Memo to: TIDI
From: W. R. Skinner
Date: 13 November 2003
Subject: RETRIEVE fitting algorithm

Introduction

This memo provides an explicit description of the fitting algorithm used by RETRIEVE. It uses an analytical model of the Fabry-Perot function and performs a non-linear least squares fit using standard linearization techniques with the addition of using constraints.

Change History

Document version B

Includes fitting for rotational temperature as well as kinetic. A constraint is included to keep them from differing too much, and to provide a value if an atomic line is observed.

Document version C

Modifies the definitions of the Fourier coefficients to be consistent with the code.

Instrument function model

The instrument function convolved with a Doppler broadened line can be expressed

$$T(\nu, T_e, T_{inst}, i) = \left(1 - \frac{L}{1-R}\right)^2 \left(\frac{1-R}{1+R}\right) \left[1 + 2\sum_{n=1}^{N_{max}} R^n e^{-\pi^2 n^2 \left(\frac{4t^2\alpha_D^2(T_{e,0})T_e}{T_{e,0}} + 8\nu_0^2 \Delta t_e^2\right)} \right.$$
$$\bullet \operatorname{sinc}\left(\frac{\pi n}{N_b}\right) \operatorname{sinc}\left(\frac{\pi n}{N_{fov}}\right) \operatorname{Jinc}\left(\frac{\pi n}{N_t}\right) \operatorname{sinc}\left(\frac{\pi n}{N_a^{'}(i)}\right)$$
$$\left. \bullet \cos\left(2\pi n\left(\frac{\nu - \nu_0}{\Delta\nu_{FSR}} - \Delta M_a(i) + \frac{1}{2N_b}\right)\right)\right]$$

with the parameters defined in Table 1 and the following function definitions are used:

$$\operatorname{sinc}(x) = \frac{\sin x}{x}$$

and

$$\operatorname{Jinc}(x) = \frac{2J_1(x)}{x}.$$

The wavenumber of the line, ν, is

$$\nu = \nu_r + \frac{\nu_r u}{c_{light}} = \nu_r\left(1 + \frac{u}{c_{light}}\right).$$

In this convention, a positive u will increase the wavenumber (a blue shift) and represents movement toward the spacecraft. The line position of the detector in terms of velocity units is

$$u(\theta) = u_{atm} + u_{sc}(\theta) + u_{ref}(\theta) - u_{rot}(\theta) + u_{therm} + u_{ltd}$$

It is convenient to combine all terms except the atmospheric component into a "zero wind"

$$u_{zero}(\theta) = u_{sc}(\theta) + u_{ref}(\theta) - u_{rot}(\theta) + u_{therm} + u_{ltd}$$

The equation for the transmission then becomes

$$T(\nu_r, T_e, T_{inst}, i, \theta, u) = \left(1 - \frac{L}{1-R}\right)^2\left(\frac{1-R}{1+R}\right)\left[1 + 2\sum_{n=1}^{N_{max}} R^n e^{-\pi^2 n^2\left(\frac{4t^2\alpha_D^2(T_{e,0})T_e}{T_{e,0}} + 8\nu_0^2\Delta t_e^2\right)}\right.$$

$$\bullet \operatorname{sinc}\left(\frac{\pi n}{N_b}\right)\operatorname{sinc}\left(\frac{\pi n}{N_{fov}}\right)\operatorname{Jinc}\left(\frac{\pi n}{N_t}\right)\operatorname{sinc}\left(\frac{\pi n}{N_a^{'}(i)}\right)$$

$$\left.\bullet \cos\left(2\pi n\left(\frac{\nu_r - \nu_0 + \frac{\nu_r}{c_{light}}\left(u_{atm} + u_{zero}(\theta)\right)}{\Delta\nu_{FSR}} - \Delta M_a(i) + \frac{1}{2N_b}\right)\right)\right]$$

This can be expanded:

$$T(\nu_r, T_e, T_{inst}, i, \theta, u) = \left(1 - \frac{L}{1-R}\right)^2\left(\frac{1-R}{1+R}\right)\left[1 + 2\sum_{n=1}^{N_{max}} R^n e^{-\pi^2 n^2\left(\frac{4t^2\alpha_D^2(T_{e,0})T_e}{T_{e,0}} + 8\nu_0^2\Delta t_e^2\right)}\right.$$

$$\bullet \operatorname{sinc}\left(\frac{\pi n}{N_b}\right)\operatorname{sinc}\left(\frac{\pi n}{N_{fov}}\right)\operatorname{Jinc}\left(\frac{\pi n}{N_t}\right)\operatorname{sinc}\left(\frac{\pi n}{N_a^{'}(i)}\right)$$

$$\bullet \left\{\cos\left(\frac{2\pi n\nu_r\left(u_{atm} + u_{zero}(\theta)\right)}{c_{light}\Delta\nu_{FSR}}\right)\cos\left(2\pi n\left(\frac{\nu_r - \nu_0}{\Delta\nu_{FSR}} - \Delta M_a(i) + \frac{1}{2N_b}\right)\right)\right.$$

$$\left.\left. - \sin\left(\frac{2\pi n\nu_r\left(u_{atm} + u_{zero}(\theta)\right)}{c_{light}\Delta\nu_{FSR}}\right)\sin\left(2\pi n\left(\frac{\nu_r - \nu_0}{\Delta\nu_{FSR}} - \Delta M_a(i) + \frac{1}{2N_b}\right)\right)\right\}\right]$$

Define

$$A_n(i) = \left(1 - \frac{L}{1-R}\right)^2\left(\frac{1-R}{1+R}\right)$$

for n=0 and for n>0

$$A_n(i) = 2\left(1-\frac{L}{1-R}\right)^2\left(\frac{1-R}{1+R}\right)R^n e^{-8\pi^2 n^2 \nu_0^2 \Delta t_e^2}\cos\left(2\pi n\left(\frac{\nu_r-\nu_0}{c_{light}\Delta\nu_{FSR}}-\Delta M_a(i)+\frac{1}{2N_b}\right)\right)$$

$$\bullet \sin c\left(\frac{\pi n}{N_b}\right)\sin c\left(\frac{\pi n}{N_{fov}}\right)Jinc\left(\frac{\pi n}{N_t}\right)\sin c\left(\frac{\pi n}{N_a^{'}(i)}\right)$$

$$B_n(i) = 2\left(1-\frac{L}{1-R}\right)^2\left(\frac{1-R}{1+R}\right)R^n e^{-8\pi^2 n^2 \nu_0^2 \Delta t_e^2}\sin\left(2\pi n\left(\frac{\nu_r-\nu_0}{c_{light}\Delta\nu_{FSR}}-\Delta M_a(i)+\frac{1}{2N_b}\right)\right)$$

$$\bullet \sin c\left(\frac{\pi n}{N_b}\right)\sin c\left(\frac{\pi n}{N_{fov}}\right)Jinc\left(\frac{\pi n}{N_t}\right)\sin c\left(\frac{\pi n}{N_a^{'}(i)}\right)$$

$$\Delta M(\nu_r, u) = \frac{\nu_r\left(u_{atm}+u_{zero}(\theta)\right)}{c_{light}\Delta\nu_{FSR}}$$

The convolved transmission equation then becomes

$$T(\nu_r, T_e, T_{inst}, i, \theta, u) = A_0 + \sum_{n=1}^{N_{max}} e^{-\frac{4\pi^2 t^2 n^2 \alpha_D^2(T_{e,0})T_e}{T_{e,0}}}\left(A_n(i)\cos 2\pi n\Delta M - B_n(i)\sin 2\pi n\Delta M\right)$$

The derivative with respect to temperature is

$$\frac{\partial T(\nu_r, T_e, T_{inst}, i, \theta, u)}{\partial T_e} = -\frac{\pi^2\alpha_D^2(T_{e,0})}{\Delta\nu_{FSR}^2 T_{e,0}}\sum_{n=1}^{N_{max}} n^2 e^{-\frac{4\pi^2 t^2 n^2 \alpha_D^2(T_{e,0})T_e}{T_{e,0}}}\left(A_n(i)\cos 2\pi n\Delta M - B_n(i)\sin 2\pi n\Delta M\right)$$

and with respect to the atmospheric velocity

$$\frac{\partial T(\nu_r, T_e, T_{inst}, i, \theta, u)}{\partial u_{atm}} = -\frac{2\pi\nu_r}{c_{light}\Delta\nu_{FSR}}\sum_{n=1}^{N_{max}} n e^{-\frac{4\pi^2 t^2 n^2 \alpha_D^2(T_{e,0})T_e}{T_{e,0}}}\left(A_n(i)\sin 2\pi n\Delta M + B_n(i)\cos 2\pi n\Delta M\right)$$

Table 1. Instrument function parameter definitions.

Parameter	Units	Description
T	None	Convolved transmission function
ν	cm^{-1}	Wavenumber of light examined
ν_r	cm^{-1}	Rest position of center of emission line (i.e. position without Doppler shift)
T_e	K	Emission kinetic temperature
T_{inst}	^oC	Instrument temperature
i	None	Spectral channel index
L	None	Loss per etalon plate
R	None	Etalon plate reflectivity
N_{max}	None	Number of terms to use in expansion (theoretically infinite), 7-15 necessary for TIDI

Parameter	Units	Description
α_D	cm^{-1}	Doppler width of emission line $\alpha_D = \frac{\nu_0}{c}\left(\frac{2kT_e}{m}\right)^{\frac{1}{2}} = 4.30x10^{-7}\nu_0\left(\frac{T_e}{M}\right)^{\frac{1}{2}}$ k=Boltzmann's constant, m=mass of emitter, M is the molecular weight, M=16 for atomic oxygen, M=32 for molecular oxygen
$T_{e,0}$	K	Reference emission kinetic temperature
$\Delta\nu_{FSR}$	cm^{-1}	Etalon free spectral range $\Delta\nu_{FSR}$=1/(2t) where t is the gap thickness, gap=2.2 cm for TIDI
ν_0	cm^{-1}	Reference wavenumber
Δt_e	Cm	rms plate separation. This is related to the defect finesse, N_D, by $\Delta t_e = \frac{1}{N_D \nu_0 \sqrt{8 \ln 2}}$
N_b	None	Bowing finesse
N_t	None	Tilt finesse
$N_a^{'}(i)$	None	Aperture finesse for channel i
N_{fov}	None	Field of view finesse $N_{fov} = \frac{c_{light}\Delta\nu_{FSR}}{\nu_0 v_{sat} \cos\theta_{dep} \sin\theta_{az,0}\Delta\theta_{az}}$ v_{sat} = spacecraft speed (~7500 ms^{-1}), θ_{dep} =telescope depression angle from horizontal (~20-22^o), $\theta_{az,0}$=azimuth angle (45, 135, 225, 315^o), $\Delta\theta_{az}$=horizontal field of view (2.5^o)
ΔM_a	None	Orders from fringe center for channel i
$T_{inst,0}$	^oC	Instrument reference temperature
c_{light}	ms^{-1}	Speed of light (c=2.998 x 10^8 ms^{-1})
u	ms^{-1}	Relative motion of emitter with respect to instrument; positive value is coming towards instrument
u_{atm}	ms^{-1}	Line of sight atmospheric motion
u_{sc}	ms^{-1}	Component of the spacecraft motion in the look direction
u_{ref}	ms^{-1}	Reference velocity
u_{rot}	ms^{-1}	Component of Earth rotation along look direction.
u_{therm}	ms^{-1}	Thermal drift $u_{therm} = \alpha_T\left(T_{inst} - T_{inst,0}\right)$
α_T	$ms^{-1}\,{}^oC^{-1}$	Instrument thermal drift coefficient
u_{ltd}	ms^{-1}	Long term drift

Linearization

The background corrected, normalized, counts on the detector can be expressed:

$$S_i = C + B\sum_{j=1}^{J} T_{F,j}P_j(T_r)T_{i,j}(u,T_e)$$

where the terms are defined in Table 2.

Table 2. Parameter Definition

Parameter	Units	Description
i	None	Spectral channel number
j	None	Rotational line number
J	None	Number of spectral lines that pass through the filter
$T_{F,j}$	None	Filter transmittance for line j
B	Rayleighs	Emission band (or line) brightness
P_j	None	Fraction of band emission that falls in line j. $P_j \equiv 1$ for a single line.
T_e	K	Emission kinetic temperature
C	Rayleighs	Continuum (Rayleighs/cm^{-1}) times the filter area (cm^{-1})
$T_{i,j}$	None	Spectral response of the Fabry-Perot at channel i for line j
T_r	K	Emission rotational temperature
$T_{r,ref}$	K	Reference rotational temperature (200K)
σ_B	Rayleighs	Constraint standard deviation for brightness
σ_C	Rayleighs	Constraint standard deviation for continuum
σ_u	ms^{-1}	Constraint standard deviation for wind
σ_{T_e}	K	Constraint standard deviation for kinetic temperature
σ_{T_r}	K	Constraint standard deviation for rotational temperature
$\sigma_{T_{r,e}}$	K	Constraint standard deviation for difference between kinetic and rotational temperature
B_{con}	Rayleighs	Constraint value for brightness
C_{con}	Rayleighs	Constraint value for continuum
$T_{e,con}$	K	Constraint value for kinetic temperature
$T_{r,con}$	K	Constraint value for rotational temperature

u_{con}	ms^{-1}	Constraint value for wind

The fitting is performed by a standard non-linear least square fitting technique. First, the parameters to be fit (B, C, u, T_e, T_r) are linearized:

$$B = B_o + \Delta B$$

$$C = C_o + \Delta C$$

$$u = u_o + \Delta u$$

$$T_e = T_{e,0} + \Delta T_e$$

$$T_r = T_{r,0} + \Delta T_r$$

and the functions T and P are linearized

$$T_{i,j}(u, T_e) = T_{i,j}(u_0, T_{e,0}) + \frac{\partial T_{i,j}(u_0, T_{e,0})}{\partial u}(u - u_0) + \frac{\partial T_{i,j}(u_0, T_{e,0})}{\partial T_e}(T_e - T_{e,0})$$

$$P_j(T_r) = P_j(T_{r,0}) + \frac{\partial P_j(T_{r,0})}{\partial T_r}(T_r - T_{r,0})$$

Note $\frac{\partial P_j(T_{r,0})}{\partial T_r} \equiv 0$ for a single line since in this case $P \equiv 1$. The equation for the signal then becomes

$$S_i = (C_0 + \Delta C) + (B_0 + \Delta B)\sum_{j=1}^{J} T_{F,j}\left\{\left(P_j(T_{r,0}) + \frac{\partial P_j(T_{r,0})}{\partial T_r}(T_r - T_{r,0})\right)\right.$$
$$\left.\left(T_{i,j}(u_o, T_{e,0}) + \frac{\partial T_{i,j}(u_o, T_{e,0})}{\partial u}(u - u_0) + \frac{\partial T_{i,j}(u_o, T_{e,0})}{\partial T_e}(T_e - T_{e,0})\right)\right\}.$$

The multiplication is performed and only the linear terms are kept, giving

$$S_i = (C_0 + \Delta C) + \sum_{j=1}^{J} T_{F,j}\left\{B_0 P_j(T_{r,0}) T_{i,j}(u_o, T_{e,0})\right.$$
$$+ \Delta B P_j(T_{r,0}) T_{i,j}(u_o, T_{e,0}) + B_0 T_{i,j}(u_o, T_{e,0}) \frac{\partial P_j(T_{r,0})}{\partial T_r}(T_r - T_{r,0})$$
$$\left. + B_0 P_j(T_{r,0}) \frac{\partial T_{i,j}(u_o, T_{e,0})}{\partial u}(u - u_0) + B_0 P_j(T_{r,0}) \frac{\partial T_{i,j}(u_o, T_{e,0})}{\partial T_e}(T_e - T_{e,0})\right\}$$

Now define

$$S_{i,0} = C_0 + B_0 \sum_{j=1}^{J} T_{F,j} P_j(T_{r,0}) T_{i,j}(u_o, T_{e,0})$$

$$x_{1,i} = \frac{\partial S_i}{\partial \Delta B} = \sum_{j=1}^{J} T_{F,j} P_j (T_{r,0}) T_{i,j}\left(u_o, T_{e,0}\right)$$

$$x_{2,i} = \frac{\partial S_i}{\partial \Delta u} = B_0 \sum_{j=1}^{J} T_{F,j} P_j (T_{r,0}) \frac{\partial T_{i,j}\left(u_o, T_{e,0}\right)}{\partial u}$$

$$x_{3,i} = \frac{\partial S_i}{\partial \Delta T_e} = B_0 \sum_{j=1}^{J} T_{F,j} P_j (T_{r,0}) \frac{\partial T_{i,j}\left(u_o, T_{e,0}\right)}{\partial T_e}$$

$$x_{4,i} = \frac{\partial S_i}{\partial \Delta T_r} = B_0 \sum_{j=1}^{J} T_{F,j} T_{i,j}\left(u_o, T_{e,0}\right) \frac{\partial P_j (T_{r,0})}{\partial T_r}$$

$$x_{5,i} = \frac{\partial S_i}{\partial \Delta C} = 1.0$$

$$g_1 = \Delta B = B - B_0$$

$$g_2 = \Delta u = u - u_0$$

$$g_3 = \Delta T_e = T_e - T_{e,0}$$

$$g_4 = \Delta T_r = T_r - T_{r,0}$$

$$g_5 = \Delta C = C - C_0$$

This gives

$$S_i (B, u, T_e, T_r, C) = S_{i,0} (B_0, u_0, T_{e,0}, T_{r,0}, C_0) + \sum_{k=1}^{5} g_k x_{k,i}$$

Constrained Least Square fit

The function to be minimized is

$$\chi^2_{\nu,\nu_c} = \frac{1}{I + \nu_c - \nu} \left\{ \sum_{i=1}^{I} \left(\frac{S_{data,i} - S_{i,0} - \sum_{k=1}^{5} g_k x_{k,i}}{\sigma_i} \right)^2 + \left(\frac{B - B_{con}}{\sigma_B} \right)^2 \right.$$

$$\left. + \left(\frac{u - u_{con}}{\sigma_u} \right)^2 + \left(\frac{T_e - T_{e,con}}{\sigma_{T_e}} \right)^2 + \left(\frac{T_r - T_{r,con}}{\sigma_{T_r}} \right)^2 + \left(\frac{T_e - T_r}{\sigma_{T_{r,e}}} \right)^2 + \left(\frac{C - C_{con}}{\sigma_C} \right)^2 \right\}$$

where ν is the number of degrees of freedom (5 in this case) and ν_c is the number of constraints (0-5) that are included in the fit. This can be rewritten in a form that breaks the parameters to be fit into their reference and perturbation terms:

$$\chi^2_{\nu,\nu_c} = \frac{1}{I+\nu_c-\nu}\left\{\sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}-\sum_{k=1}^{5}g_k x_{k,i}}{\sigma_i}\right)^2 + \left(\frac{B_0+g_1-B_{con}}{\sigma_B}\right)^2 + \left(\frac{u_0+g_2-u_{con}}{\sigma_u}\right)^2\right.$$

$$+\left(\frac{T_{e,0}+g_3-T_{e,con}}{\sigma_{T_e}}\right)^2 + \left(\frac{T_{r,0}+g_4-T_{r,con}}{\sigma_{T_r}}\right)^2 + \left(\frac{T_{r,0}+g_4-T_{e,0}-g_3}{\sigma_{T_{r,e}}}\right)^2$$

$$\left.+\left(\frac{C_0+g_5-C_{con}}{\sigma_C}\right)^2\right\}$$

The derivatives with respect to the parameters to be fit (g's) are then taken

$$\frac{\chi^2_{\nu,\nu_c}}{\partial g_1} = 0 = \frac{1}{I+\nu_c-\nu}\left\{-\sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}-\sum_{k=1}^{5}g_k x_{k,i}}{\sigma_i^2}\right)x_{1,i} + \left(\frac{B_0+g_1-B_{con}}{\sigma_B^2}\right)\right\}$$

$$\frac{\partial\chi^2_{\nu,\nu_c}}{\partial g_2} = 0 = \frac{1}{I+\nu_c-\nu}\left\{-\sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}-\sum_{k=1}^{5}g_k x_{k,i}}{\sigma_i^2}\right)x_{2,i} + \left(\frac{u_0+g_2-u_{con}}{\sigma_u^2}\right)\right\}$$

$$\frac{\partial\chi^2_{\nu,\nu_c}}{\partial g_3} = 0 = \frac{1}{I+\nu_c-\nu}\left\{-\sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}-\sum_{k=1}^{5}g_k x_{k,i}}{\sigma_i^2}\right)x_{3,i}\right.$$

$$\left.+\left(\frac{T_{e,0}+g_3-T_{e,con}}{\sigma_{T_e}^2}\right)-\left(\frac{T_{r,0}+g_4-T_{e,0}-g_3}{\sigma_{T_{r,e}}^2}\right)\right\}$$

$$\frac{\partial\chi^2_{\nu,\nu_c}}{\partial g_4} = 0 = \frac{1}{I+\nu_c-\nu}\left\{-\sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}-\sum_{k=1}^{5}g_k x_{k,i}}{\sigma_i^2}\right)x_{4,i}\right.$$

$$\left.+\left(\frac{T_{r,0}+g_4-T_{r,con}}{\sigma_{T_r}^2}\right)+\left(\frac{T_{r,0}+g_4-T_{e,0}-g_3}{\sigma_{T_{r,e}}^2}\right)\right\}$$

$$\frac{\partial\chi^2_{\nu,\nu_c}}{\partial g_5} = 0 = \frac{1}{I+\nu_c-\nu}\left\{-\sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}-\sum_{k=1}^{5} g_k x_{k,i}}{\sigma_i^2}\right)x_{5,i} + \left(\frac{C_0+g_5-C_{con}}{\sigma_C^2}\right)\right\}$$

Now define a 5 element vector **Y** with elements

$$Y(m) = \sum_{i=1}^{I}\left(\frac{S_{data,i}-S_{i,0}}{\sigma_i^2}\right)x_{m,i} \, ,$$

a 5 element vector $\mathbf{Y_0}$ given by

$$\mathbf{Y_0} = \begin{bmatrix} \dfrac{B_0-B_{con}}{\sigma_B^2} \\ \dfrac{u_0-u_{con}}{\sigma_u^2} \\ \dfrac{T_{e,0}-T_{e,con}}{\sigma_{T_e}^2} - \dfrac{T_{r,0}-T_{e,0}}{\sigma_{T_{r,e}}^2} \\ \dfrac{T_{r,0}-T_{r,con}}{\sigma_{T_e}^2} + \dfrac{T_{r,0}-T_{e,0}}{\sigma_{T_{r,e}}^2} \\ \dfrac{C_0-C_{con}}{\sigma_C^2} \end{bmatrix},$$

a 5 by 5 kernel, **K**, with elements

$$K(m,n) = \sum_{i=1}^{I}\frac{x_{m,i}x_{n,i}}{\sigma_i^2} \, ,$$

and finally a 5 by 5 constraint matrix, $\mathbf{K_c}$,

$$\mathbf{K_C} = \begin{bmatrix} \frac{1}{\sigma_B^2} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sigma_u^2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sigma_{T_e}^2}+\frac{1}{\sigma_{T_{r,e}}^2} & -\frac{1}{\sigma_{T_{r,e}}^2} & 0 \\ 0 & 0 & -\frac{1}{\sigma_{T_{r,e}}^2} & \frac{1}{\sigma_{T_r}^2}+\frac{1}{\sigma_{T_{r,e}}^2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sigma_C^2} \end{bmatrix}.$$

This gives a matrix equation

$$\mathbf{Y} = \mathbf{Y_0} + (\mathbf{K}+\mathbf{K_C})\mathbf{g}$$

that has the solution

$$\mathbf{g} = (\mathbf{K} + \mathbf{K_C})^{-1}(\mathbf{Y} - \mathbf{Y_0}).$$

The vector **g** is used to update the parameters and a new value of chi-square is determined. If the relative change in chi-square is greater than a tolerance (~0.001) and the number of iterations is less than the maximum allows, the process is repeated.

Fitting procedure notes

The key to fitting Fabry-Perot spectra with a linearized fitting procedure as outlined here is to start with an initial guess for the velocity that is close so that the fitting will converge to the proper minima. If the starting guess is too far off, it is quite possible to converge on a solution approximately one-half order away, with the brightness and/or continuum significantly negative. The algorithm must be "tuned" so the initial guesses are close. Operationally, this means the reference or zero velocities must be known rather well. If that is true, then the initial guess on the atmospheric velocity can be set to 0; a starting guess that will rarely be off more than 100 ms^{-1}. The other parameters need not be chosen so carefully. The brightness and continuum are linear coefficients and are readily fit. It is required that the initial guess for the brightness be greater than 0 if the constraints are not used. The temperature is not linear, but there are not false minima in the temperature fitting so its value is also not critical.

The constraints could be very useful in processing TIDI data since the spectra contain much more noise than anticipated because of the light leak and ice scattering. As a consequence a straightforward least-square fit will contain many more bad values than desired. Noise spikes will on some occasions cause the fitting to be off a significant amount, and very importantly, the error bars will be underestimated (but probably still large) since they are based on a perturbation about an incorrect starting point. Constraints can be used to keep the initial guess where is should be. The atmospheric wind in the region that TIDI is examining rarely exceeds ±100 ms^{-1}, so a realistic constraint is $u_{con} = 0$ ms^{-1} and $\sigma_u = 100 ms^{-1}$.

Partitioning among O_2 A band emission lines

The fraction of the energy of a vibration transition that falls in a single rotational line in the O_2 Atmospheric band can be expressed

$$P_j(T_r) = \frac{P_j(T_{r,ref})T_{r,ref}}{T_r} \exp\left(\frac{hcE'}{k}\left(\frac{1}{T_{r,ref}} - \frac{1}{T_r}\right)\right)$$

where $T_{r,ref}$ is a reference temperature, $P_j(T_{r,ref})$ is the fraction of energy in rotational line j at the reference temperature, h is Planck's constant, k is Boltzmann's constant and E′ is the upper state energy. The parameters for the O_2 lines observed by TIDI are shown in Table 3. The derivative with respect to temperature is

$$\frac{\partial P_j(T_e)}{\partial T_r} = P_j(T_{r,ref})\left(\frac{hcE'}{kT_r^2} - \frac{1}{T_r}\right).$$

For small values of E′ or at high temperatures, the second term will dominate and the derivative is negative. As E′ increases or the temperature decreases, the first term becomes increasingly important and the derivative will be positive.

Table 3. Parameters for the O_2 lines observed by TIDI

Wavenumber (cm^{-1})	E′ (cm^{-1})	$P_j(T_{r,ref})$ [$T_{r,ref}$=200K]
13100.8070	58.43	0.0442
13098.8342	58.43	0.0524
13093.6407	100.15	0.0424
13091.6958	100.15	0.0485
13086.1095	152.98	0.0356
13084.1883	152.98	0.0398
13078.2116	216.92	0.0267
13076.3118	216.92	0.0293
13069.9459	291.94	0.0180
13068.0662	291.94	0.0195
13061.3115	378.04	0.0110
13059.4512	378.04	0.0118