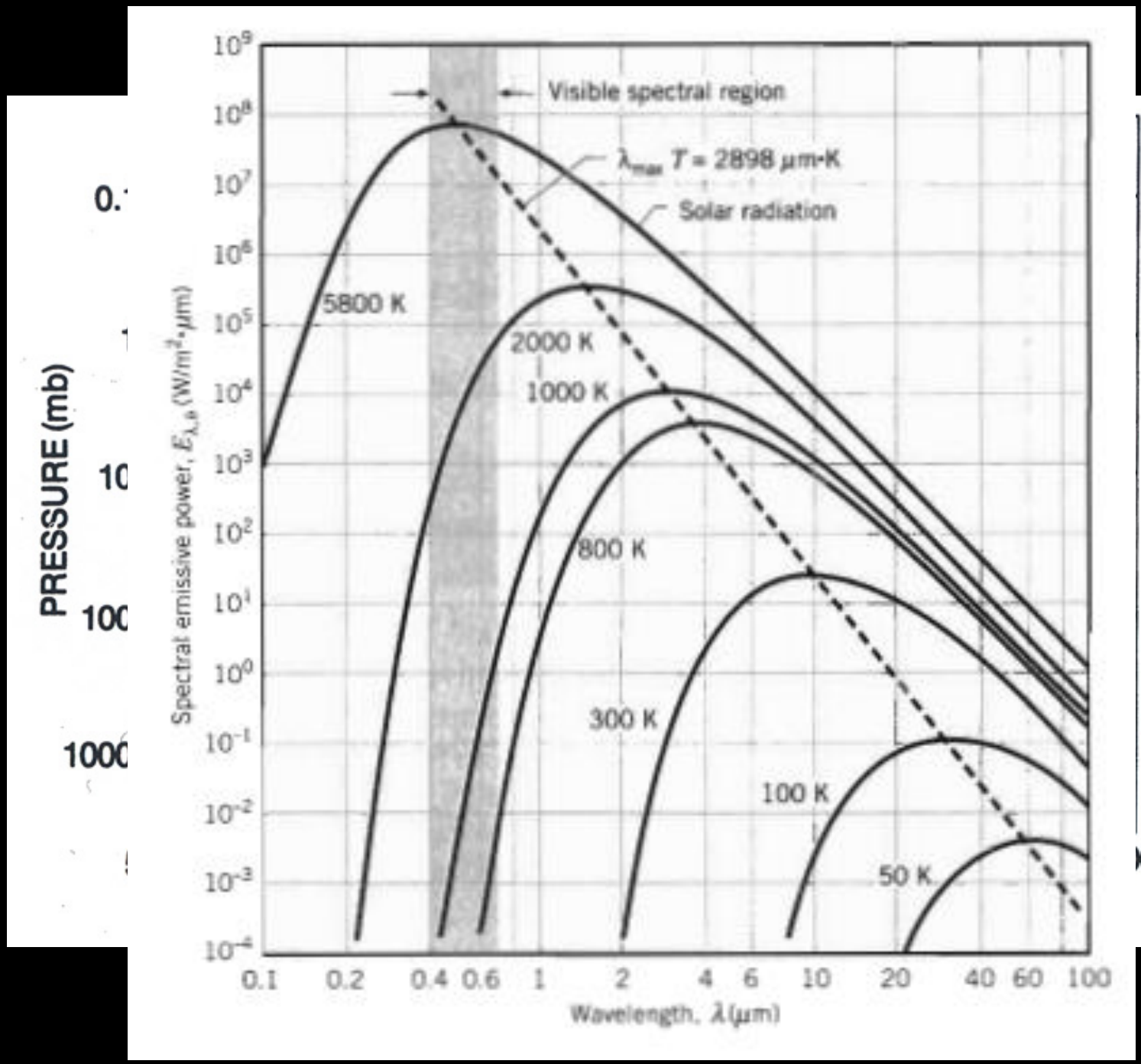
Atmospheric Radiative Transfer Modeling

Conor A. Nixon
Richard K. Achterberg
Department of Astronomy
University of Maryland
June 26th 2012

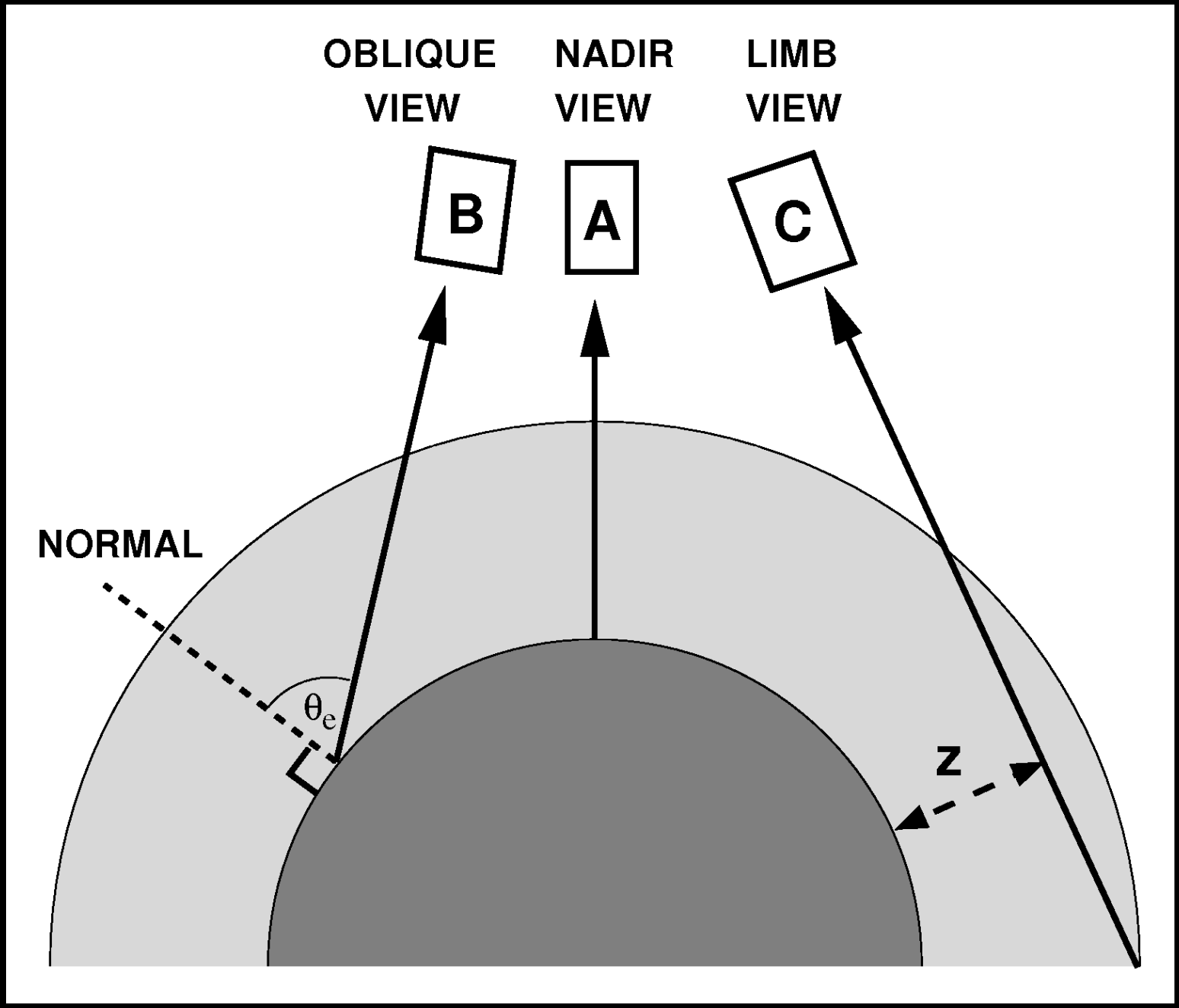
Overview

- Part 1 (Nixon):
  - Statement of problem
  - Parameterizing the atmosphere
  - Forward model/synthetic spectrum calc.
  - Sample results
- Part 2 (Achterberg):
  - Information content of thermal IR spectra
  - Retrieval of atmospheric structure
  - More sample results

Planetary Thermal Emission



Remote sensing



1D-radiative transfer

- Absorption (Beer-Lambert Law):

$$dI = -Ik\rho dz$$

- Where: I= radiance (W cm^{-2} sr^{-1} (freq)$^{-1}$

  k= absorption co-efficient <u>*and*</u> scattering

  ρ= absorber density

  z= distance along optical path

- Similarly emission (Kirchoff's law):

$$dI = Jk\rho dz$$

Schwarzchild Equation

- Combining these two is known as the Schwarzchild equation:

$$dI = Jk\rho dz - Ik\rho dz$$

$$\frac{dI}{d\chi} = I - J; \quad \chi = -k\rho dz$$

- Where we have defined the optical depth χ
- Note that the source function J is often the Planck function when the atmosphere is in local thermodynamic equilibrium (LTE):

$$B_\upsilon(T) = \frac{2h\nu^3}{c^2 \exp\left[(h\nu / kT - 1)\right]}$$

Solution to Schwarzchild Equation

- Integrating the Schwarzchild equation from $\chi=0$ to ∞ gives the emerging radiance at the top of the atmosphere:

$$I_0 = \int_0^\infty J e^{-\chi} \, d\chi$$

- So the forward radiance calculation is therefore typically a numerical computation of the form:

$$I_0 = \sum_{i=1}^{n} B_i \left(\tau_{i+1} - \tau_i \right)$$

- Where $\tau=e^{-\chi}$ is the transmission (range 0 to 1).

Solution to Schwarzchild Equation

- Integrating the Schwarzchild equation from $\chi=0$ to ∞ gives the emerging radiance at the top of the atmosphere:

$$I_\infty = \int_0^\infty J e^{-\chi}\, d\chi$$

- If we define $\tau=e^{-\chi}$ as the transmission (range 0 to 1), change the integrating variable to altitude (z) and add a planetary surface then:

$$I_\infty = \int_0^{z_\infty} \frac{\partial \tau(z_\infty, z)}{\partial z} B(T(z))\, dz + \varepsilon_s B(T_s)\tau_s + (1-\varepsilon_s)\tau_s \int_{z_\infty}^{0} \frac{\partial \tau(0,z)}{\partial z} B(T(z))\, dz$$

Emission from each layer at B(T) multipled by transmission to space

Surface emission at $B(T_s)$ transmitted to space

Downward radiation from atmosphere $B(T_s)$ reflected to space from surface

Numerical computation

- For unit surface emissivity we can write the integration as a sum over atmospheric model layers:

$$I_\infty = B_s \tau_{N_L} + \sum_{l=1}^{N_L} \left[B_l \exp\left(-\sum_{i=1}^{l} \Delta\chi_i \right) \right]$$

- Typically the opacity of each layer $\Delta\chi_i$ has contributions from three sources:

$$\Delta\chi_{L,i}(\tilde{\nu}) = \sum_{j=1}^{N_g} \left[k_j(\tilde{\nu}) q_{ij} \right] \rho_i \Delta z_i$$

SPECTRAL LINES

$$\Delta\chi_{C,i}(\tilde{\nu}) = \sum_{j=1}^{N_g} \sum_{k=1}^{N_g} \alpha_{jk}(\tilde{\nu}) q_{ij} q_{ik} \left(\frac{p_i}{p_0} \right)^2 \left(\frac{T_0}{T_i} \right)^2 \Delta z_i$$

COLLISION-INDUCED OPACITY (CIA)

$$\Delta\chi_{P,i}(\tilde{\nu}) = \sum_{j=1}^{N_P} \sigma_j(\tilde{\nu}) n_{ji} \Delta z_i$$

PARTICULATES

Definition of terms

- k_j = spectral line absorption co-efficient per unit mass for j^{th} of N_g gases in atmosphere
- q_{ij} = volume mixing ratio of jth gas at level i
- P_i = total atmospheric mass density at layer i
- Δz_i = thickness of layer i
- α_{jk} = spectral CIA co-efficient for gas pair (j,k) at pressure p_0 and temperature T_o
- p_i = pressure of layer i.
- T_i = temperature of layer i.
- σ_j = extinction cross-section of jth particle type
- n_{ji} = number density of jth particle type in layer i.

Spectral Line Formation I

- Spectral line opacity is defined by the line strength and shape:

$$k_\nu = Sf\left(\nu - \nu_0\right)$$

- where

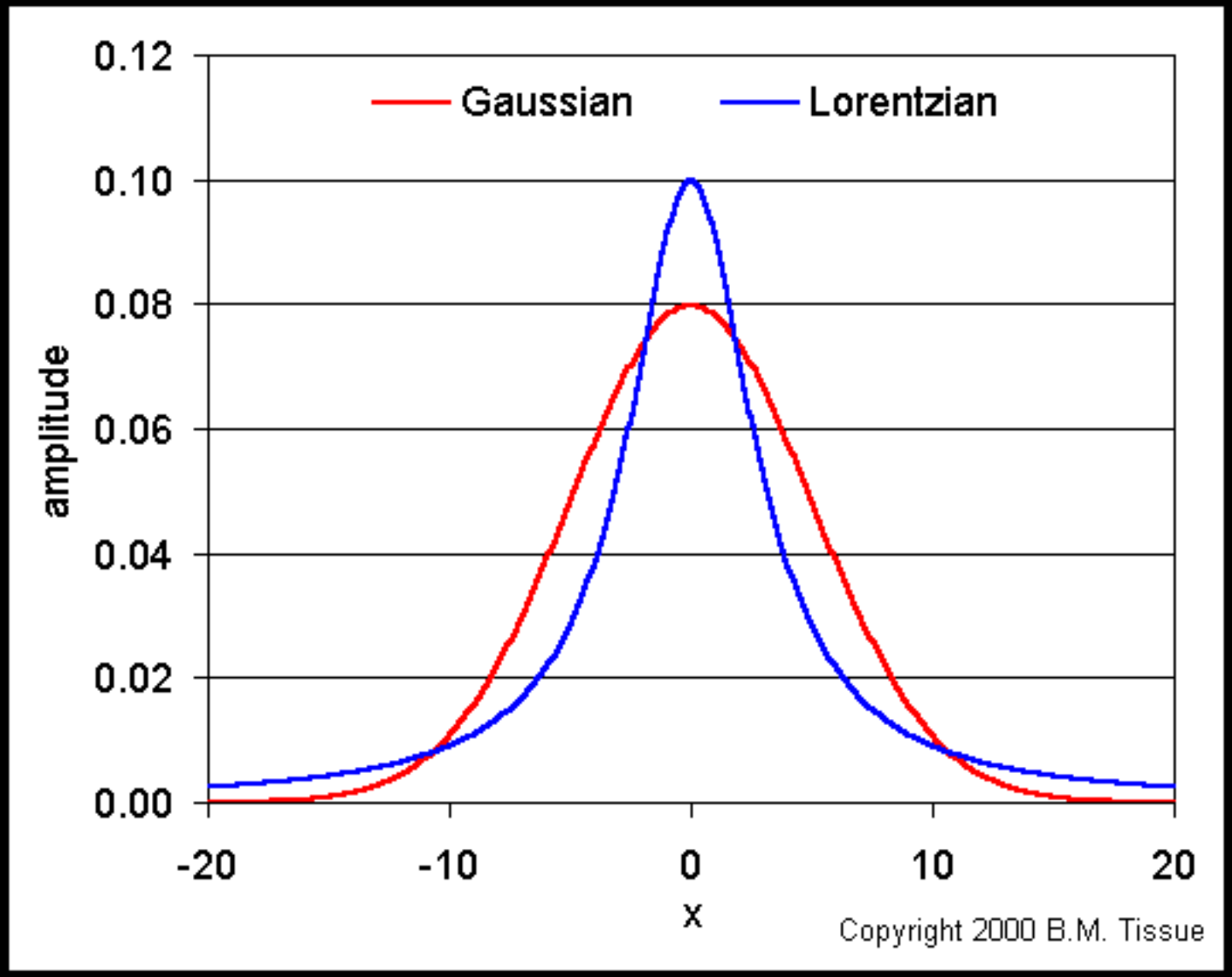
$$S = \int k_\nu \, d\nu$$

- The line shape function *f* is often given by the Voigt profile, a combination of Lorentz (pressure) and Doppler (temperature) broadening:

$$f\left(\nu - \nu_0\right) = \int_{-\infty}^{+\infty} \frac{\left(\alpha_L/\pi\right)}{\left[\left\{\left(\nu - \nu_0\right) - \left(u\nu_0/c\right)^2\right\} + \alpha_L^2\right]} \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(\frac{-mu^2}{2kT}\right) du$$

- Where k, h and c are the usual constants; m is the molecular mass, T is temperature and α_L is the Lorentzian HWHM.
- α_L and S are usually obtained from tabulated line lists.

Line broadening



- The Voigt profile (previous slide) combines both Doppler and Lorentz line shapes.

Spectral Line Formation II

- However we must allow for temperature dependence.
- For α_L:

$$\alpha_L(P,T) = \alpha_{L.0}\frac{P}{P_0}\left[\frac{T_0}{T}\right]^n$$

- Where the parameter 'n' is known as the 'temperature dependence of width'.
- For S:

$$S = S_0\frac{V_0 R_0}{VR}\exp\left\{\frac{hc}{k}E''\left[\frac{1}{T_0}-\frac{1}{T}\right]\right\}$$

- Where E'' is the lower state energy of the transition, and R and V are the rotational and vibrational partition functions:
- For R: $R(T) = T^x$ where x=1 for linear molecules
  x=1.5 otherwise
- For V can use: $V(T) = \prod_j \left(1-\exp\left(-h\nu_j/kT\right)\right)^{-g_j}$
- quantum harmonic oscillator approximation, with frequencies ν_j and degeneracies g_j

Where does opacity data come from? I: spectral lines

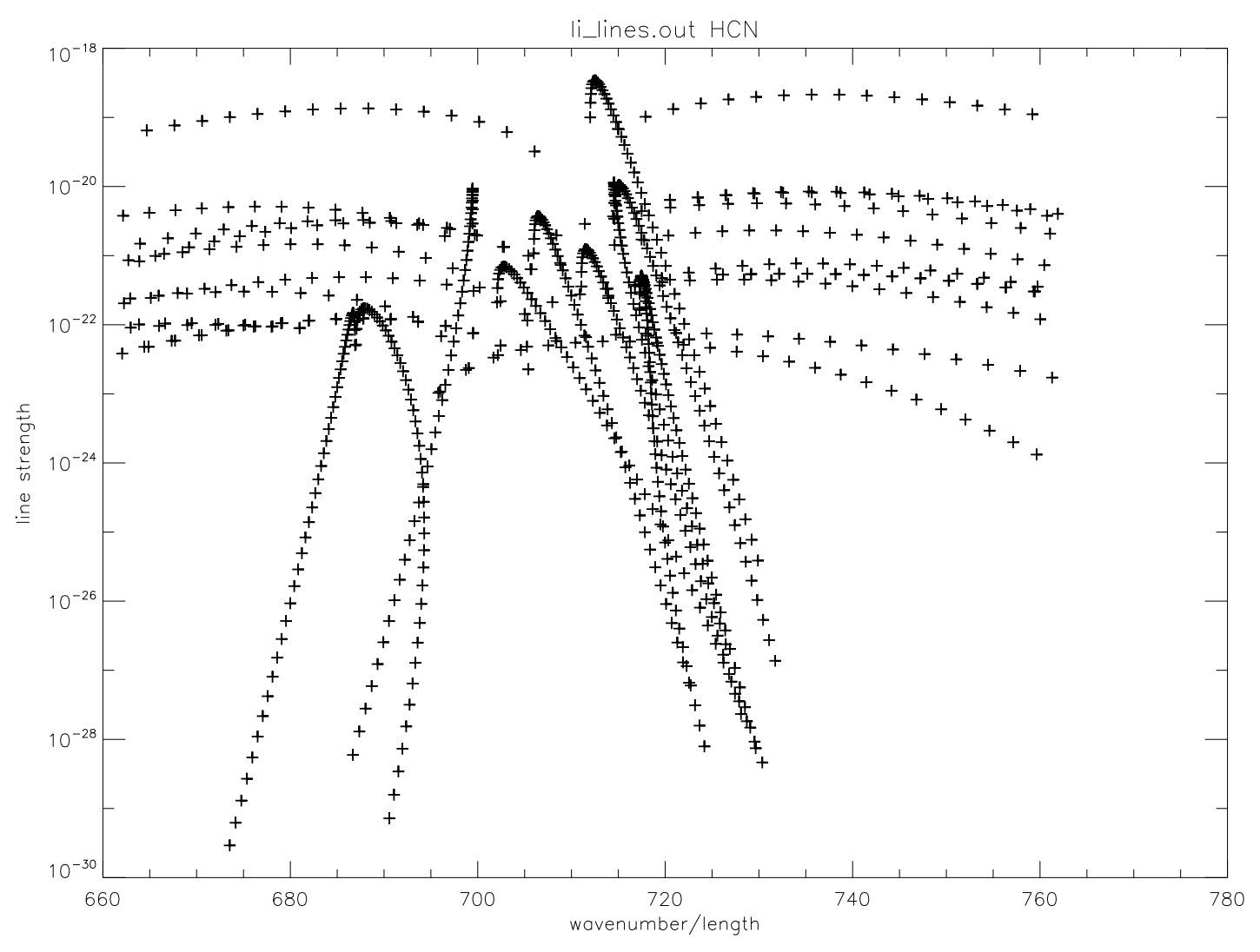
- For spectral lines, position, strength and broadening and other information is available in line atlases: the two main public ones being:
  - GEISA: Gestion et Etude des Informations Spectroscopiques Atmosphériques (Management and Study of Atmospheric Spectroscopic Information): best coverage for planets

    http://ether.ipsl.jussieu.fr/etherTypo/?id=950
  - HITRAN: **hi**gh-resolution **tran**smission molecular absorption database: best coverage for Earth gases

    http://www.cfa.harvard.edu/hitran/

Example line strengths

- Example of line positions and strengths for HCN v_2 band at 712 cm^{-1}



Exact or approximate?

- The calculation of spectral lines (esp. the Voigt func.) is slow and computationally intensive.
- Dense bands may have 10^4-10^5 lines: e.g. CH_4 v_4 band, ~25,000 lines from 1100-1500 cm^{-1}.
- Therefore approximate methods sometimes used.
- Several decades ago, analytical <u>band models</u> were popular:
  - 'Regular' Model (Elsasser): assumes grid of identical strength lines spaced by δ:

$$\tau_\nu = \exp\left(-\sum_{-\infty}^{+\infty} k_{\nu-n\delta}\rho z\right)$$

… so only have to calculate line shape for one line!!!

  - 'Random' Model (Goody): assumes lines have some probability distribution of strengths:

$$\bar{\tau} = \exp\left(-\sum_{i=1,N} \frac{W_i}{\Delta\nu}\right)$$

$$W = \int_{-\infty}^{+\infty} k_\nu m \, d\nu = Sm$$

$$P(S) = \frac{1}{S}\exp\left(-\frac{S}{S_m}\right)$$

Correlated-k approximation

- The most popular approximate method for rapid radiative transfer computations in recent years is the <u>correlated-k</u> method.
- This technique uses a frequency analysis of the fundamental line distributions, replacing the slow computation of individual lines with a parameterization of the cumulative absorption co-efficient distribution in each spectral bin.

- Freq dist.:

$$f(k_i) = \frac{1}{\nu_2 - \nu_1} \sum_j^M \left| \frac{\Delta \nu_j}{\Delta k_i} \right| W(k_i, k_i + \Delta k_i)$$

- Cum. dist g(k):
- And inverse, k(g):

$$g(k_n) = \sum_{i=1}^{n} f(k_i) \Delta k_i; \quad k_n(g) = g^{-1}(k_n)$$

Correlated-k approximation

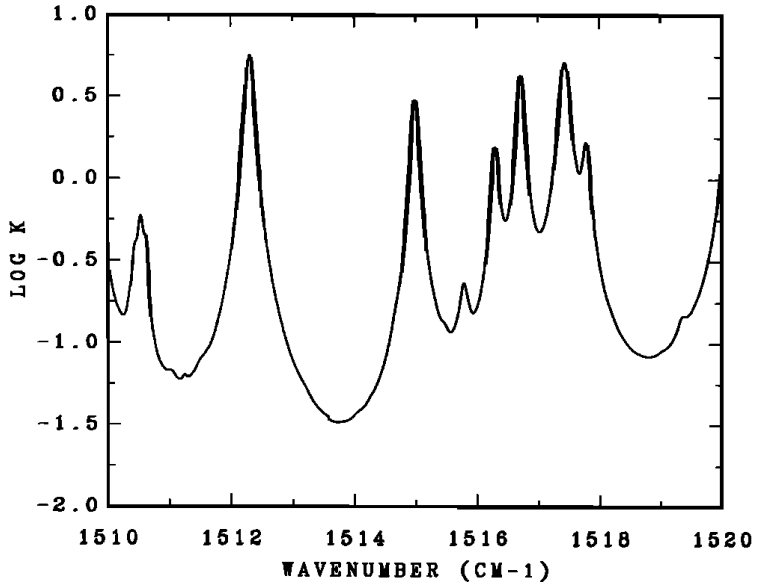


Fig. 1*c*

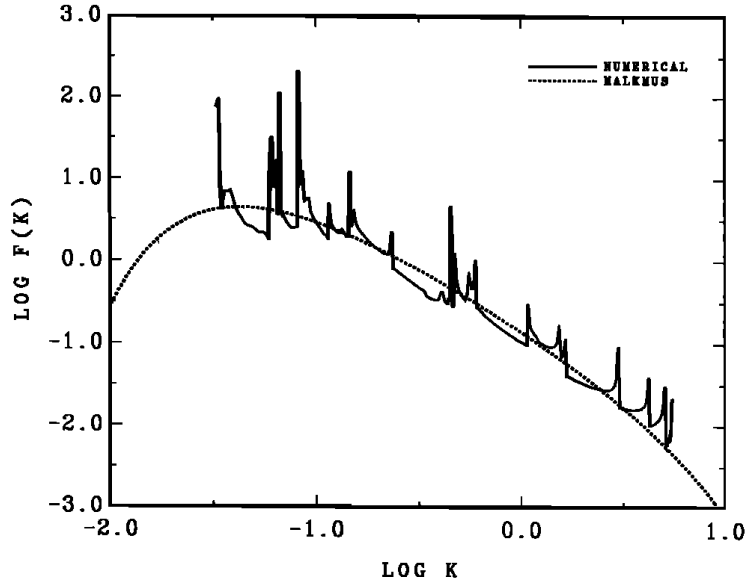
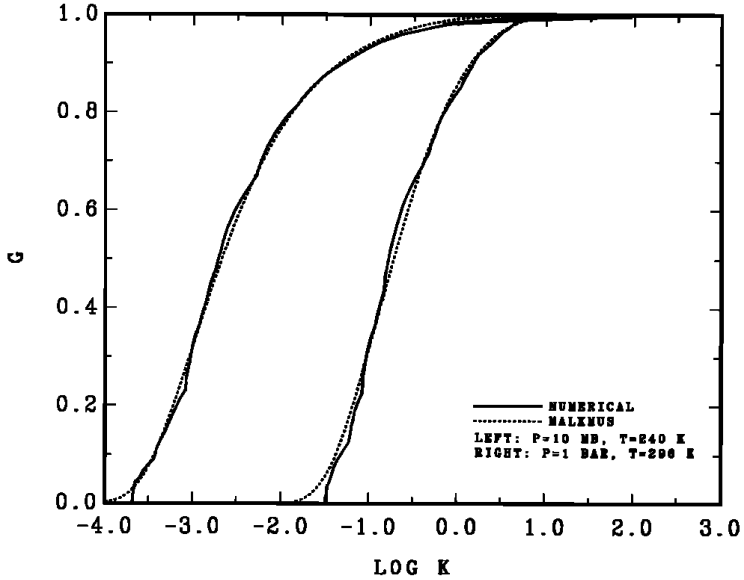
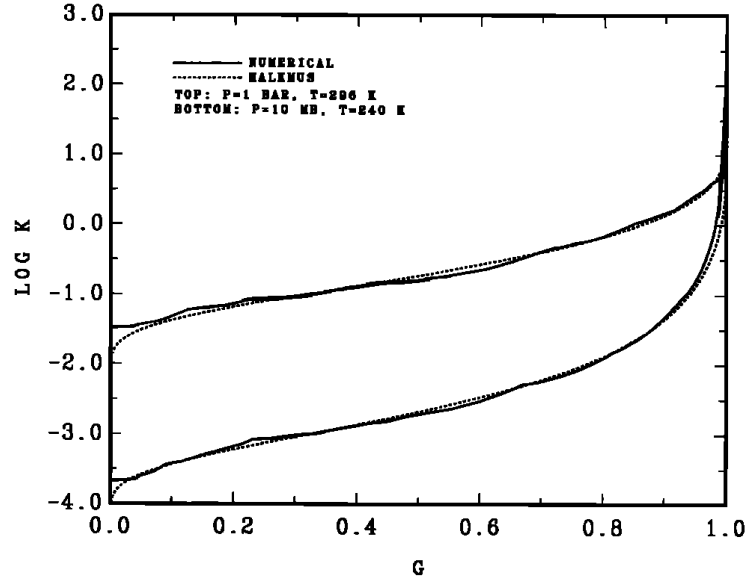


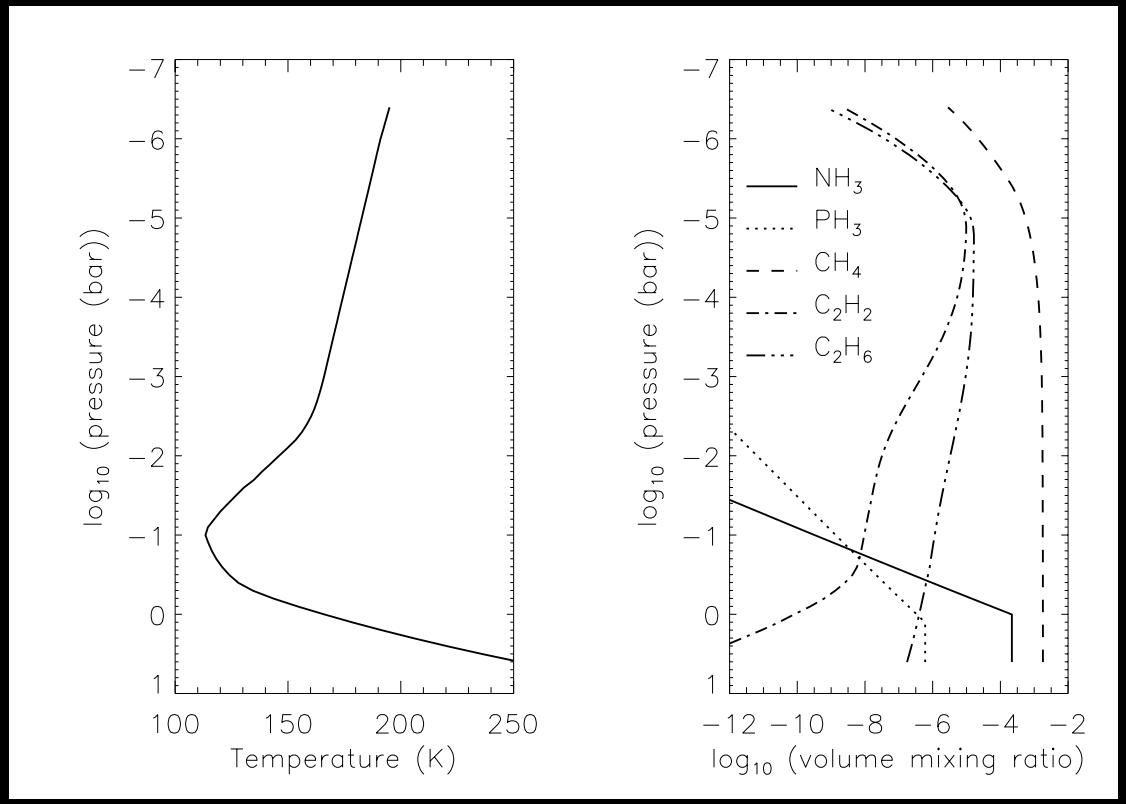
Fig. 1*d*





Model Atmosphere

- The <u>model atmosphere</u> defines the vertical (1D) dependence of atmospheric quantities including:
- **Temperature**
- **Gas abundances**
- **Particle abundances**
- E.g. Jupiter model from Nixon et al. (2007):



Some further definitions

- Weighting function: the opacity contribution from each model layer:

$$WF(i) = \Delta\tau_i = \exp\left(-k_i \rho_i \Delta z_i\right)$$

- Contribution function: the WF multiplied by the Planck function of the layer:

$$CF(i) = B\left(T_i\right)\Delta\tau_i = B\left(T_i\right)\exp\left(-k_i \rho_i \Delta z_i\right)$$

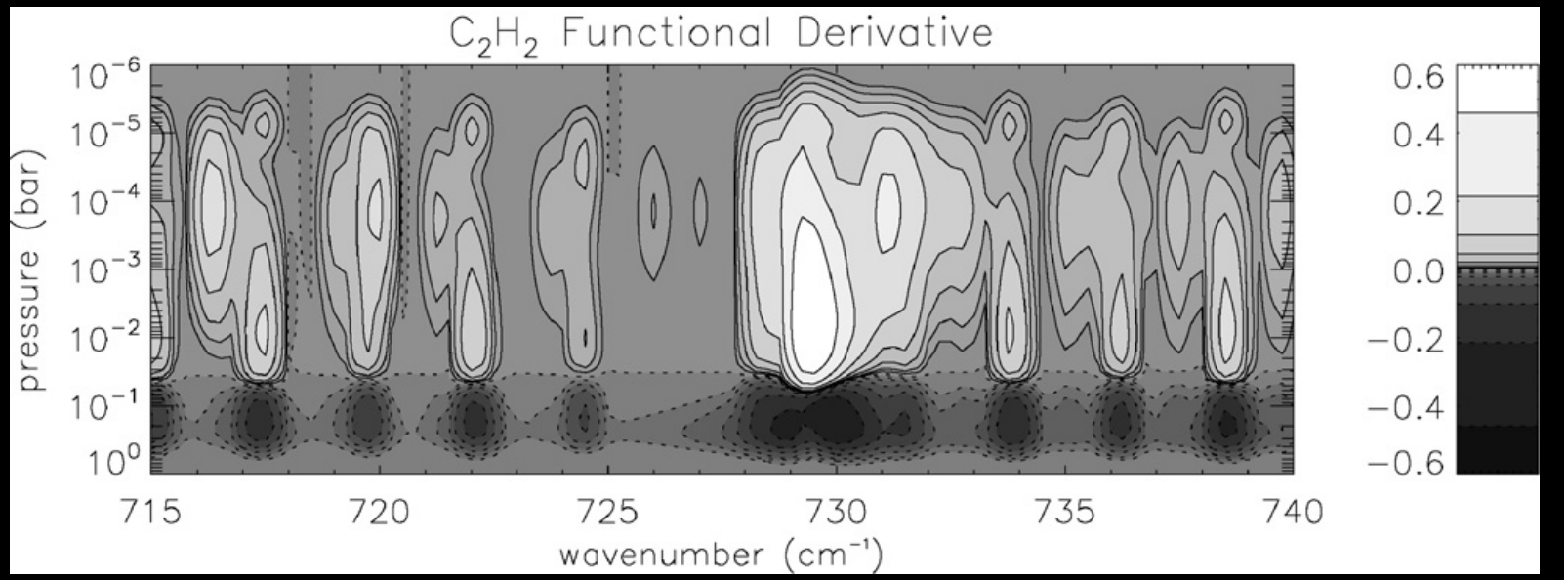
- Both the WF and CF refer to the opacity from all sources. Therefore it is also useful to know the Jacobian matrix or Functional Derivative:

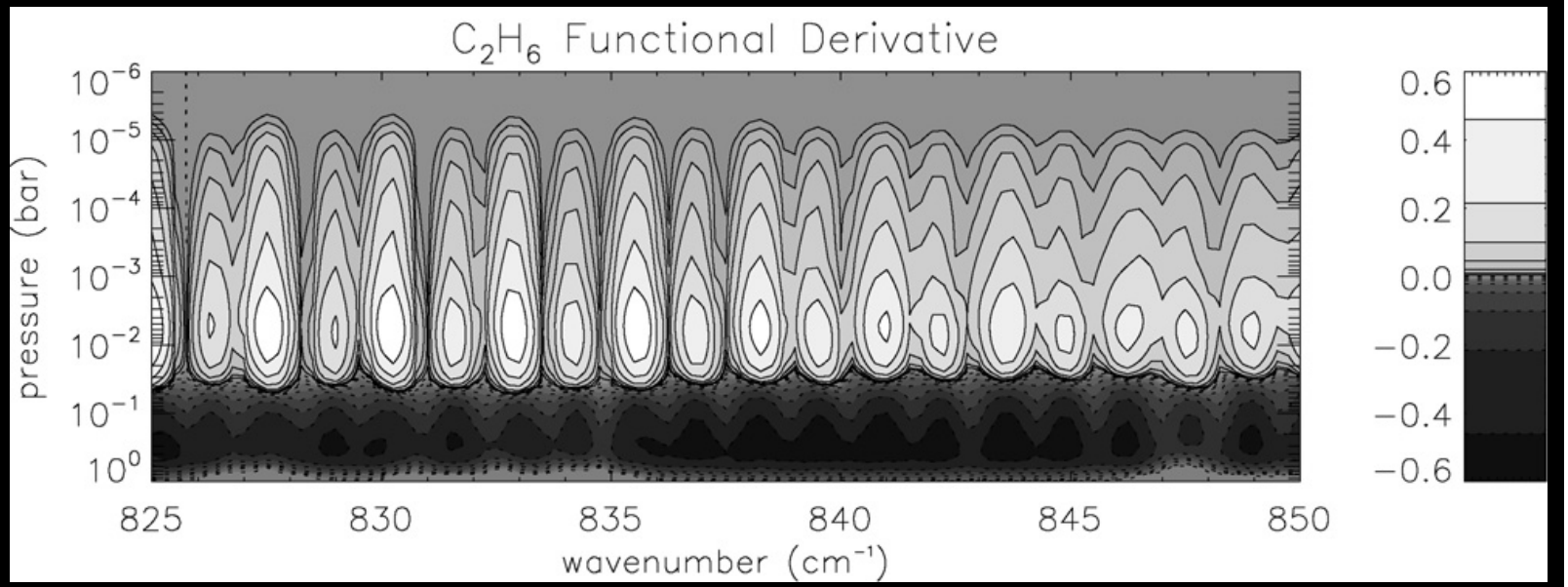
$$FD_{i,j} = \frac{\delta}{\delta q_j} I(\nu_i, q)$$

Example 1: Jupiter Hydrocarbons

- We now look at a worked example of fitting Jupiter hydrocarbon emission

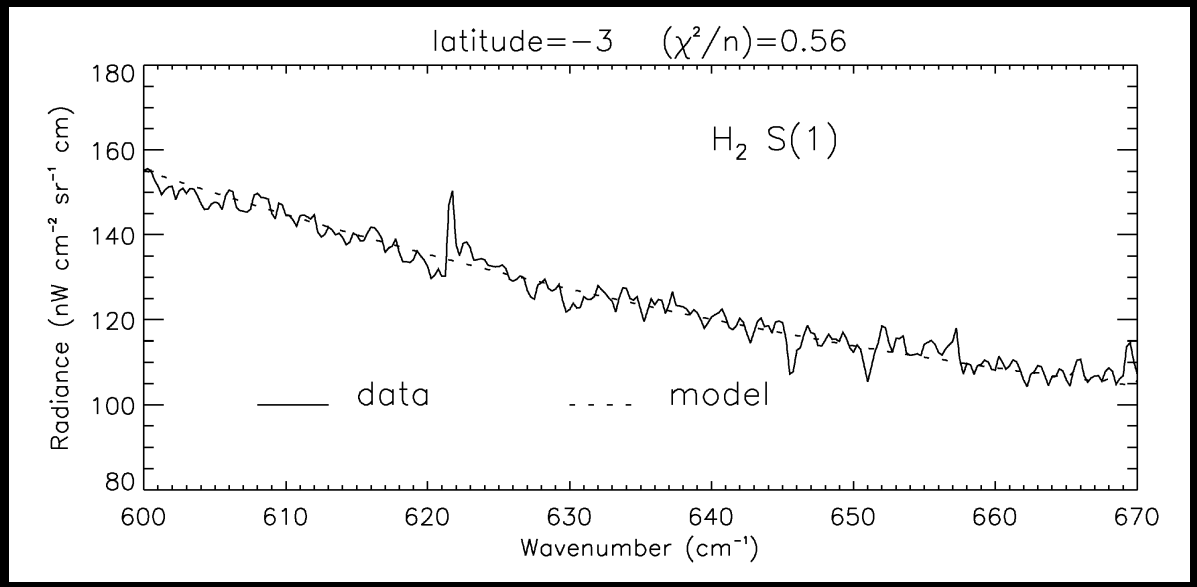
Example 1: functional derivatives



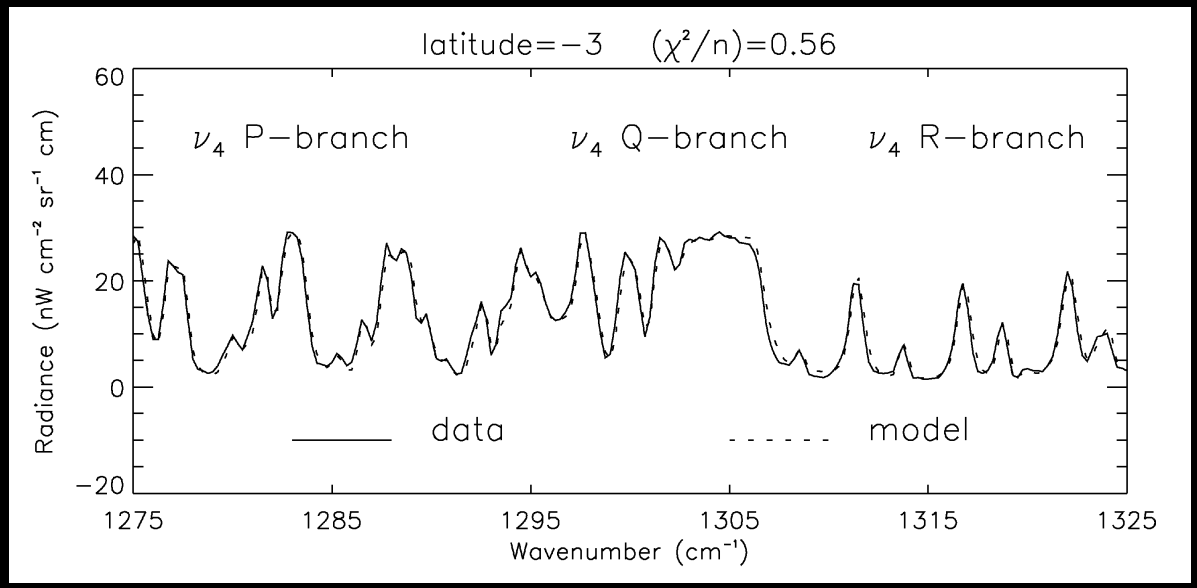


Example 1: spectral fits

H_2 band fit

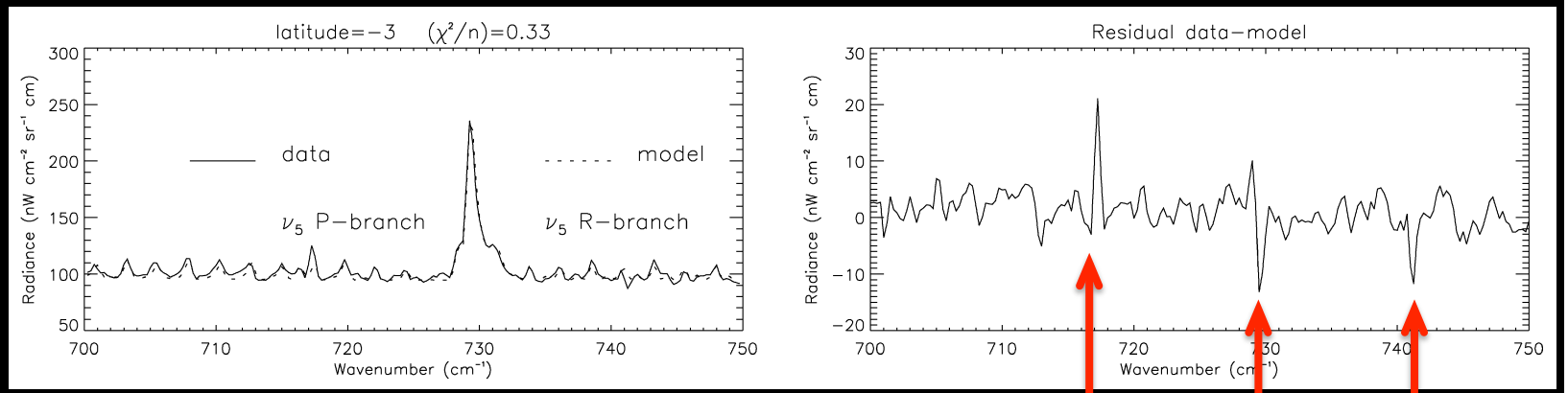


CH_4 band fit



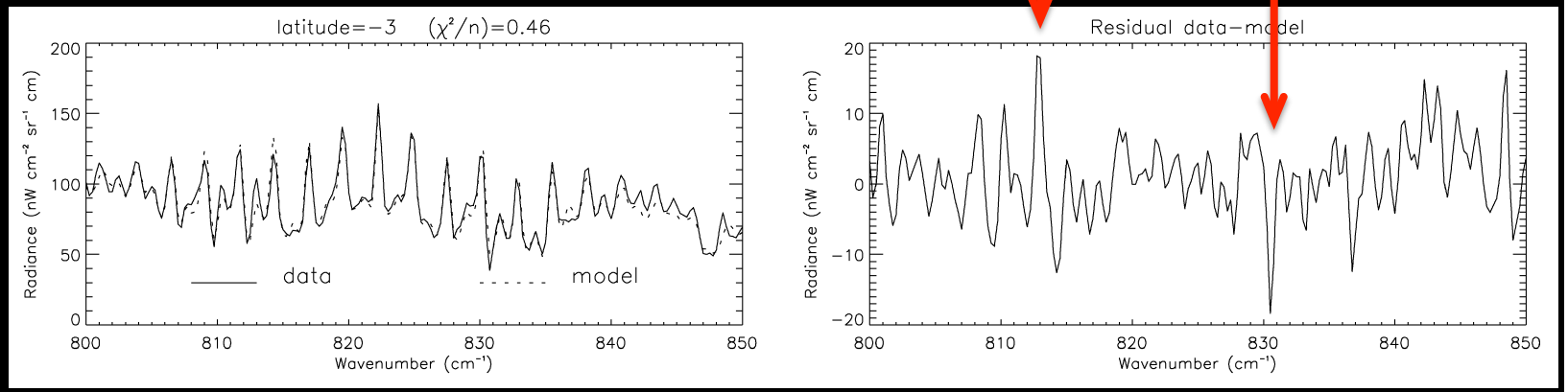
Example 1: spectral fits

C_2H_2 band fit

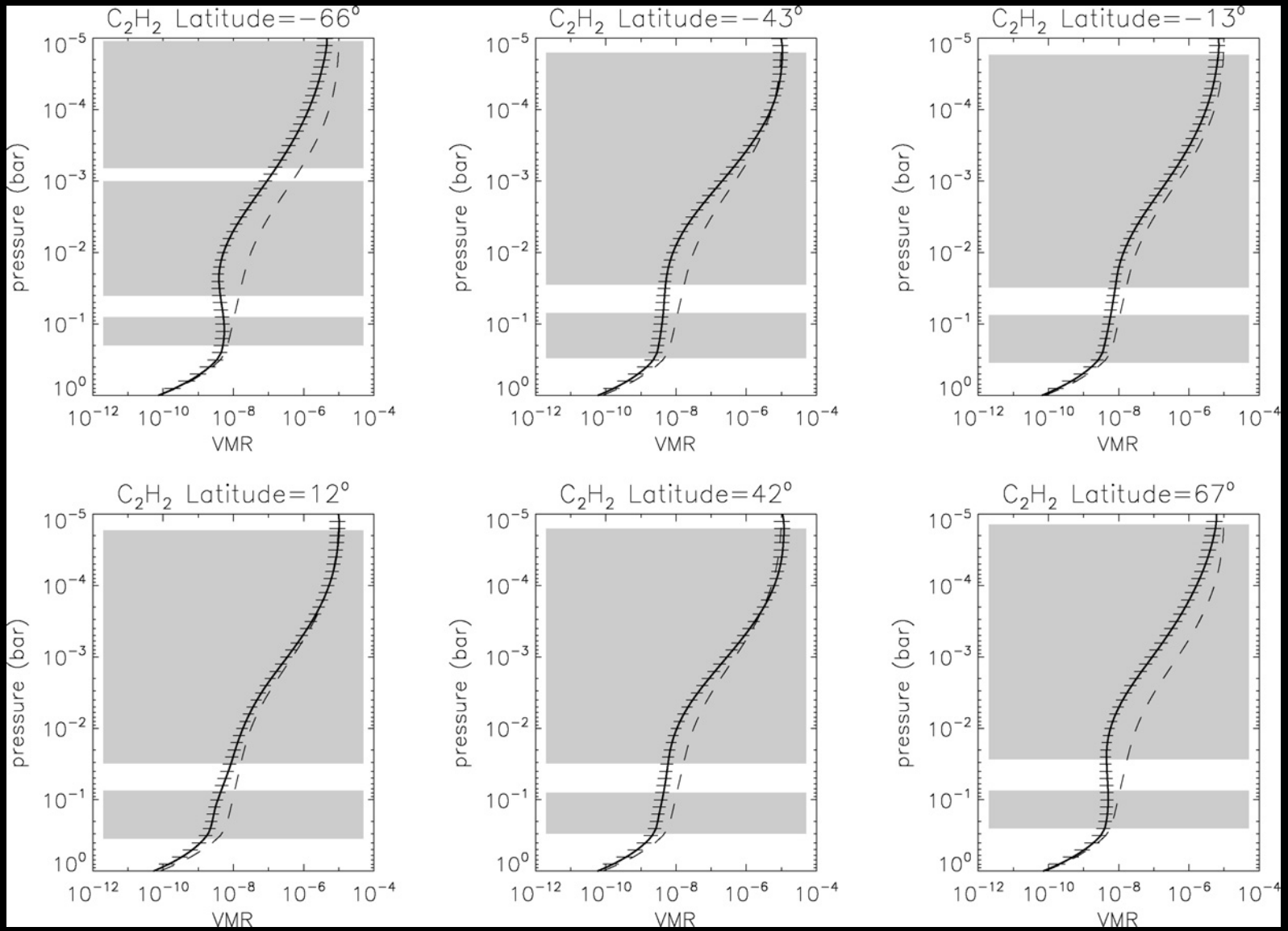


Electrical interference 'spikes'

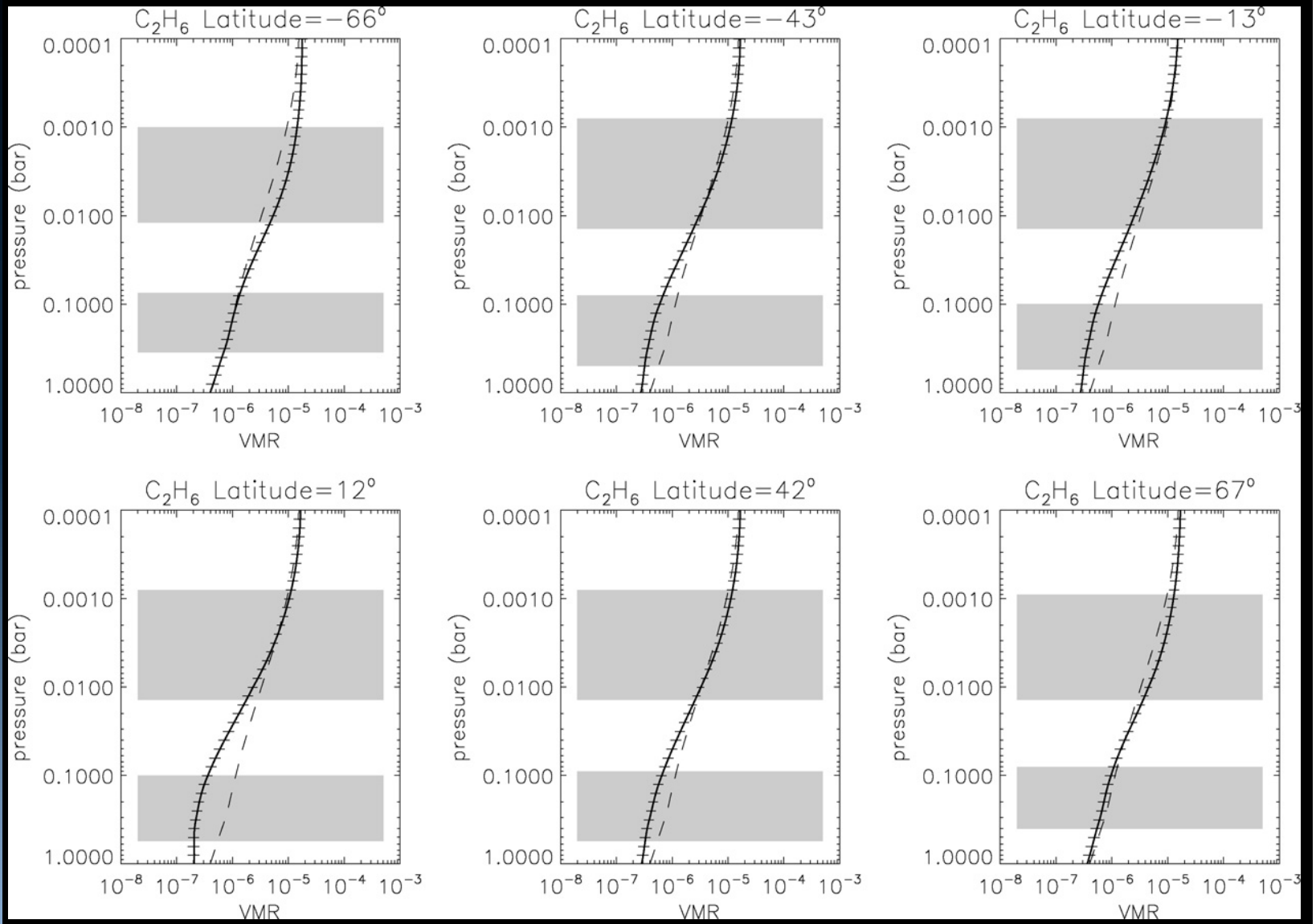
C_2H_6 band fit



Example 1: C_2H_2 profiles



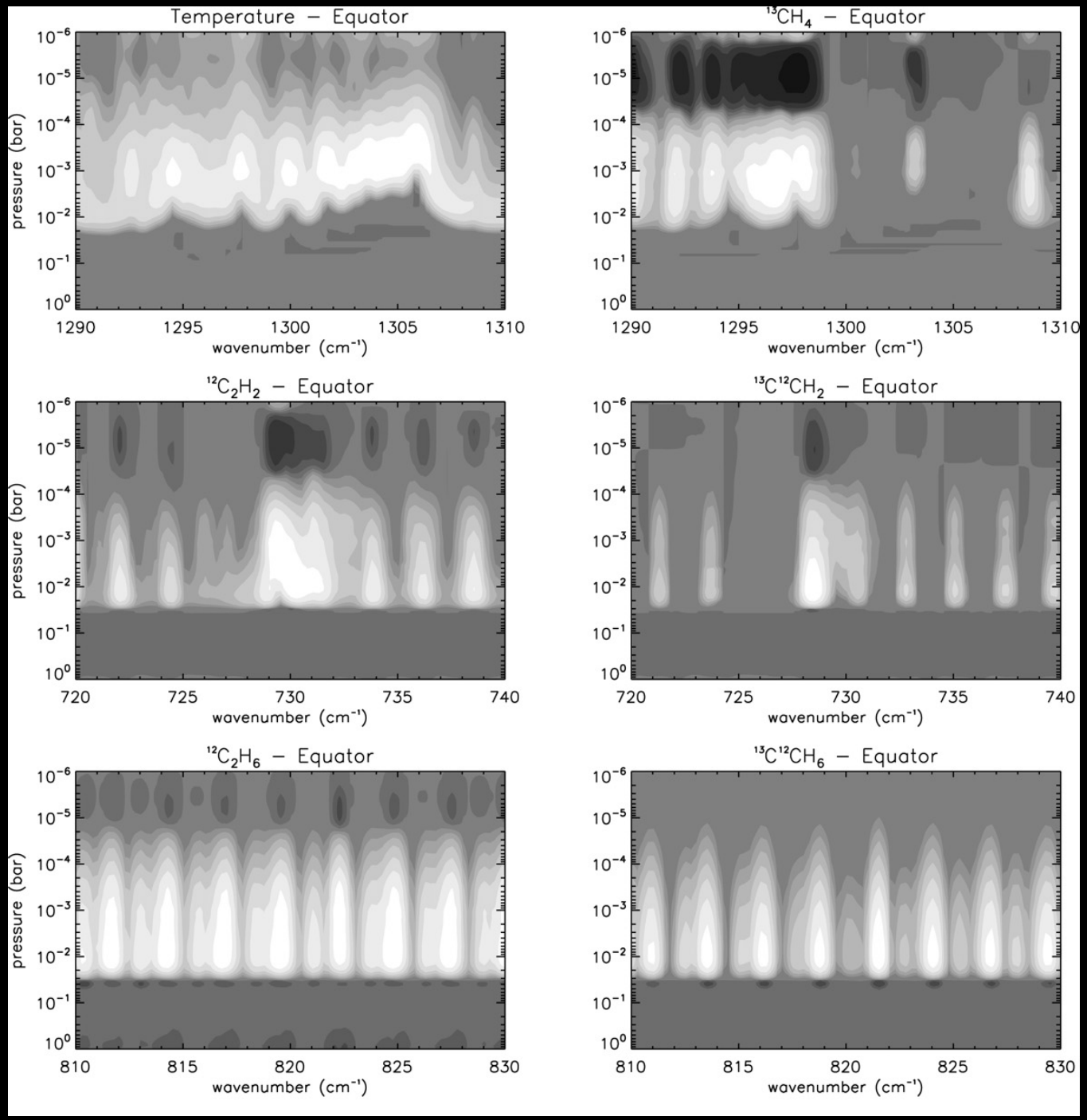
Example 1: C_2H_6 profiles



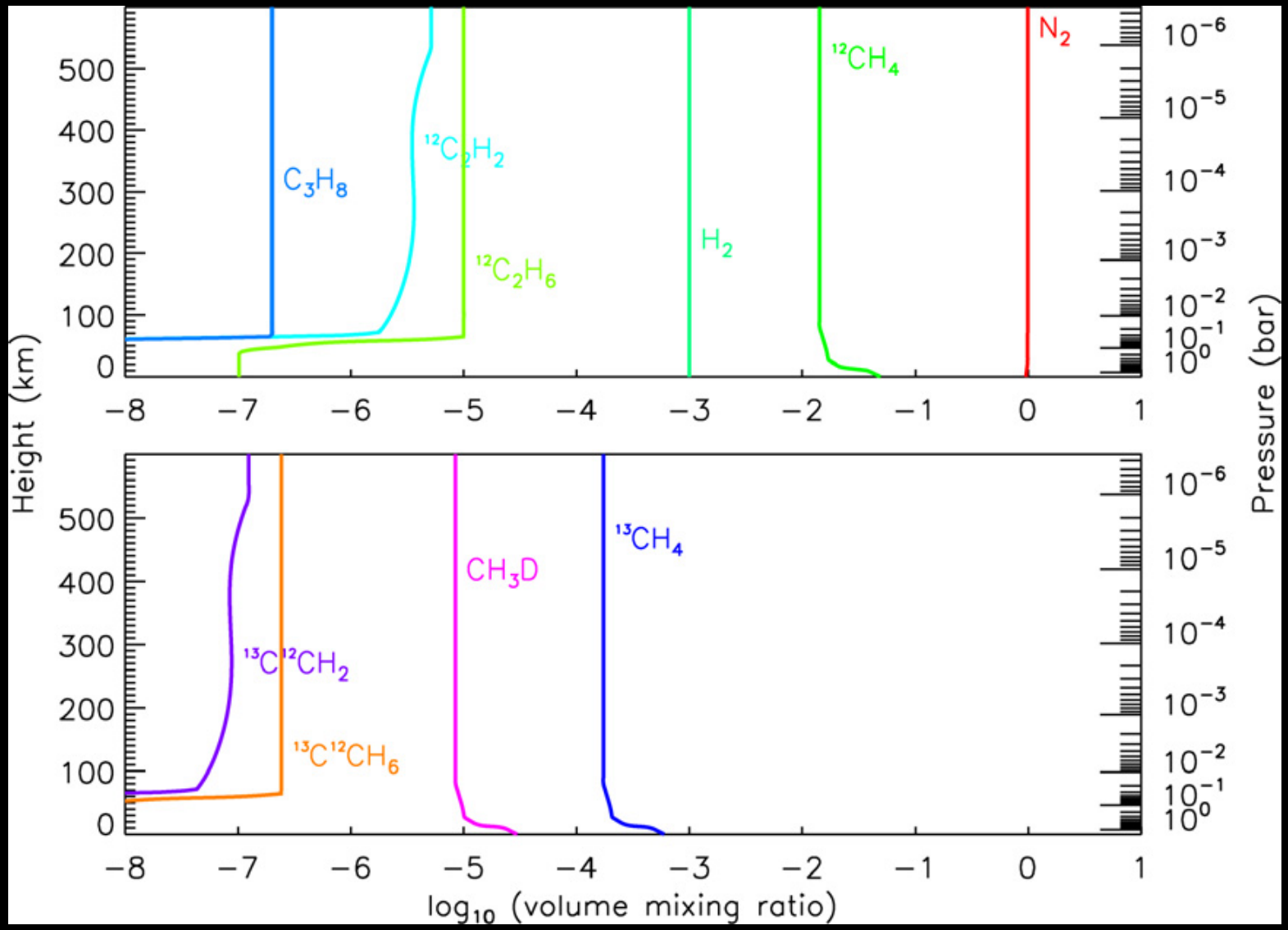
Example 2: Titan isotopes

- Worked example on missing bands/ isotopes

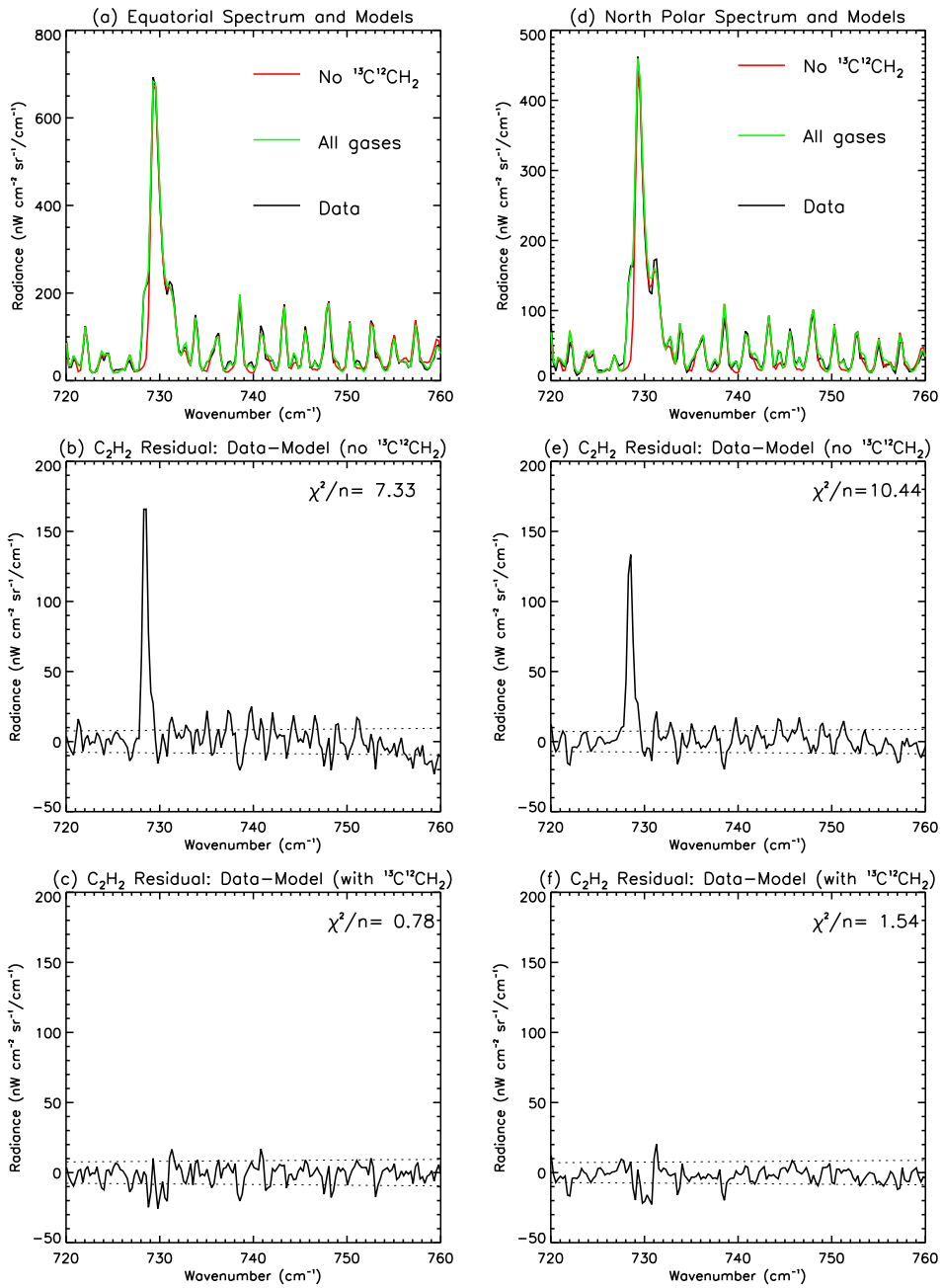
Example 2: spectral information



Example 2: trial gas profiles



Example 2: isotopic band fitting



The Inverse Problem

- Given:
  - a set of m measurements y_i with uncertainties ε_i,
  - An atmospheric state vector $\mathbf{x}$ with n elements,
  - A forward model **F(x)** relating the measurements to the state vector
- Solve $\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\varepsilon}$ for the atmospheric state $\mathbf{x}$.

The inverse problem is, in general, under-constrained: there are multiple solutions within the measurement uncertainty.

Information content (1)

- Linearize the inverse problem about a reference atmospheric state $\mathbf{x_0}$:

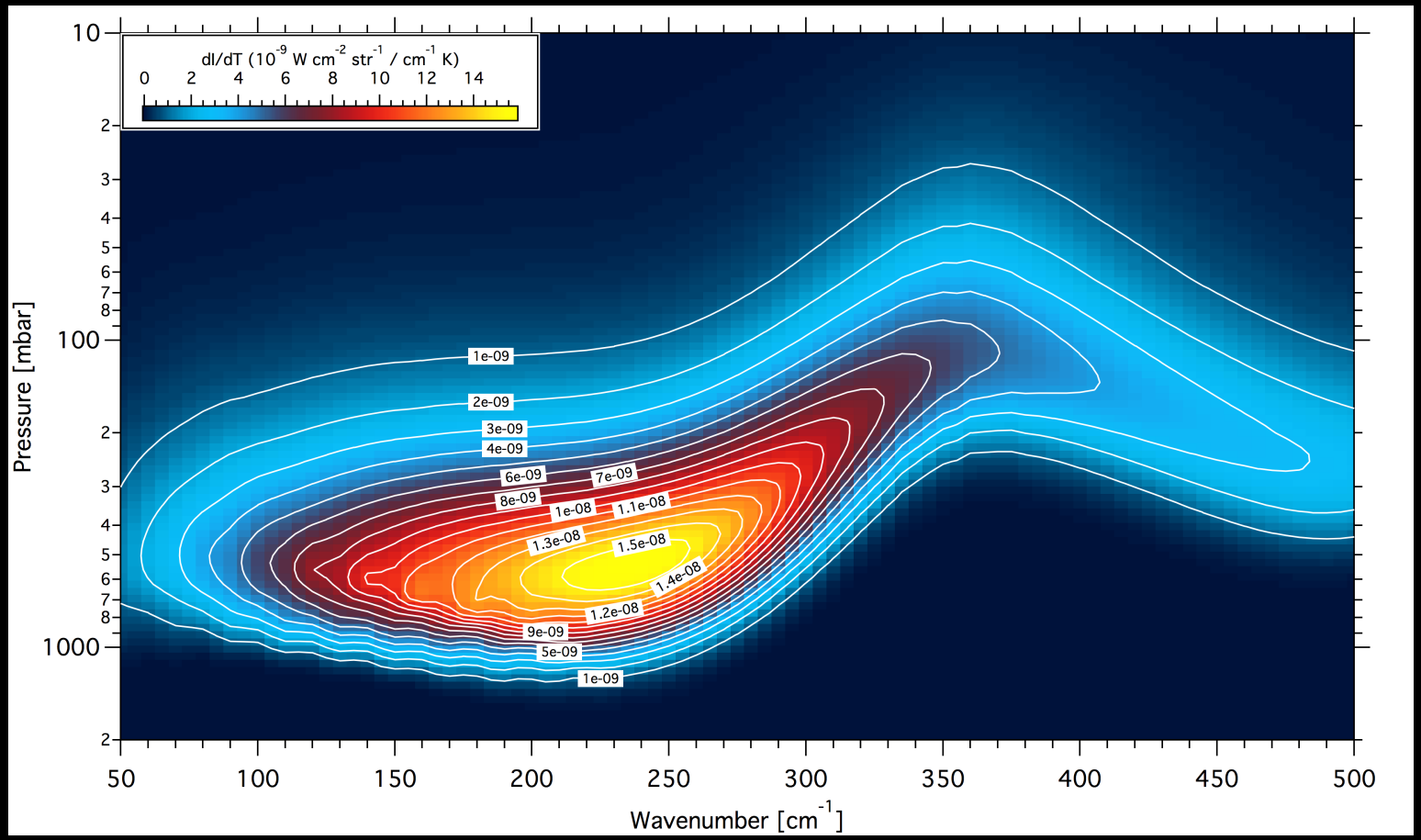
$$\mathbf{y} - \mathbf{F}(\mathbf{x}_0) = \mathbf{K}(\mathbf{x} - \mathbf{x}_0) + \varepsilon$$

$$K_{ij} = \frac{\partial F_i(\mathbf{x})}{\partial x_j}$$

- $\mathbf{K}$ (the inversion kernel) gives the change in observed radiance for a given change in the atmospheric state vector.

Example Kernel

Inversion kernel for tropospheric temperatures on Saturn (20 – 200 µm)



Information Content (2)

- Two common features of inversion kernels:
- Rows of **K** are linearly dependent
  - Rank(**K**) < min(m,n)
    - m measurements gives < m independent pieces of information about the atmosphere
  - $\mathbf{K}^T\mathbf{K}$ is singular, or nearly so
    - Standard least-squares techniques do not work (greatly amplify measurement noise)
- Individual measurements average over a broad altitude range (~scale height)
  - Little to no information on structure at small vertical scales

Information Content (3)

- **K** can be expressed in the form (Singular Value Decomposition)

$$\mathbf{K} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^{\mathbf{T}},$$

where **U** ($m \times p$) and **V** ($n \times p$) are orthonormal ($\mathbf{U}^{\mathbf{T}}\mathbf{U}=\mathbf{I}$) and $\boldsymbol{\Lambda}$ ($p \times p$) is diagonal, p = rank(**K**)

- Using **U** and **V** as basis functions,

$$\mathbf{y} - \mathbf{F}(\mathbf{x}_0) = \mathbf{U}\mathbf{y}', \quad \mathbf{x} - \mathbf{x}_0 = \mathbf{V}\mathbf{x}'$$

the linearized inverse problem can be written as

$$\mathbf{y}' = \boldsymbol{\Lambda}\mathbf{x}' + \mathbf{U}^{\mathbf{T}}\boldsymbol{\varepsilon}$$

Information Content (4)

- Solving for **x'** and setting **ε = 0** gives:

$$\mathbf{x'} = \mathbf{\Lambda}^{-1}\mathbf{y'}$$

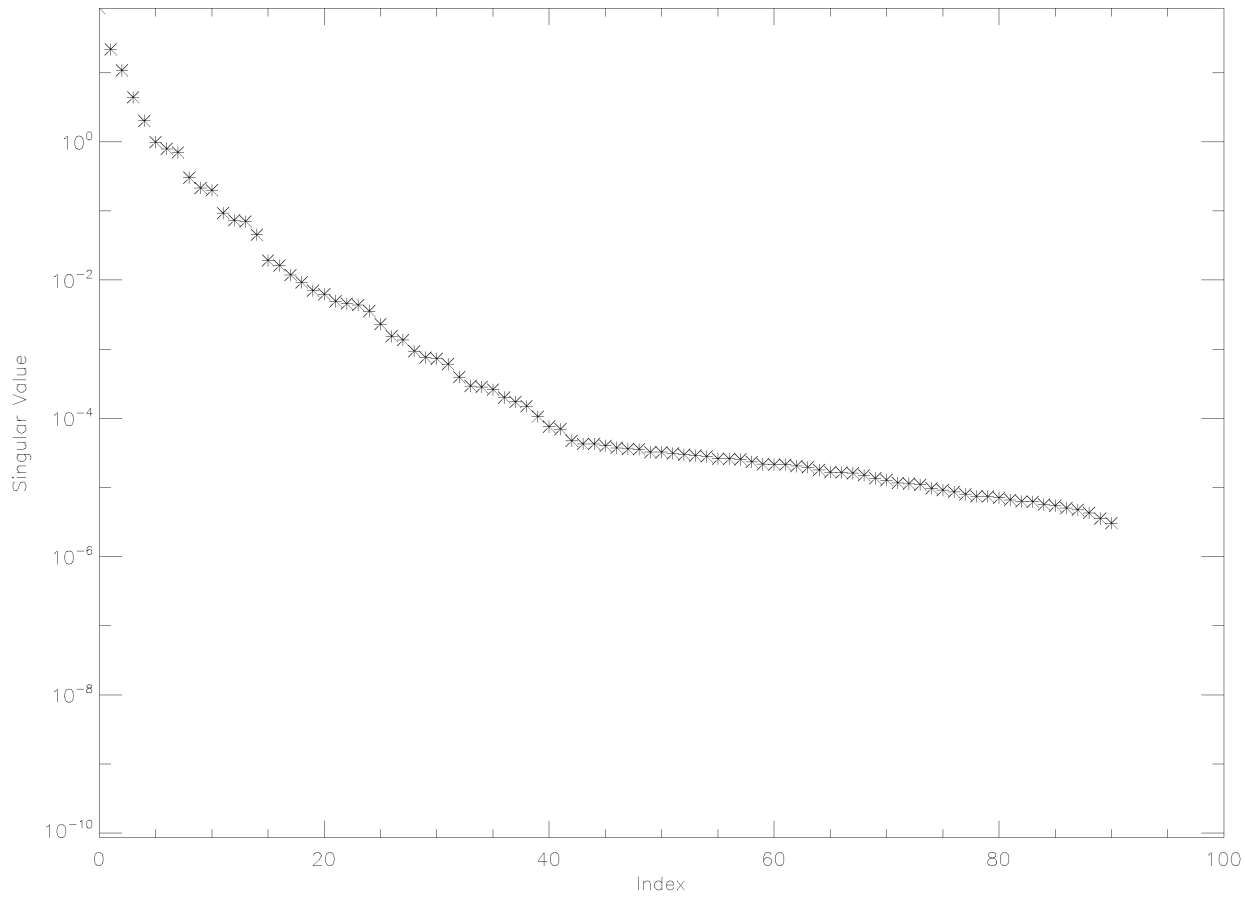
  – If $n = m = p$, this is exact, if $n < p$, it is the least-squares solution, if $n > p$, it is the solution that minimizes $||\mathbf{x'}||^2$.

- For realistic problems, **K** is usually nearly singular: many Λ_{ii} are small (several orders of magnitude < $\max(\Lambda_{ii})$)

  – The reconstructed **x** = **Vx'** is dominated by terms for which Λ_{ii} is small, which are just the terms for which **y'** is dominated by noise.

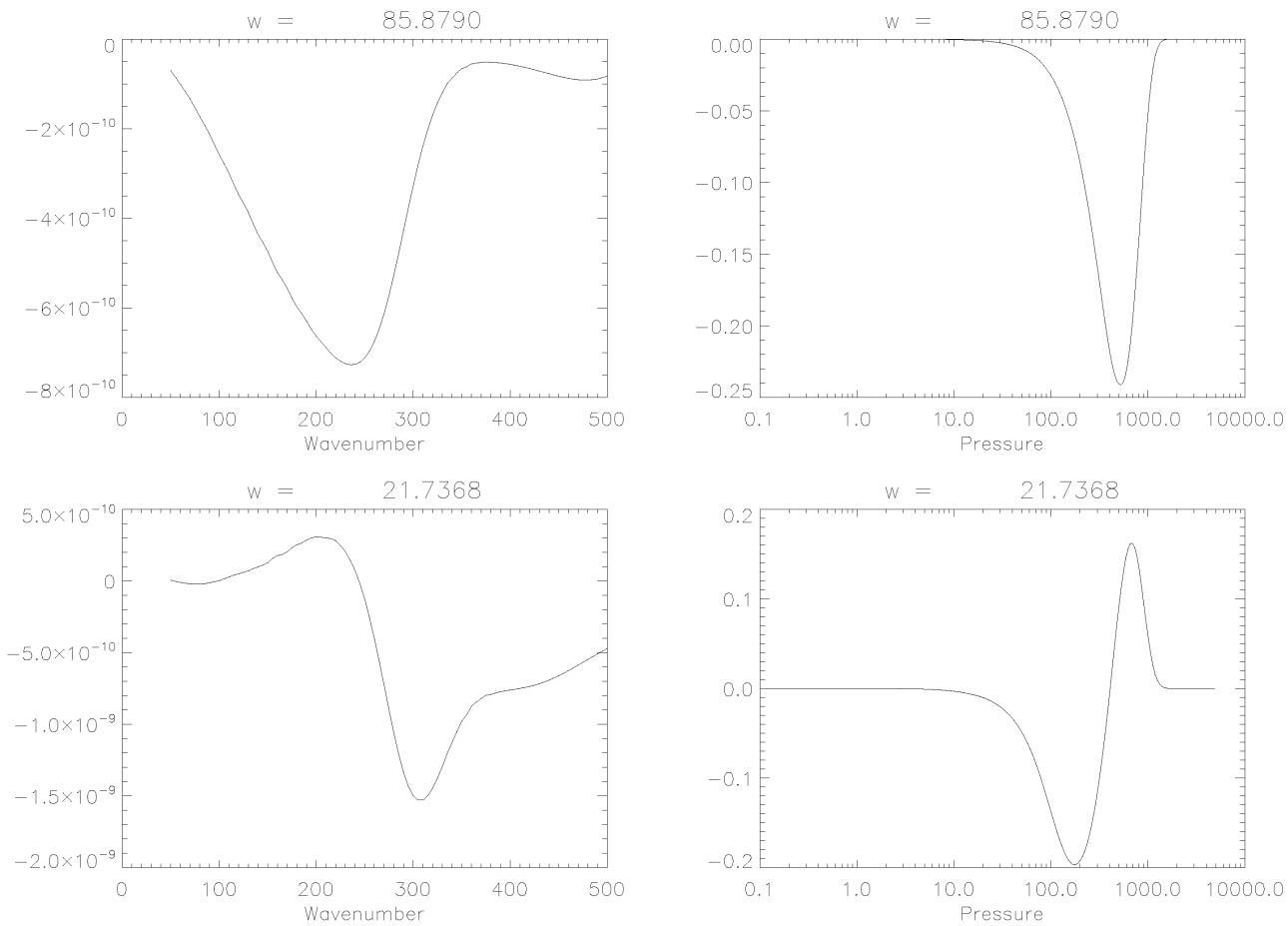
Example SVD: Saturn T kernel

Λ_{ii} for Saturn tropospheric temperature kernel



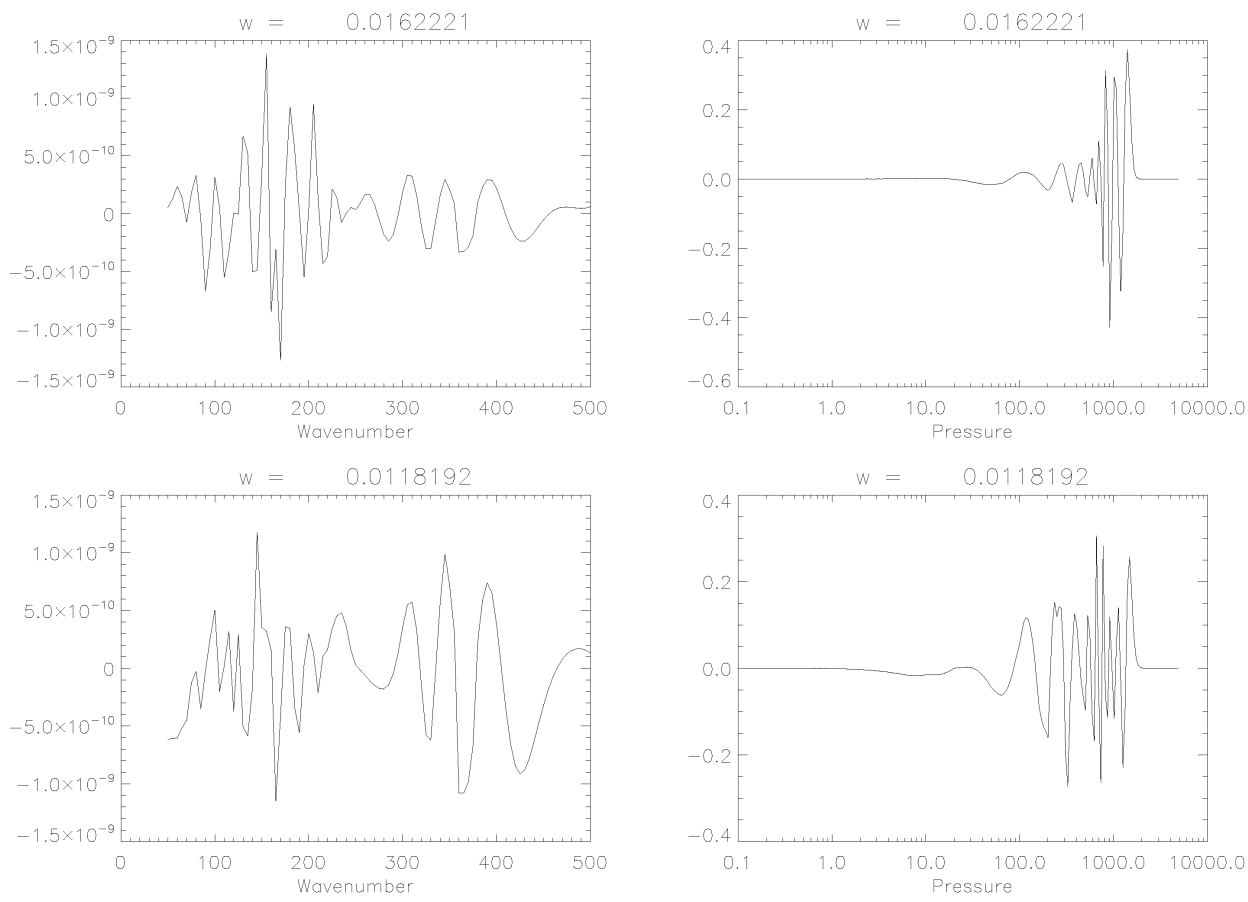
Example SVD: Saturn T kernel

Rows of U,V for 2 largest Λ_{ii}



Example SVD: Saturn T kernel

Rows of U,V for 2 small Λ_{ii}



Information Content (5)

- In practice, the number of independent parameters that can be usefully retrieved above the noise level is the number of singular values of **K** with Λ_{ii} larger than about ε/σ_x, where σ_x is the "expected" deviation of the atmospheric state from the reference state.
- A useful retrieval method must suppress those components of the state vector that are dominated by noise

Constrained Linear Inversion

- To suppress noise in the retrieval, expand the deviation of the state vector from the reference value in a set of basis vectors **F**

$$\mathbf{\Delta x} = \mathbf{x} - \mathbf{x_0} = \mathbf{Fa}$$

- minimize a penalty function of the form

$$\chi^2 = (\mathbf{\Delta I}\text{-}\mathbf{KFa})^T\mathbf{E}^{-1}(\mathbf{\Delta I}\text{-}\mathbf{KFa}) + \gamma\mathbf{a}^T\mathbf{a}$$

  - **E** is the measurement error covariance matrix
  - $\mathbf{\Delta I} = \mathbf{y} - \mathbf{F}(\mathbf{x_0})$
  - First term is usual chi-squared used in least-squares
  - Second term penalizes deviations from the reference state; γ determines the relative strength of the constraint
  - Constraint term and basis functions **F** both act to smooth the solution.

Solution

- Minimization of χ^2 gives

$$\mathbf{\Delta x} = \mathbf{G\Delta I}$$

$$\mathbf{G} = \mathbf{SK}^T(\gamma^{-1}\mathbf{KSK}^T + \mathbf{E})^{-1}$$

  - $\mathbf{S} = \mathbf{FF}^T$ is the correlation matrix of the basis vectors
  - Usually assume **S** of the form

$$S_{ij} = \exp[-(z_i - z_j)^2 / 2c^2]$$

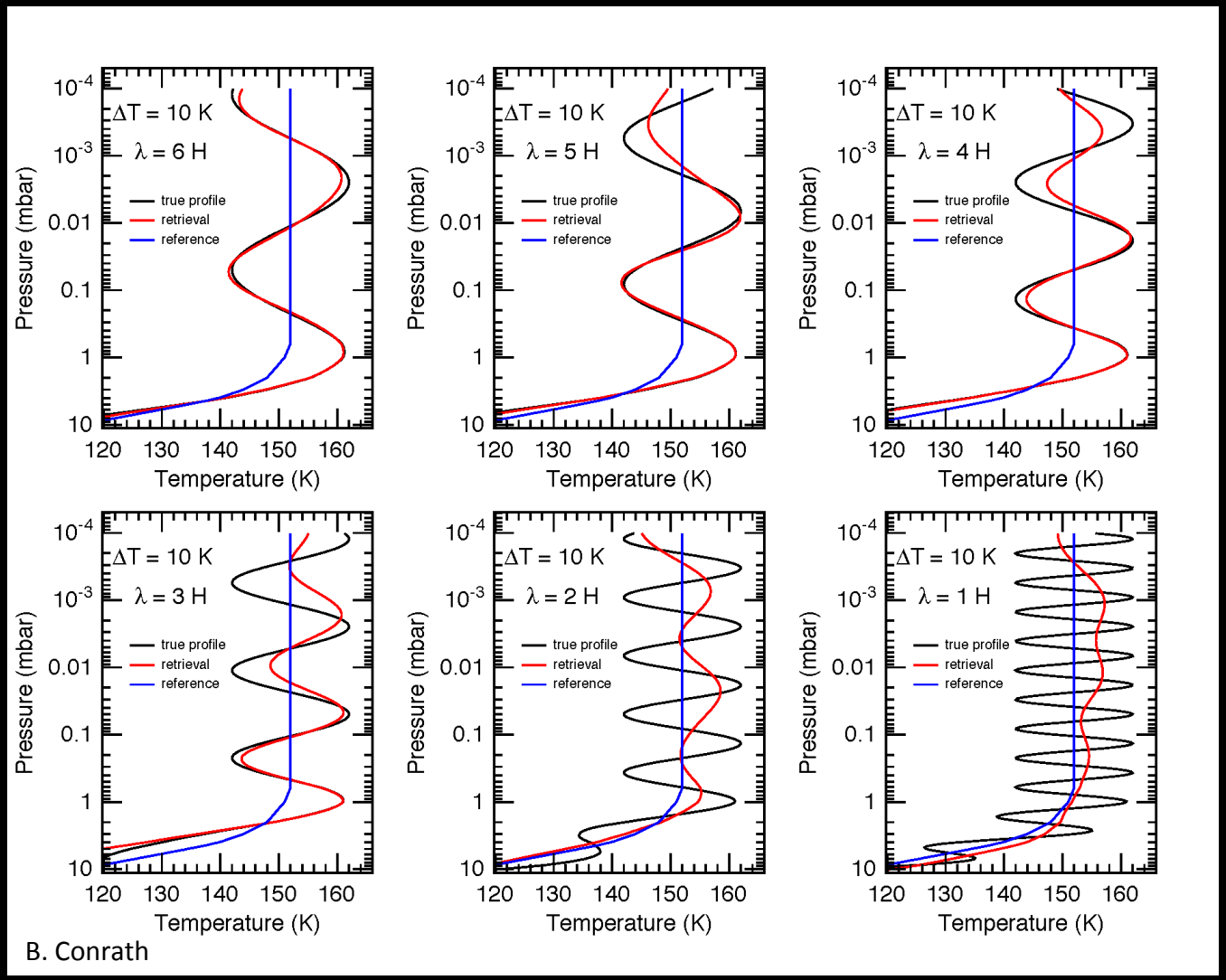
  - Setting $\gamma \approx \mathrm{Tr}(\mathbf{KSK}^T) / \mathrm{Tr}(\mathbf{E})$ will usually give good noise suppression without overly smoothing the result.
- Statistical estimation theory (Rogers, 2000) gives the same solution (with $\gamma = 1$), but in this case **S** is interpreted as the *a-priori* covariance matrix for the ensemble of expected solutions.
- Above solution assumes the problem is linear; in practice the solution must be iterated to account for nonlinearities.

Retrieval Uncertainty

- Error covariance matrix for the retrieved solution is $\boldsymbol{\sigma}_x = \mathbf{GEG}^T$.
  - Diagonal elements give an estimate of how much the retrieved solution will vary if the measurements are varied by their estimated uncertainty.
  - This estimate assumes the problem is linear.
  - Real errors will be somewhat larger (~factor of 2).

Example 3: Saturn Limb

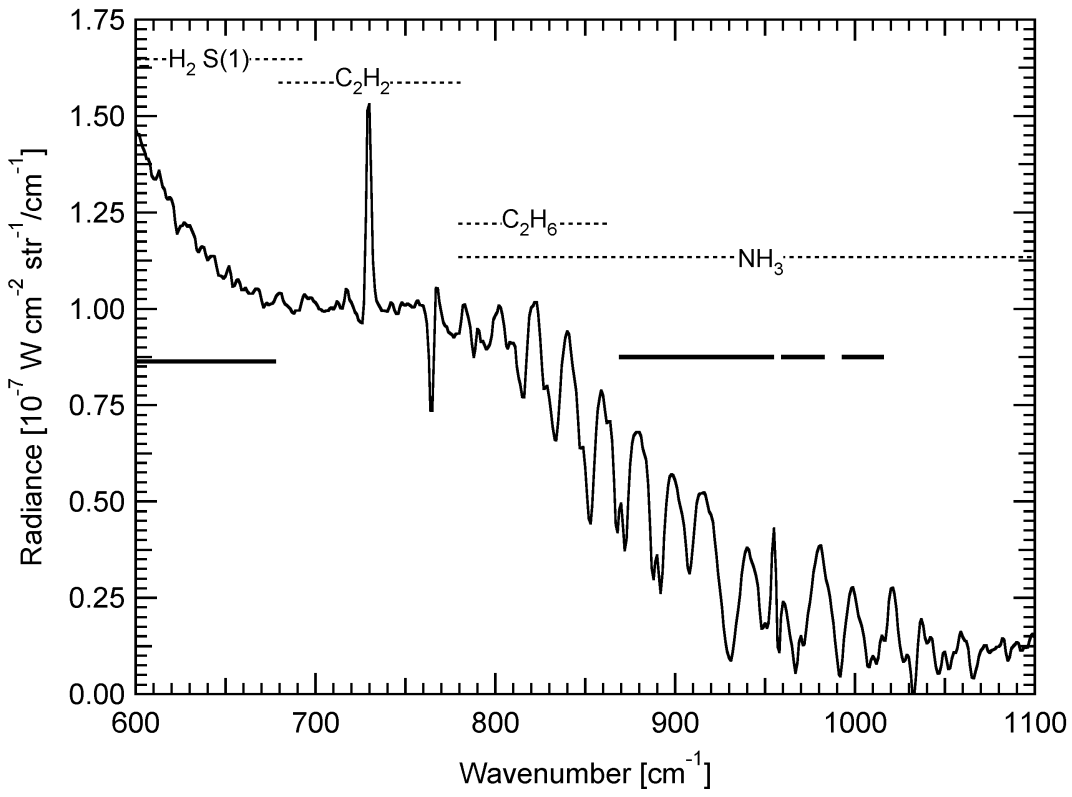
Saturn limb temperature retrievals (using synthetic data): sensitivity to scale of vertical variations



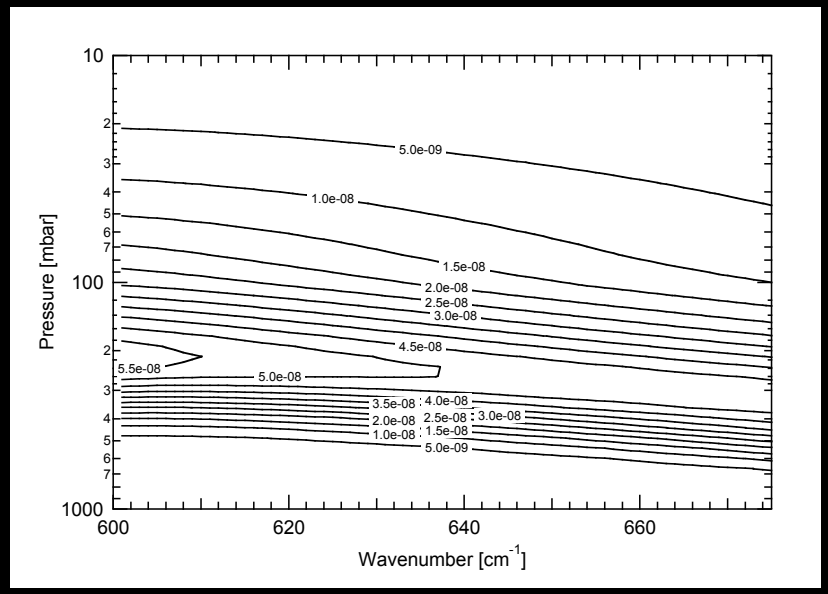
B. Conrath

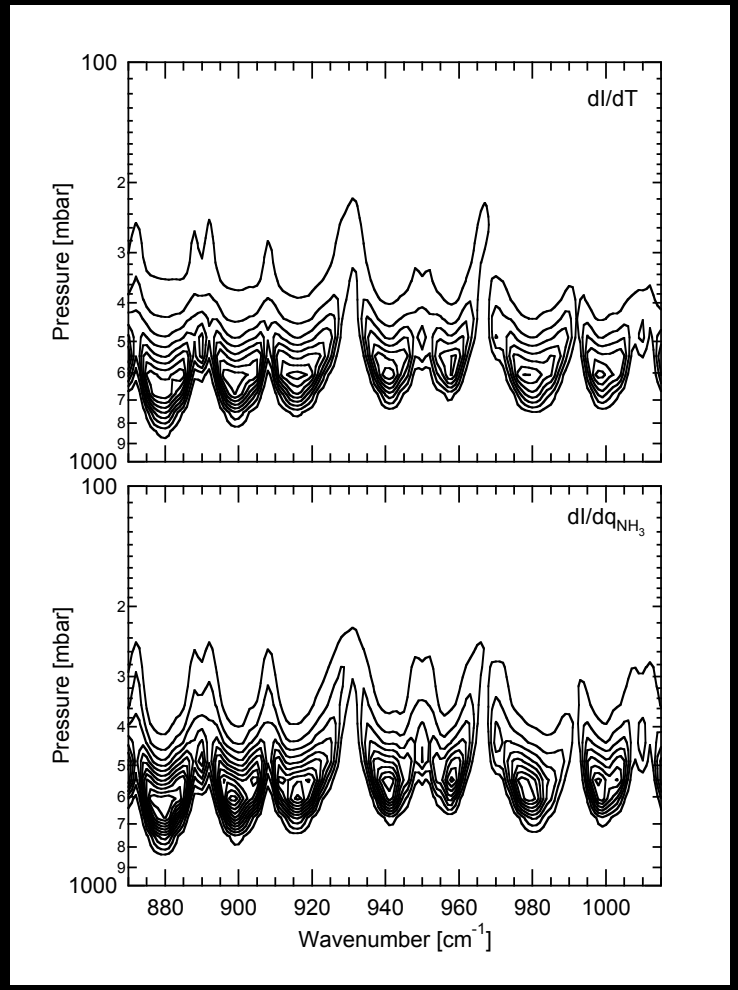
Example 4: Retrieval of NH_3 on Jupiter (Achterberg et al 2006)

CIRS equatorial spectrum of Jupiter



Jupiter T & NH_3 Kernels

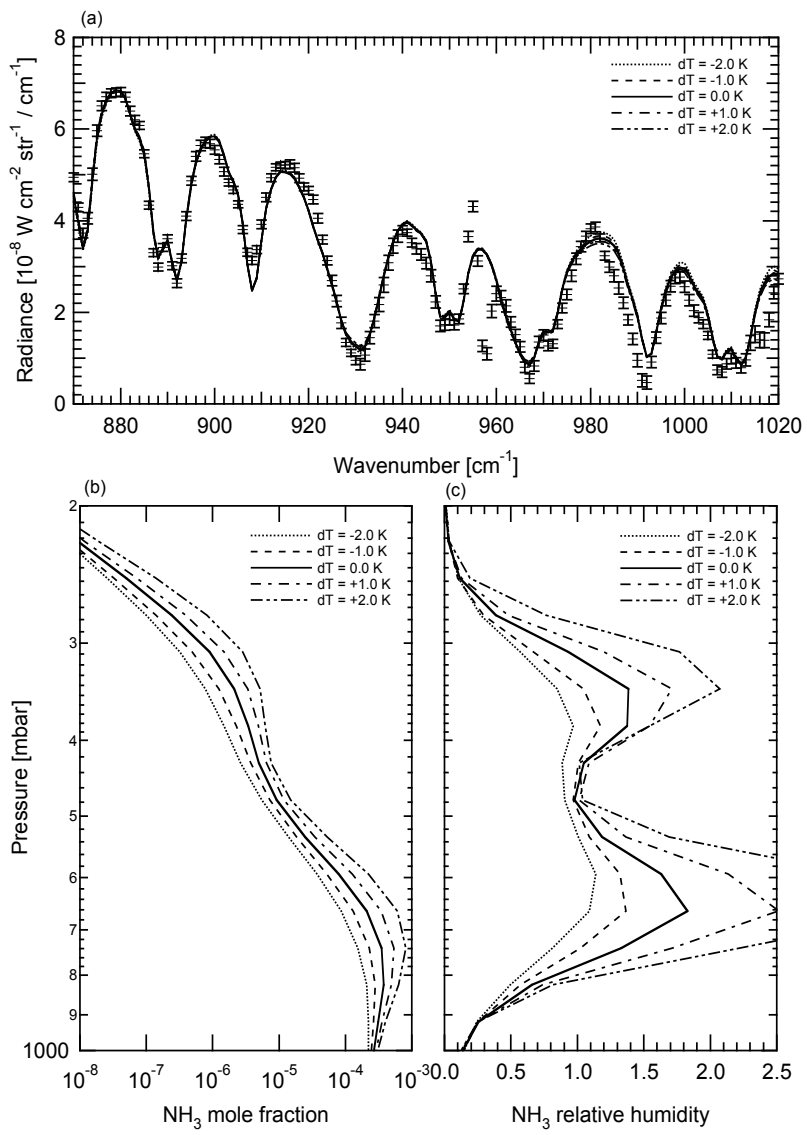




- Spectrum from 600-675 cm^{-1} is sensitive to T from ~100-400 mbar
- Spectrum from 870 – 1020 cm^{-1} is sensitive to both T & NH_3 from ~400-700 mbar

- Use 600 – 676 cm^{-1} to retrieve temperature
- Use 870 – 1020 cm-1 to retrieve ammonia abundance
  - Use log(ammonia mole fraction) as retrieved quantity

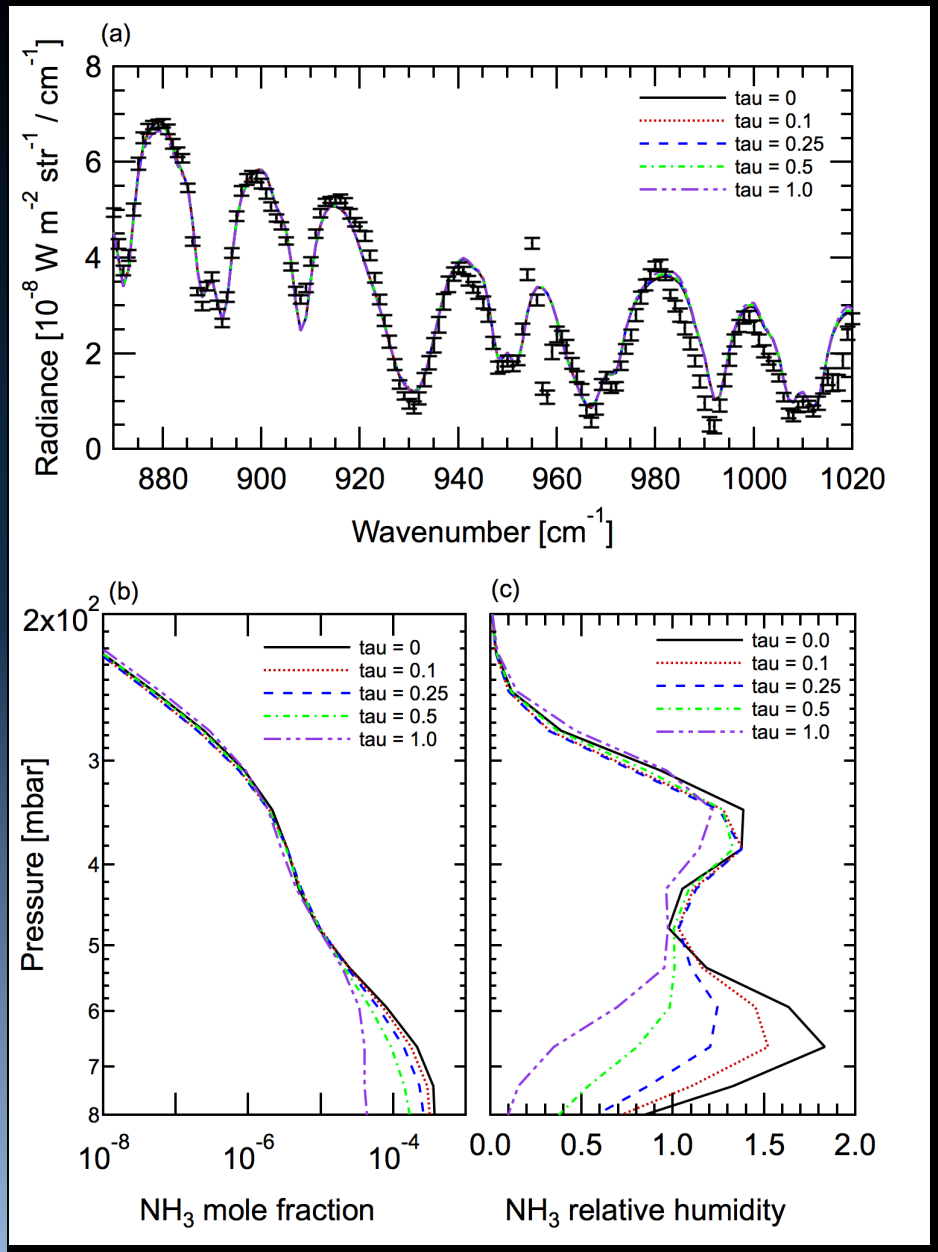
Sensitivity of NH_3 to T



Effect of temperature errors on NH_3 retrieval

Relative humidity is less sensitive to errors in the temperature than the absolute mole fraction when absorber profile is controlled by condensation, dT/dz and relative humidity are constant (Killen & Flasar, 1996)

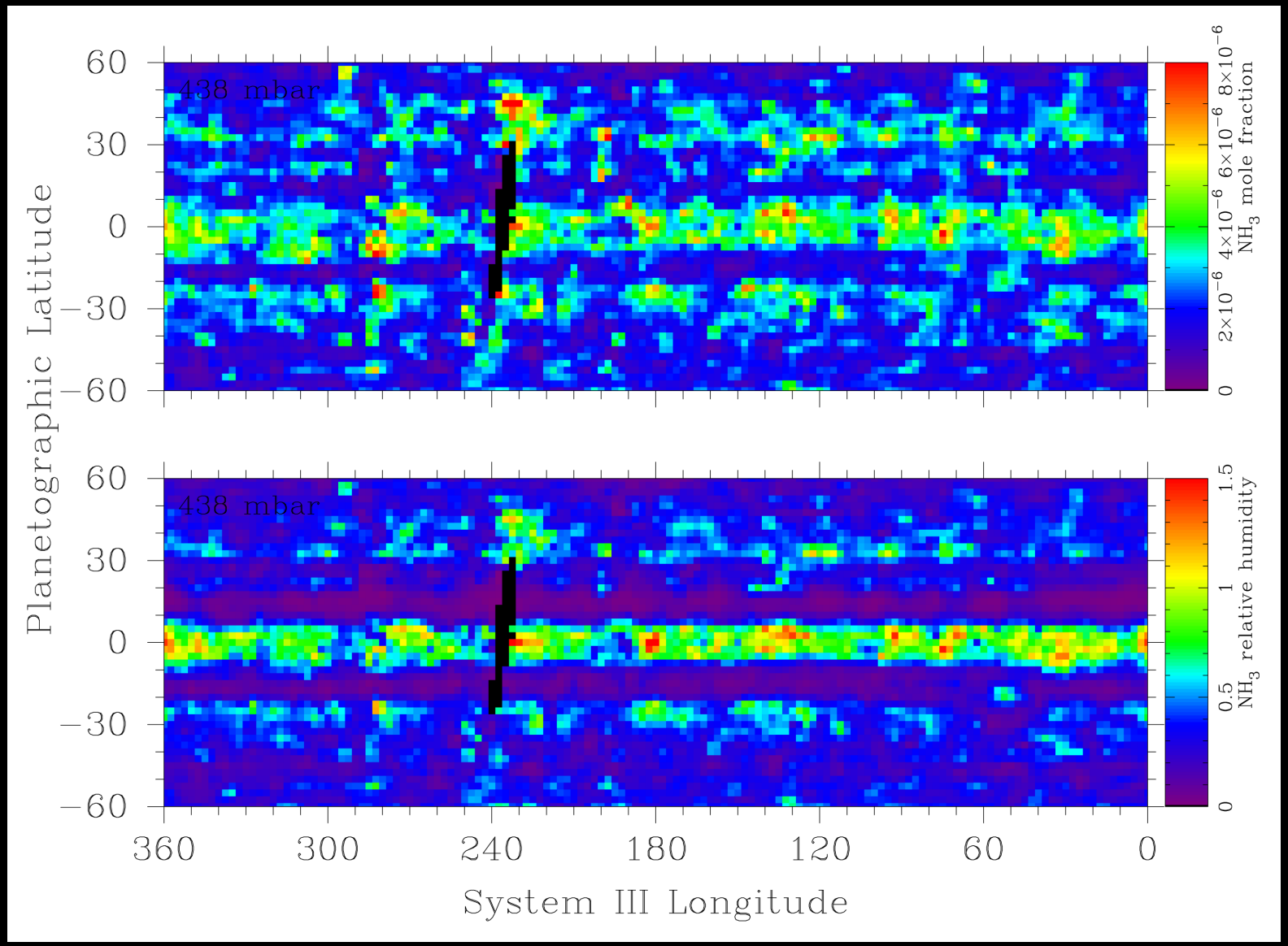
Sensitivity of NH_3 to cloud



- Effect of assuming cloud of varying optical depth with base at 690 mbar (expected location of NH3 cloud)
- For p >~ 500 mbar, NH_3 retrieval is sensitive to assumed cloud opacity
- CIRS spectra are sensitive to NH3 relative humidity at ~400 – 500 mbar

Jupiter NH_3: Results

Map of NH3 on Jupiter at 438 mbar



Summary

- Scoping the problem:
  - Parameterizing the atmosphere
  - Fundamental input information, spectral line lists etc
  - Radiative transfer code
- Forward calculation:
  - Produce a sample spectrum
  - Compute sensitivity (dI/dq) to model parameters
  - Understand information content of spectrum
- Optimize/solve inverse problem:
  - Compute cost function (χ^2)
  - Adjust parameters to minimize model-data difference, subject to constraints
  - Compute errors on retrieved parameters

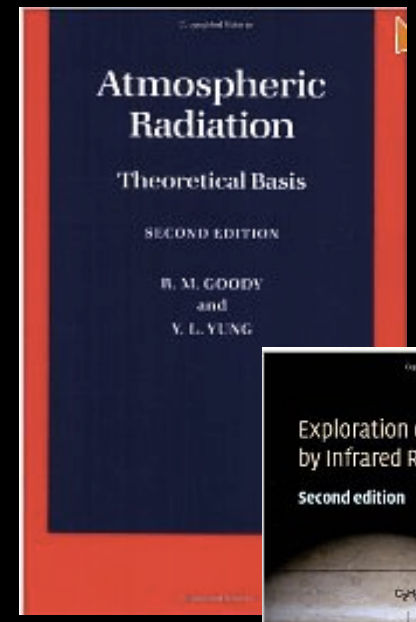
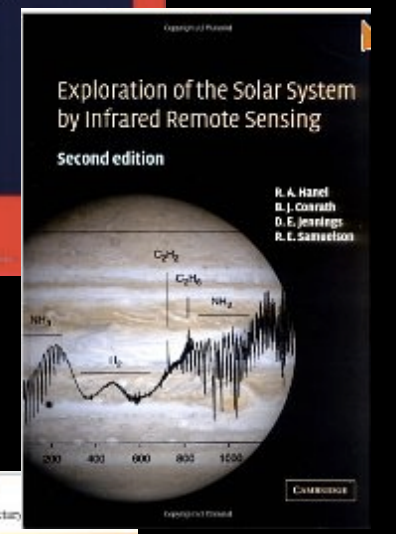
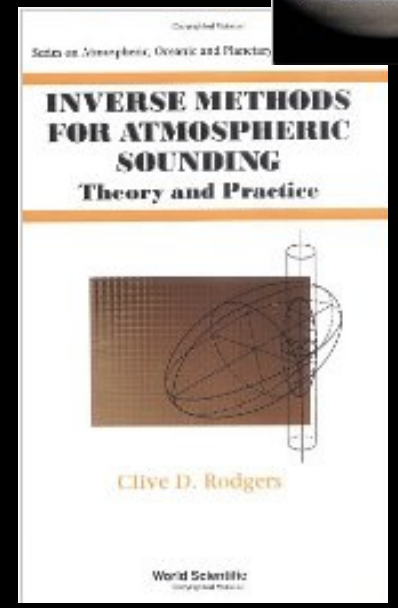
Further Reading

- <u>Radiative Transfer</u>:

  Goody and Yung *"Atmospheric Radiation,"* 2nd Edition, OUP, 1989

- <u>Remote Sensing</u>:

  Hanel et al. *"Exploration of the Solar System by Infrared Remote Sensing,"* 2nd Edition, CUP, 2003

- <u>Retrievals</u>:

  Rodgers *"Inverse methods for atmospheric sounding,"* World Scientific, 2000.