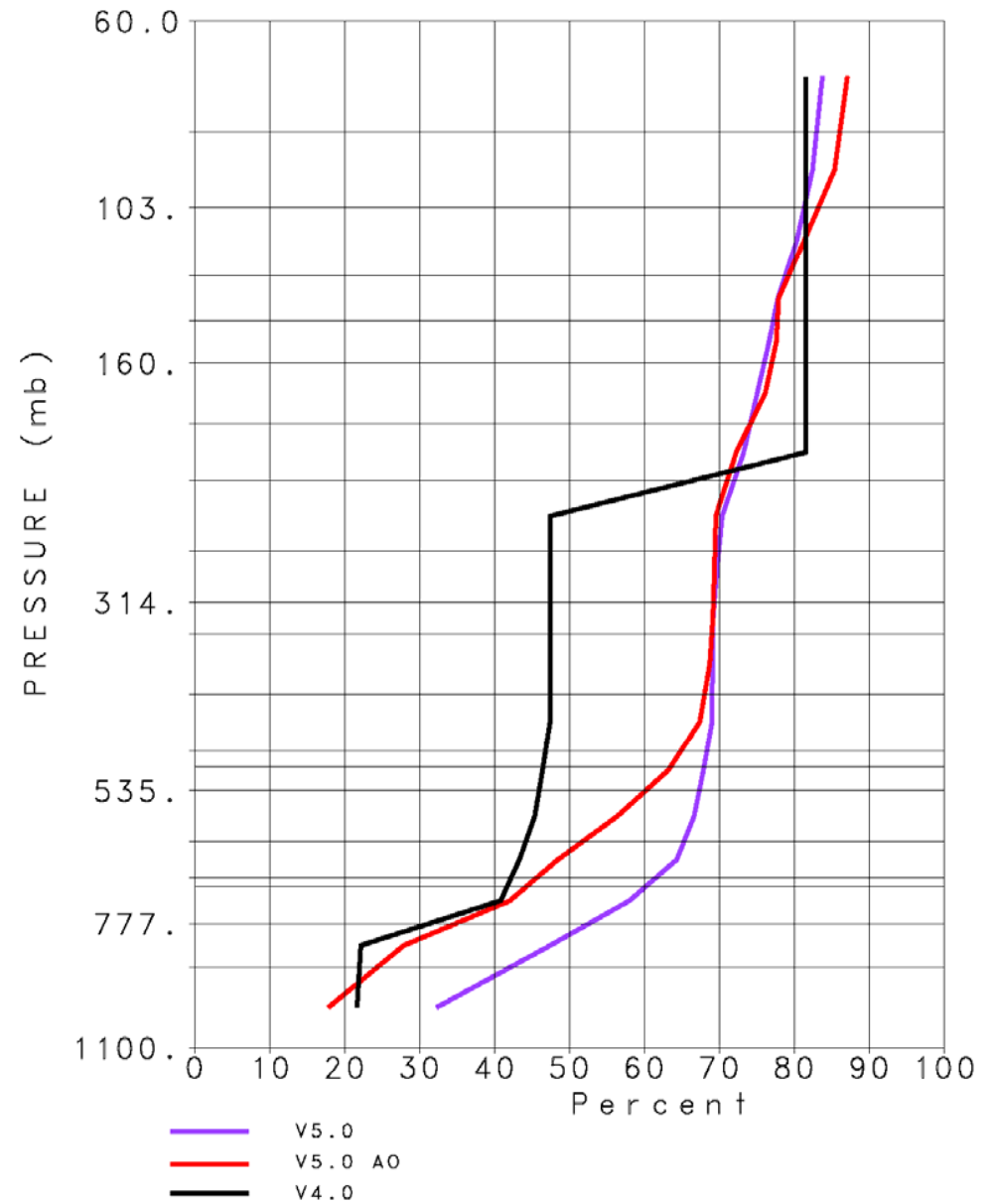
Mean Observed minus Computed
Brightness Temperature Difference (K)
Clear Ocean Day minus Clear Ocean Night



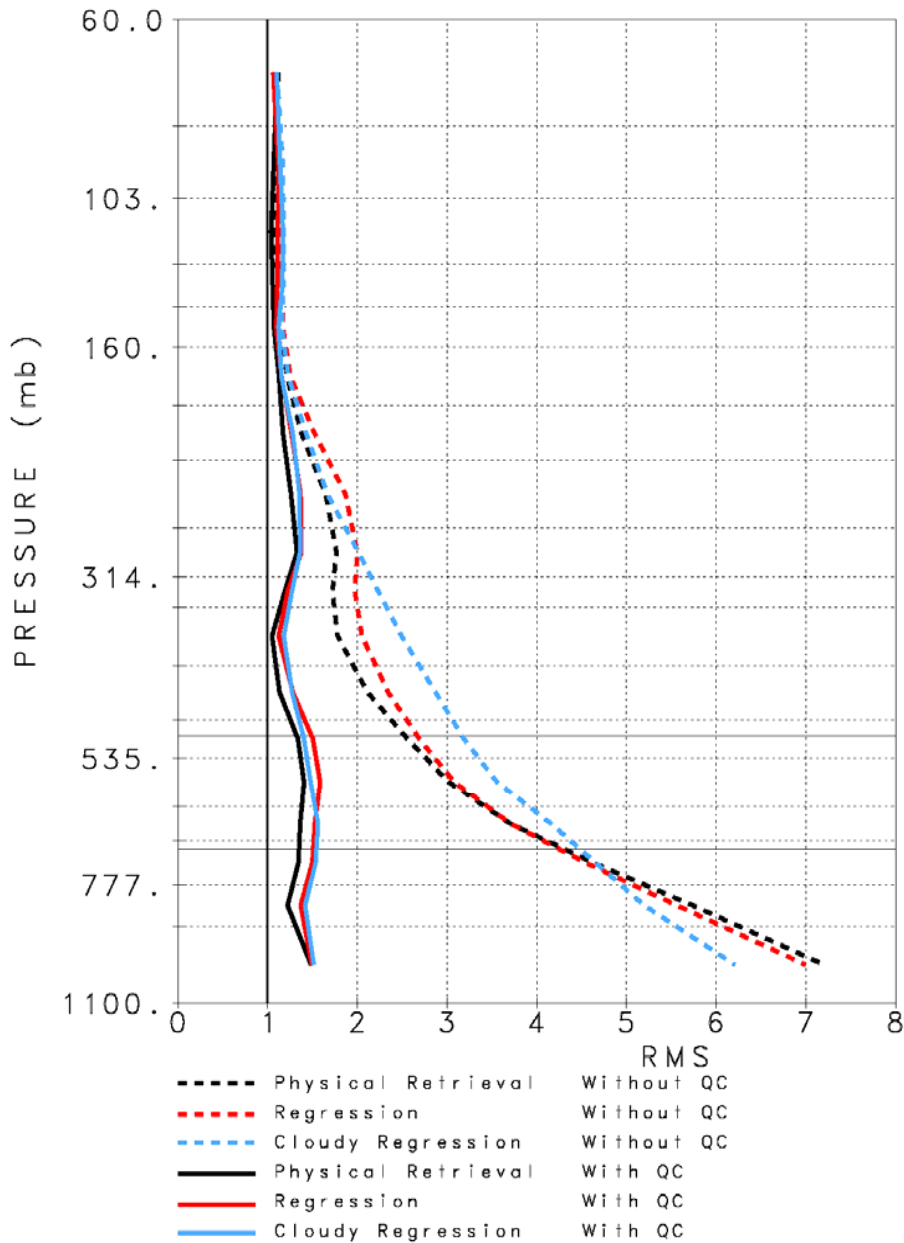
LAYER MEAN RMS TEMPERATURE ($^{\circ}\text{C}$)
 GLOBAL DIFFERENCES FROM "TRUTH"
 January 25, 2003
 Global



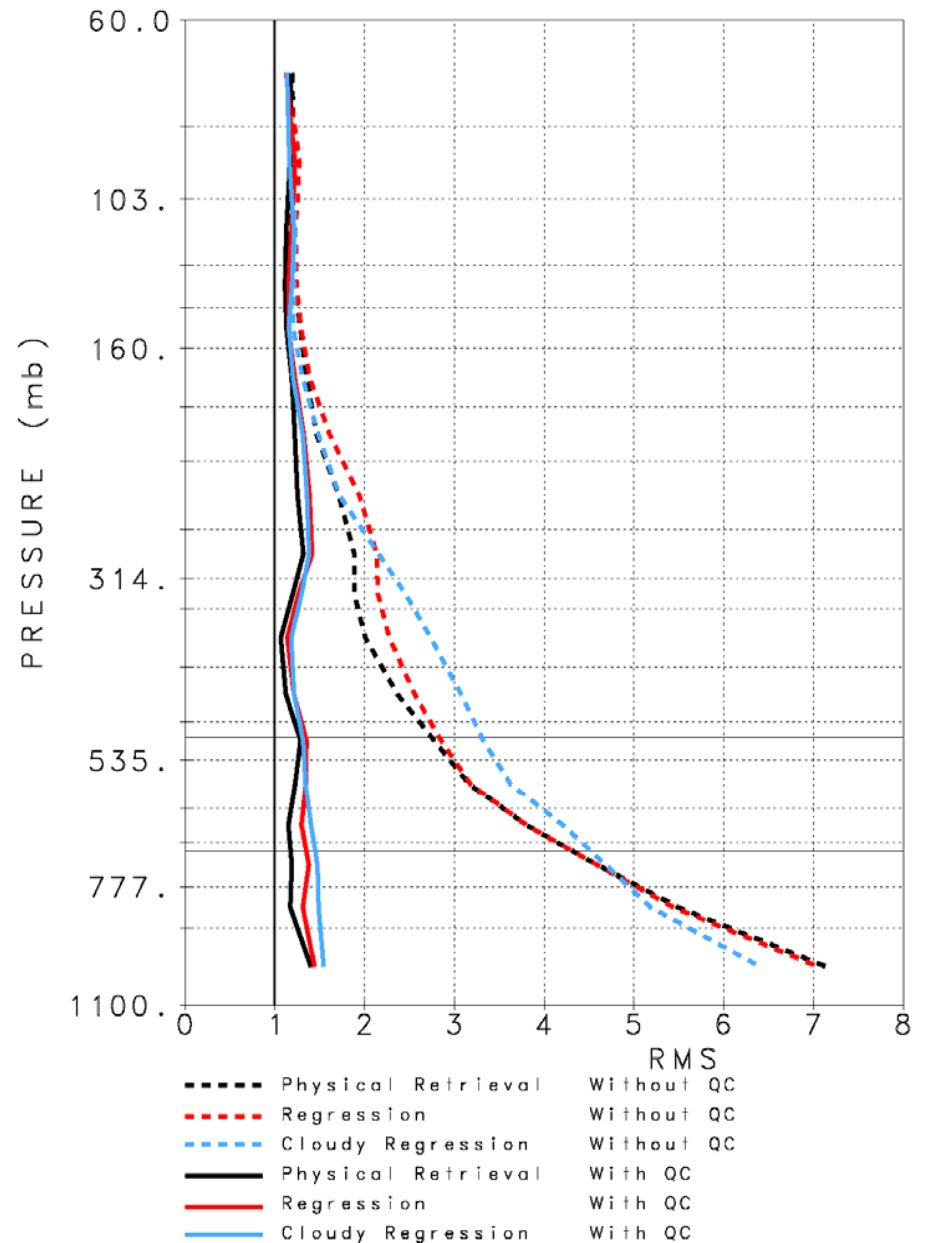
Percent of IR/MW Cases Included
 January 25, 2003
 Global



LAYER MEAN RMS TEMPERATURE ($^{\circ}\text{C}$)
 GLOBAL DIFFERENCES FROM "TRUTH"
 Version 5 AIRS Only
 Global
 January 25, 2003 Nighttime



LAYER MEAN RMS TEMPERATURE ($^{\circ}\text{C}$)
 GLOBAL DIFFERENCES FROM "TRUTH"
 Version 5 AIRS Only
 Global
 January 25, 2003 Daytime



Comparison of CrIS and AIRS

Both instruments are functionally equivalent

Both instruments have similar spectral coverage, spatial resolution

AIRS is a grating spectrometer

$$\nu / \Delta\nu \approx 1200 \quad \Delta\nu = 0.54 \text{ cm}^{-1} \text{ at } 650 \text{ cm}^{-1}$$

$$\Delta\nu = 2.25 \text{ cm}^{-1} \text{ at } 2670 \text{ cm}^{-1}$$

$f_i(\nu - \nu_i)$ is essentially Gaussian

$$\text{Channel spacing} = 2 \text{ channels per } \Delta\nu \quad 0.27 \text{ cm}^{-1} \text{ at } 650 \text{ cm}^{-1}; 1.13 \text{ cm}^{-1} \text{ at } 2670 \text{ cm}^{-1}$$

CrIS is an interferometer

Spectral characteristics of CrIS are poorer than AIRS

Noise characteristics of CrIS should be better than AIRS

Factors should roughly compensate each other

Spectral Characteristics of an Interferometer

Interferometer measures Fourier transform of the spectrum, $I(x)$ from $x= 0-L$ cm

Unapodized spectrum is Fourier transform of $I(x)$

$$\Delta\nu_{\text{un}} \approx \frac{0.6}{L} \text{ cm}^{-1}$$

Spectral response function is unlocalized and has negative sidelobes - undesirable

Apodized spectrum is Fourier transform of the product of $I(x)$ and the apodization function $A(x)$

Hamming apodization provides optimal balance between half-width and side lobes

$$\Delta\nu_{\text{HAM}} \approx \frac{0.9}{L} \text{ cm}^{-1} = \text{effective resolution of } I(x)$$

Spectral response function is highly localized

Spectral sampling = $\frac{1}{2L} \text{ cm}^{-1}$ independent of apodization

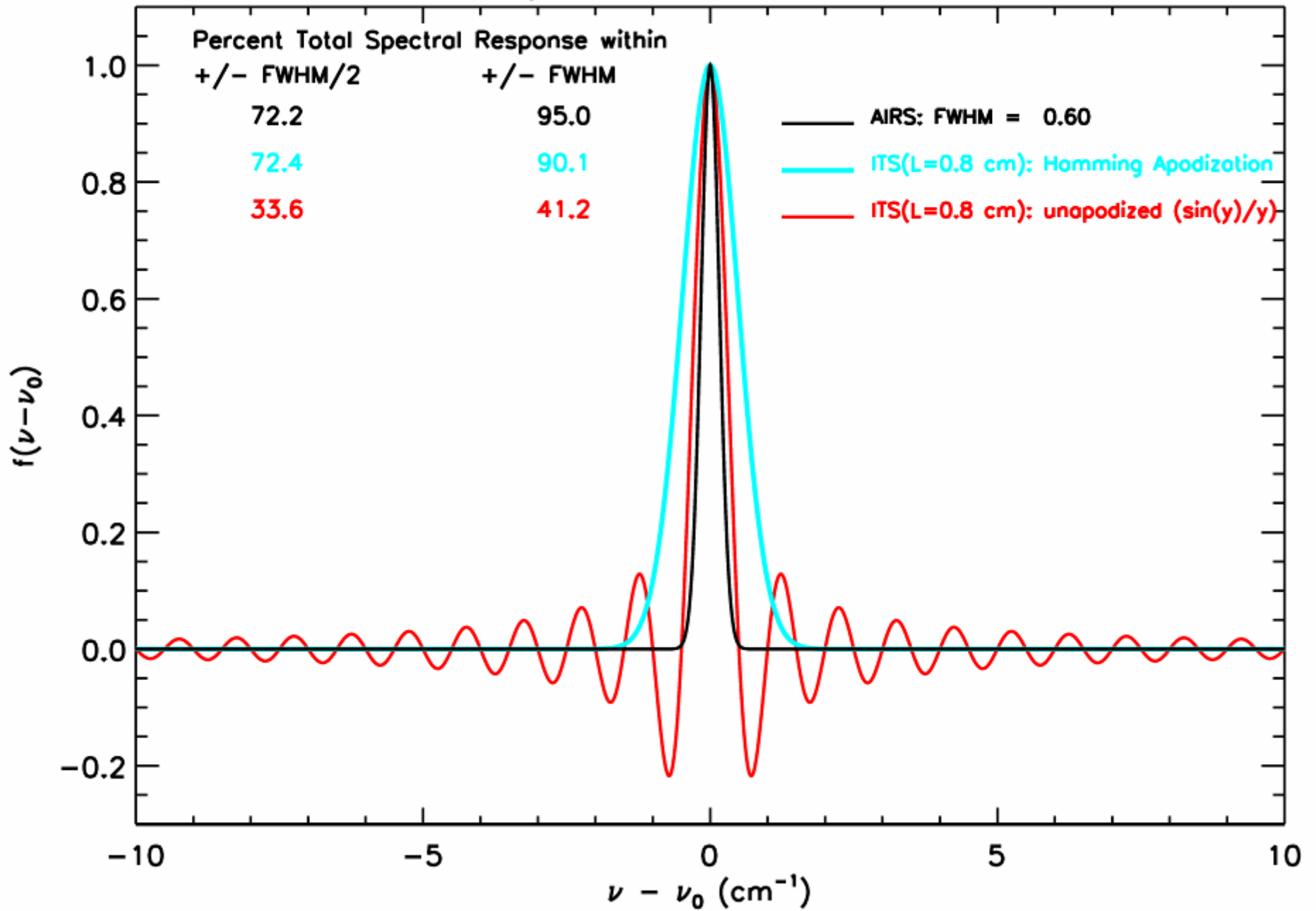
CrIS has 3 bands

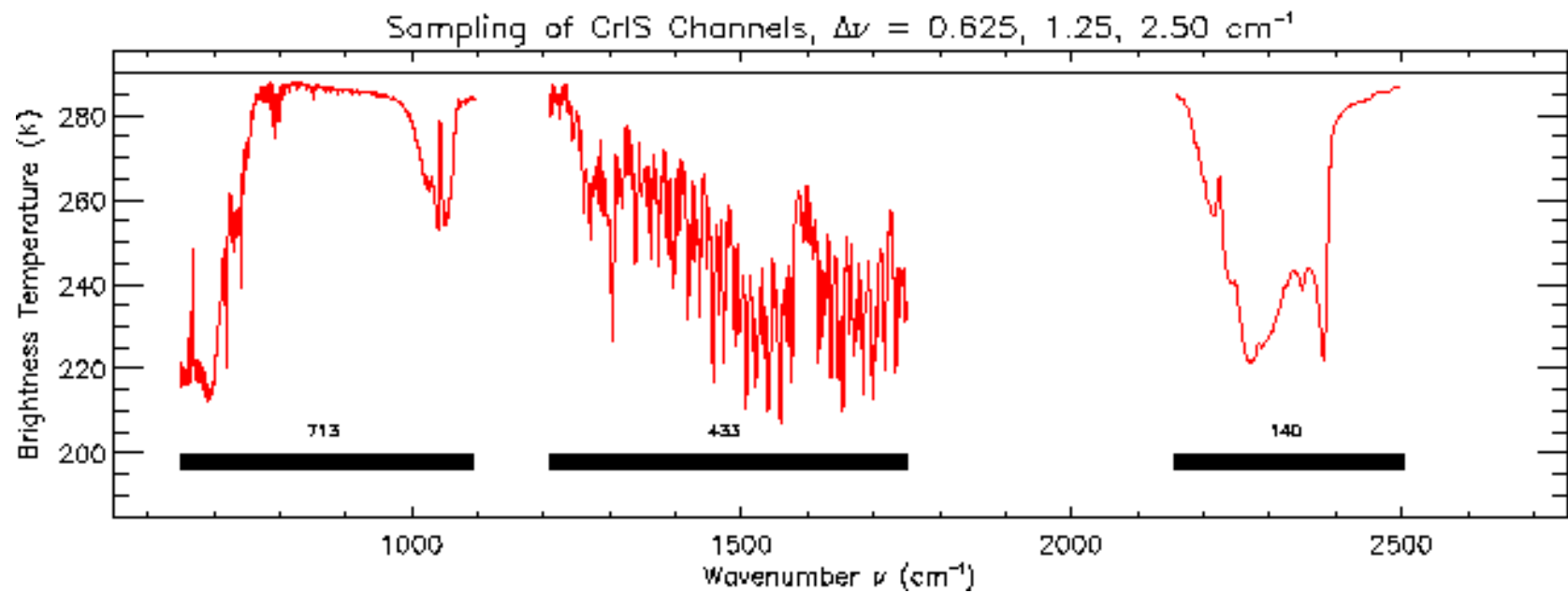
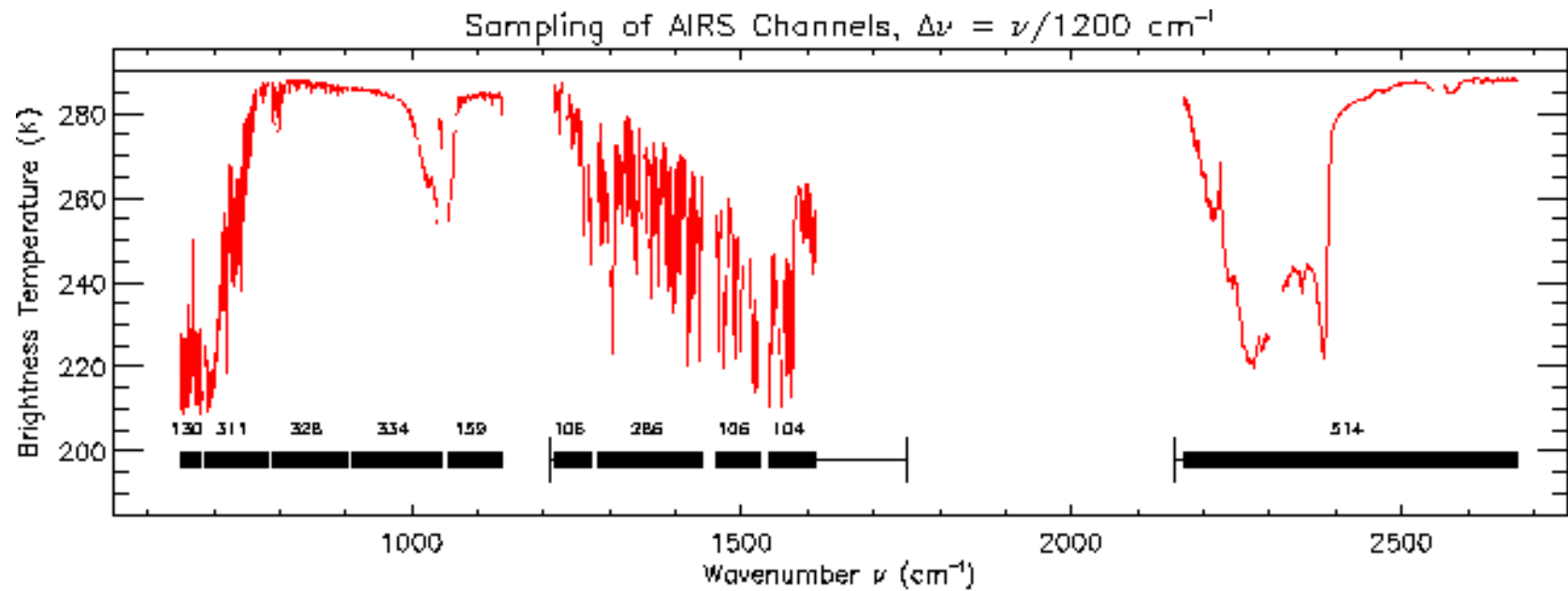
650 cm^{-1} - 1095 cm^{-1}	L = 0.8 cm	$\Delta\nu_{\text{HAM}} = 1.125 \text{ cm}^{-1}$	sampling = 0.625 cm^{-1}
1210 cm^{-1} - 1750 cm^{-1}	L = 0.4 cm	$\Delta\nu_{\text{HAM}} = 2.25 \text{ cm}^{-1}$	sampling = 1.25 cm^{-1}
2155 cm^{-1} - 2550 cm^{-1}	L = 0.2 cm	$\Delta\nu_{\text{HAM}} = 4.5 \text{ cm}^{-1}$	sampling = 2.5 cm^{-1}

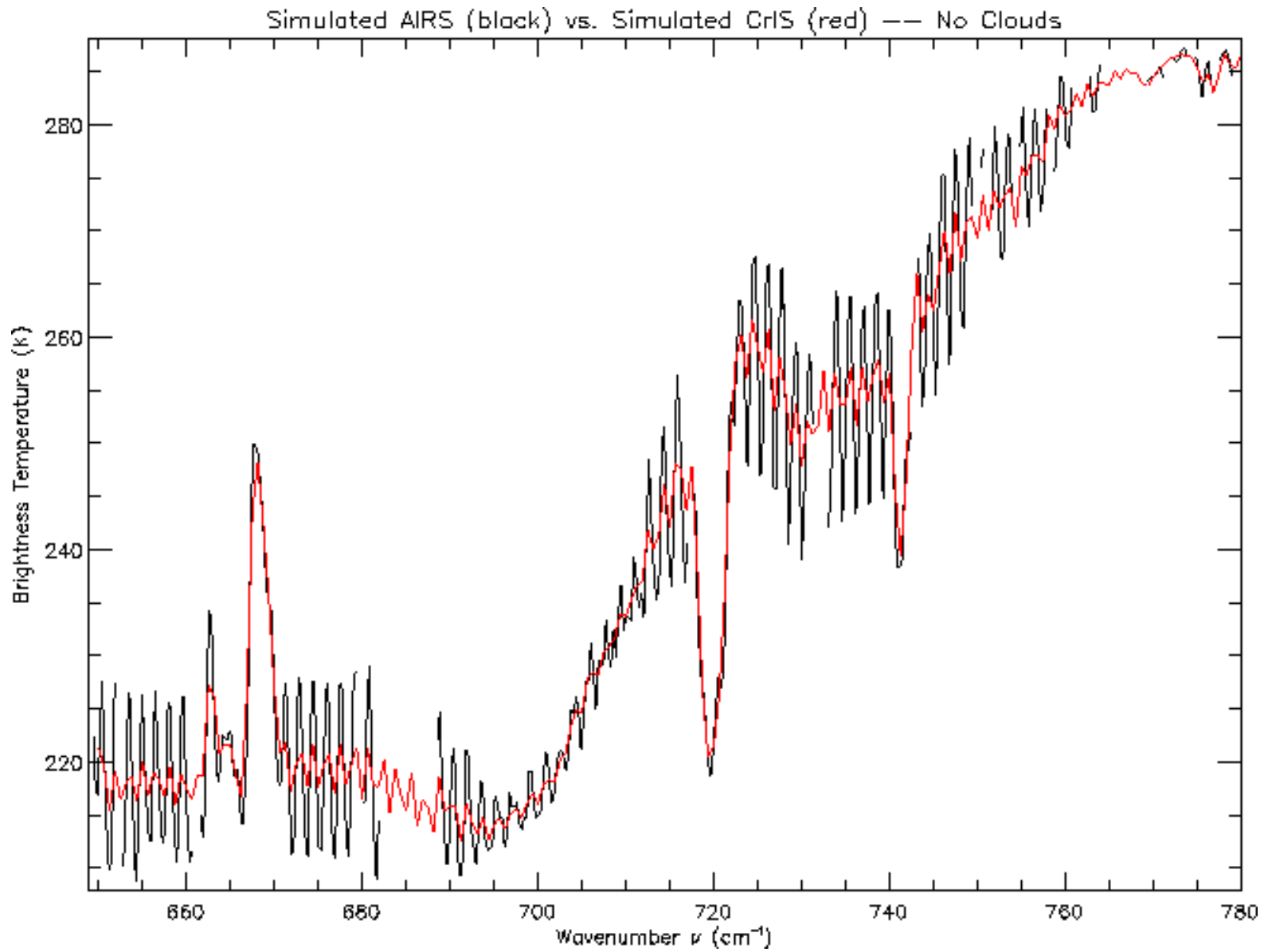
IASI has 1 band

645 cm^{-1} - 2760 cm^{-1}	L = 2.0 cm	$\Delta\nu_{\text{GAUS}} = 0.5 \text{ cm}^{-1}$	sampling = 0.25 cm^{-1}
--	------------	---	----------------------------------

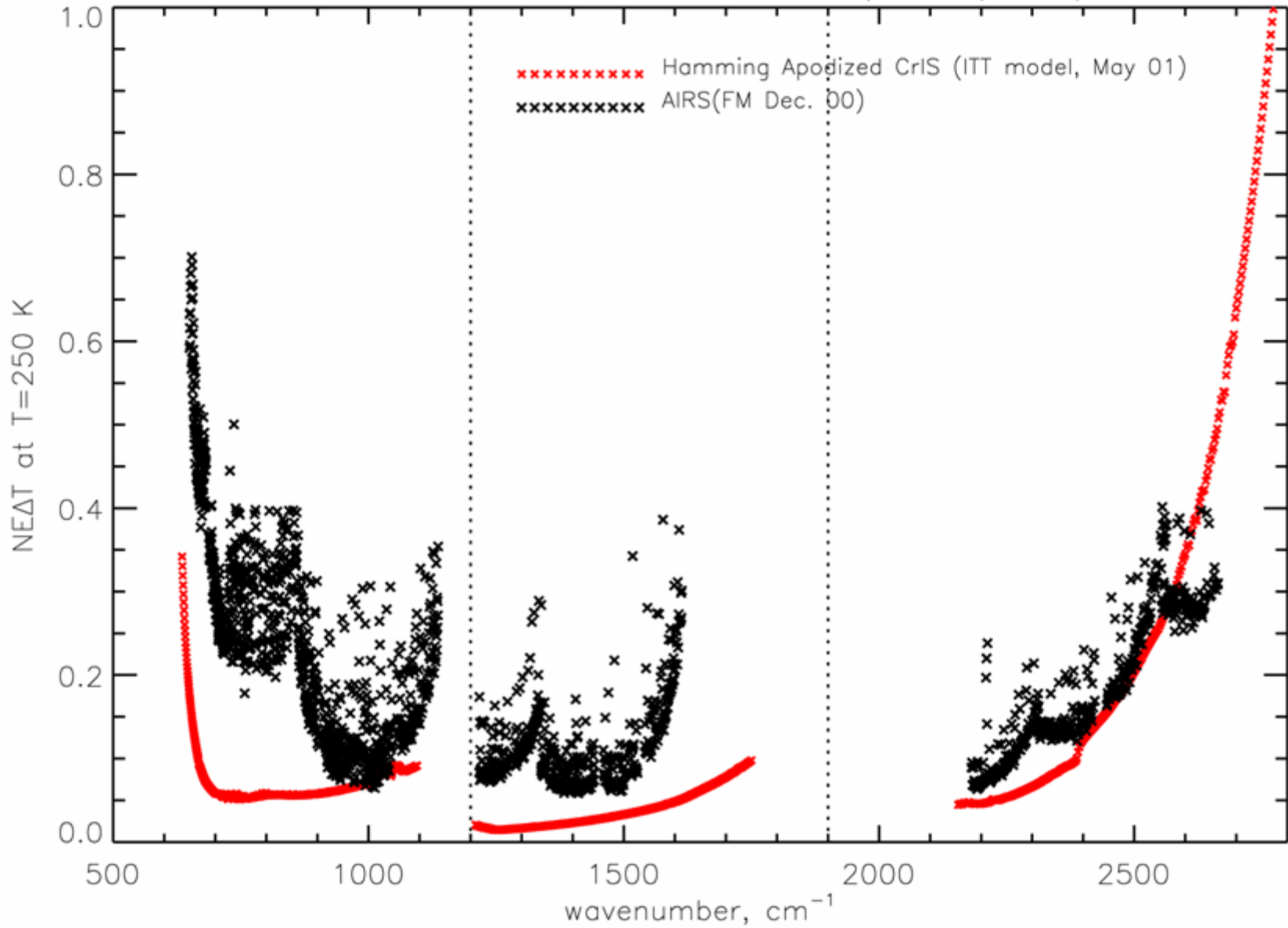
Channel Response Functions @ 720.50 cm⁻¹







AIRS measured noise versus CrIS ITT model (NE Δ T per spectral sample)



Advanced IR Imaging Sounders

Produce AIRS-like sounding capability but with higher spatial resolution

Use 2 D detector array technology - a few hundred by a few hundred detectors

Interferometers

2 D detector array images the ground

Interferogram provides spectrum for each detector - spatial pixel

Usually multiple detector arrays for different spectral ranges

Spatial pixels must be well co-aligned

Grating spectrometer

One detector dimension is spectral array (like AIRS)

Other detector dimension is linear spatial array

Instrument scans in other spatial dimension (like AIRS)

Same spectral channels for different spatial detectors must match well (low smile distortion)

Spatial pixels for entire channel set must match well (low keystone distortion)

Possible Future Missions

HES - GOES-S (2016) or GOES-T (2019)

Goal requirements are for AIRS spectral resolution, noise

680 cm^{-1} - 1040 cm^{-1} , 1210 cm^{-1} - 1645 cm^{-1} or 1689 cm^{-1} - 2150 cm^{-1} , 2150 cm^{-1} - 2400 cm^{-1}

5 km contiguous spatial resolution

3000 km x 3000 km spatial coverage in 35 minutes

STATUS of HES - 3 vendors finished formulation phase with satisfactory designs

2 spectrometer designs, 1 interferometer design

Project goal is to have an REP to down-select to single vendor in near future

This approach will lead to a HES on GOES-S

No money is committed yet for this step by either NOAA or NASA

ARIES - NASA polar orbiting satellite

2 D detector array spectrometer design

Will have AIRS sounding capability at 1 km spatial resolution

Further improvements in AIRS sounding capability

Especially around storms and hurricanes

Bob Atlas, Head of AOML, really wants ARIES

We have to convince NASA to fly it

Important for global weather, severe storms, climate

Summary

Accurate quality controlled temperature soundings are produced from AIRS under most cloud conditions

Most tropospheric temperature sounding information comes from the 4.2 μm spectral region

Soundings are as accurate during day as at night

AMSU observations aid in cloud clearing and quality control but are not critical

Accurate AIRS only retrievals are also produced globally but with lower tropospheric yield

It is essential to have spectral coverage from 2360 cm^{-1} - 2400 cm^{-1} with low $\text{NE}\Delta\text{T}$ to achieve this

GOES S or GOES T will have an advanced IR sounder with no microwave instrument

Spectral coverage to 2400 cm^{-1} with low $\text{NE}\Delta\text{T}$ is critical

GIFTS extends only to 2150 cm^{-1} - this is sub-optimal

