HIGH RESOLUTION ATMOSPHERIC RADIATIVE TRANSFER CODE (H A R T C O D E)

Version No. 01

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Technical Report

August 1989

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* The author is visiting scientist from the University of Calabar, Department of Physics, P.M.B. 1115 Calabar, C.R.S. Nigeria ...The only way, therefore, to assure the highest accuracy in calculating atmospheric transmittance is to use the lineby-line method with a set of accurate line parameters and appropriate meteorological data.

A. J. LaRocca

ACKNOWLEDGEMENT

The author wishes to express his thanks for the financial support received from the International Centre for Theoretical Physics (ICTP) under the Programme for Training and Research in Italian Laboratories. The permanent assistance of Prof. G. Furlan, the Director of the Programme, and his staff is particularly appreciated. The constant interest and encouragement of Prof. R. Guzzi, the Director of IMGA-CNR, are also greatly appreciated. Several helpful discussions on the recent development of the IR spectroscopy were held with Dr. R. Rizzi who was also supplying me with most of the necessary background material moreover, the interest and willingness to help of G. Zibordi, F. Parmiggiani, M. Bonzagni, A. Ghelli and my other colleagues at the IMGA-CNR are gratefully acknowledged.

ABSTRACT

This document is the detailed description of the High-resolution Atmospheric Radiative Transfer Code (HARTCODE) recently developed at IMGA-CNR and an account on the first results of its application. The code was designed to improve the accuracy of infrared remote sensing and the parameterization of the basic infrared radiative processes in the atmosphere.

The HARTCODE computes the integrated optical depth, transmittance or radiance spectrum of a layered atmosphere for any viewing geometry with the desired resolution using the line-by-line integration method. The ultimate spectral resolution is not limited and - due to numerical reasons - the accuracy of the channel transmittances/radiances is more than six significant figures.

The first part of the report is a short mathematical summary of the IR atmospheric radiative transfer from the point of view of a line-by-line code.

The second part deals with the basic structure of the HARTCODE explaining the operation of the individual programme modules in detail.

The third part is devoted to the validation of the HARTCODE. The validation was based on comparisons with homogeneous transmittance measurements, comparisons with transmittance and radiance calculations for model atmospheres made by other authors and comparisons with measured radiances by the HIS interferometer under real atmospheric conditions.

The appendices contain the listing of the HARTCODE and the auxiliary routines.

The HARTCODE is not fully developed yet and the validation is still in progress. Accordingly, this version should not be regarded as an operative one and this report is not a "User's Manual" for immediate application. Instead, this report intends to give some assistance to those who are willing to go into the very details of the code for its further improvement.

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I. INTRODUCTION

1. The Aim of the Study

In the late 1987 a project was initiated by the ICTP to improve the efficiency of the weather forecasts and the related research activity in the developing countries of the equatorial areas.

The original idea was to prepare a large set of IR transmittance function profiles calculated for carefully selected model atmospheres taking into account the special features of the wet tropical climate. Having this type of data set one can calculate either the actual IR fluxes within the atmosphere for modeling purposes or the actual emission spectrum of the Earth- atmosphere system for remote sensing purposes by simple and fast interpolation method avoiding the enormous mathematical and computational difficulties arising from the subsequent solution of the IR radiative transfer equation.

Consequently the application of the IR satellite spectral measurements would become easier and more common and also the above set of transmittances could be the basis of the accurate parameterization of the radiative processes needed for the general circulation or large-scale climate models. (From practical point of view it is essential that the solution of both problems can be based on the same data set.)

To complete the above aim it is necessary to have a proper, on-line transmittance computer code. Because of the deviations between the results of the recently existing codes exceed the accuracy of the laboratory and field measurements and because there was not available a fully documented high resolution transmittance code which could serve as a starting point to develop a more accurate one, we had to prepare a new code which satisfies the necessary requirements of computational accuracy.

Generally the accuracy of such type of calculations merely depends on the outcome of the competition between the required accuracy and the available computer time. However, it should be understood that to investigate the effect of slight changes in the input spectroscopic data requires extreme numerical accuracy.

As a result of the permanent improvement of instrumentation, in atmospheric applications to evaluate high resolution measured radiance spectra - for example in the 600 - 1200 cm^{-1} spectral region - the required spectral resolution is around 0.01 cm^{-1} and the absolute error in the calculated channel radiance must be below 0.05 $mW/(cm^{-1}sterrad m^2)$.

The only hope to achieve this magnitude of absolute accuracy is to develop a high resolution transmittance/radiance code with numerical accuracy high enough to discover the deficiencies of the input spectroscopic data which themselves can also include our - sometimes insufficient - knowledge of the nature of the molecular absorption bands.

2. Recent Activity in the Field of IR Atmospheric Transmittance and Radiance Calculations

From 1982 till the present time a transmittance/radiance model comparison study is being conducted under the auspices of the IAMAP-IRC (International Association of Meteorology and Atmospheric Physics - International Radiation Commission) and with the coordination of the WGRS (Working Group on Remote Sensing).

This international activity - called ITRA (Intercomparison of Transmittance and Radiance Algorithms) - was organized to work on three different fields :

IR Nadir Group, convener D. Spankuch, IR Limb Group, convener H. Fischer, Microwave Group, convener K. F. Kunzi,

with the overall coordination of A. Chedin. In the three sub-groups the high resolution LBL (Line-by-line) computer codes were studied and compared for several model conditions.

Another working group, the ICRCCM (Intercomparison of Radiation Codes in Climate Models) is dealing with the problems of implementation and validation of the radiance algorithms related to climate models.

All over the world about nine or ten scientific teams were joining to the activity of the ITRA subgroups. The ITRA proved to be an excellent basis to monitor the accuracy and development of the individual high resolution IR transmittance codes.

So far two exercises were completed by the ITRA. The first one was concerned to homogeneous CO_2 transmittances and the basis of the comparisons were the well-documented transmittance spectra obtained under laboratory conditions in the 600-800 cm⁻¹ spectral region by Gryvnak et al.^[1] and Bulanin et al.^[2]. In the second exercise the calculations were performed for different model atmospheres and both the CO_2 and H_2O were involved.

We are very thankful to A. Chedin who was kindly supplying us with the detailed documentation of the first exercise^[3] and with the reports on the second exercise edited by D. $Spankuch^{[4]}$ and H. $Fischer^{[5]}$.

In the present stage of development of the HARTCODE we are able to join to the exercises conducted by the Nadir and Limb Sub-Groups and further on to perform extended validations by measurements that are going to be taken under fully monitored real atmospheric conditions.

3. Equation of the IR Radiative Transfer

For sake of simplicity in deriving the equations of the IR radiative transfer for atmospheric conditions we are making some assumptions.

• The atmosphere is in local thermodynamical equilibrium (LTE). This is true up to the height of 60-70 km. Above this level correction must be applied to the Planck function to obtain correct source functions. (This problem is rather pronounced in the cooling rate calculations for the upper atmosphere.)

• The atmosphere is plane-parallel and horizontally homogeneous and the refraction is negligible. To consider a spherically stratified refractive geometry correction must be applied to the relative optical path.

• Light scattering in the IR spectral region is also negligible. (This is true for the gas components but we do not have sufficient information about the aerosol particles.)

The differential equation may be written according to $Chandrashekar^{[6]}$:

$$\mu \frac{dI_{\nu}(\tau_{\nu},\mu)}{d\tau_{\nu}} = I_{\nu}(\tau_{\nu},\mu) - J_{\nu}(\tau_{\nu}), \qquad (1)$$

where I_{ν} is the monochromatic radiance, J_{ν} is the source function, ν is the wave number, $\mu = cos(\theta)$ and θ is the zenith angle, τ_{ν} is the monochromatic optical thickness (or optical depth) generally defined by:

$$\tau_{\nu}(s_2) - \tau_{\nu}(s_1) = \int_{s_1}^{s_2} k_{\nu}(s) du(s), \qquad (2)$$

where k_{ν} is the monochromatic mass absorption coefficient u is the optical mass of the absorbing gas and s is the optical path. For $\theta < 60^{\circ}$ $1/\mu = \mu^*$ where $\mu^* = ds/dz$ is the relative optical path and z is the vertical coordinate. Under suitable (LTE) conditions J_{ν} can be approximated by the Planck blackbody function :

$$J_{\nu} = B_{\nu}(T) = c_1 \nu^3 \left[exp\left(\frac{c_2 \nu}{T}\right) - 1 \right]^{-1},$$
(3)

where $c_1 = 1.1909596 \times 10^{-5}$, $c_2 = 1.43879$ if the wave number is given in cm^{-1} and T is the absolute temperature of the absorbing gas.

For an optical path in the Earth's atmosphere we shall follow the usual convention that τ_{ν} is measured vertically, $\tau_{\nu} = 0$ at the top of the atmosphere and increasing downward ($\tau_{\nu} = \tau_{\nu}^{g}$ at the ground) and $\mu > 0$ indicates the outward direction. In this case the proper boundary conditions are : $I_{\nu}(0, \mu^{-}) = 0$ for $\mu = \mu^{-} < 0$ and $I_{\nu}(\tau_{\nu}^{g}, \mu^{+}) = B_{\nu}(T_{g})$ for $\mu = \mu^{+} > 0$. The first one implies that the solar radiation is negligible - which is not true in the NIR regions - while the second one assumes that the Earth's surface is a perfect black-body which is again an approximation. We should also note that the temperature of the air at the ground, the ground temperature and the brightness temperature of the radiating surface are normally not the same.

With respect the boundary conditions given above Eq. (1) can easily be integrated to obtain the up- and down-welling radiance at level τ_{ν} :

$$I_{\nu}(\tau_{\nu},\mu^{+}) = B_{\nu}(T_{g})exp\left[-\frac{(\tau_{\nu}^{g}-\tau_{\nu})}{\mu^{+}}\right] + \int_{\tau_{\nu}}^{\tau_{\nu}^{g}} B_{\nu}(T(\tau_{\nu}^{,}))exp\left[-\frac{(\tau_{\nu}^{,}-\tau_{\nu})}{\mu^{+}}\right]\frac{d\tau_{\nu}^{,}}{\mu^{+}} \quad (4)$$
$$I_{\nu}(\tau_{\nu},\mu^{-}) = \int_{0}^{\tau_{\nu}} B_{\nu}(T(\tau_{\nu}^{,}))exp\left[-\frac{(\tau_{\nu}-\tau_{\nu})}{\mu^{-}}\right]\frac{d\tau_{\nu}^{,}}{\mu^{-}}. \quad (5)$$

Eqs. (4) and (5) weighted with the normalized instrumental response function and setting the limits of the integral properly to the condition of the particular measurement are the fundamental equations for the IR remote sensing. In case of a satellite radiance measurement in the channel ν_i with an instrumental response function $\Phi_{\nu_i}(\nu)$ and with a viewing angle $\theta < 90^{\circ}$ Eq. (4) takes the following form:

$$I_{\overline{\nu_i}}(\mu) = \int_{0}^{\infty} \left[B_{\nu}(T_g) exp(-\frac{\tau_{\nu}^g}{\mu}) + \int_{0}^{\tau_{\nu}^g} B_{\nu}(T(\tau_{\nu})) exp(-\frac{\tau_{\nu}}{\mu}) \frac{d\tau_{\nu}}{\mu} \right] \Phi_{\nu_i} d\nu.$$
(6)

To obtain the flux across a horizontal surface at level p the monochromatic radiance must be integrated over the full solid angle and the whole wave number interval (by definition). Assuming cylindrical symmetry the flux divergence is :

$$\frac{dF(p)}{dp} = 2\pi \int_{0}^{\infty} \int_{-1}^{1} \mu \frac{dI_{\nu}(\tau_{\nu},\mu)}{dp} d\mu d\nu.$$
(7)

For $\mu > 0$ $I_{\nu}(\tau_{\nu}, \mu)$ is equivalent with Eq. (4) and for $\mu < 0$ $I_{\nu}(\tau_{\nu}, \mu)$ is equivalent with Eq. (5). This last equation gives the rate of loss of radiant energy at pressure level p and is directly related to cooling rate calculations via the next equation : $c_p(dT/dt) = -g(dF(p)/dp)$ where c_p is the specific heat of the air at constant pressure, t is the time and g is the gravity acceleration.

It is obvious that Eqs. (6) and (7) have some common characteristic. Both equations involve wave number integration and integration with respect to the vertical coordinate. More important however, that both integrand contain the same mathematical expression which is called the monochromatic transmission function or transmittance:

$$\gamma_{\nu}(\tau_{\nu}^{,},\tau_{\nu}) = exp\left(-\frac{\tau_{\nu}^{,}-\tau_{\nu}}{\mu}\right) \tag{8}$$

This expression has a fundamental role in the IR radiative transfer and will be discussed in the next section.

4. Transmission Function and Weighting Function

In terms of the transmission function one can rewrite Eqs. (4) and (5) into a more convenient form :

$$I_{\nu}(\tau_{\nu},\mu^{+}) = B_{\nu}(T_{g})\gamma_{\nu}(\tau_{\nu}^{g},\tau_{\nu}) - \int_{\tau_{\nu}}^{\tau_{\nu}^{g}} B_{\nu}(T(\tau_{\nu}^{,})) \frac{\partial\gamma_{\nu}(\tau_{\nu}^{,},\tau_{\nu})}{\partial\tau_{\nu}^{,}} d\tau_{\nu}^{,}$$
(9)

$$I_{\nu}(\tau_{\nu},\mu^{-}) = \int_{0}^{\tau_{\nu}} B_{\nu}(T(\tau_{\nu})) \frac{\partial \gamma_{\nu}(\tau_{\nu},\tau_{\nu})}{\partial \tau_{\nu}} d\tau_{\nu}^{,}.$$
 (10)

The partial derivatives in the integrand are the weighting functions and practically the information content of any kind of spectral measurements will depend on the behavior of these functions.

Recalling the original definition of the optical thickness we can introduce pressure coordinates. With the pressure coordinates $d\tau_{\nu} = k_{\nu}\omega(p)dp$ where $\omega(p) = \rho(p)/[g\rho_a(p)]$ is the mass mixing ratio profile of the absorber and ρ and ρ_a are the density profiles of the absorber and the air. (In the HARTCODE ω is measured in *atm-cm/mb*.) Now considering only the looking-down geometry the measured radiance at the top of the atmosphere is :

$$I_{\overline{\nu_i}} = \int_{0}^{\infty} \left[B_{\nu}(T_g) \gamma_{\nu}(p_g) + \int_{0}^{p_g} B_{\nu}(T(p)) W_{\nu}(p) dp \right] \Phi_{\nu_i} d\nu,$$
(11)

where

$$W_{\nu}(p) = \frac{\partial \gamma_{\nu}(p)}{\partial p} \tag{12}$$

is the weighting function and

$$\gamma_{\nu}(p) = exp\left[-\mu^* \int_{0}^{p} \omega k_{\nu} dp\right]$$
(13)

is the transmittance of an atmospheric layer from the top of the atmosphere to the pressure level p.

To calculate $I_{\overline{\nu_i}}$ by Eq. (11) both the wave number and the pressure integral must be evaluated by numerical methods. Generally the half-power bandwidth of the IR spectrometers normally used in satellite remote sensing is in the range of 0.1-20.0 cm^{-1} and the shape of the $\Phi_{\nu_i}(\nu)$ function can be approximated by a rectangular, triangular or Gaussian function. Compared with the oscillating nature of the absorption coefficient the wave number dependence of the response function is smooth. Since within the spectral range of the response function the Planck function is also approximately constant the only problem which arises at the numerical evaluation of the wave number integral in Eq. (11) is the integration of the transmittance function over a suitable short wave number interval.

5. The Monochromatic Mass Absorption Coefficient

As we mentioned before the source of the computational difficulties is in the spectral behavior of the absorption coefficient. In case of several absorber and slant optical path the total monochromatic optical thickness of an atmospheric layer is defined as :

$$\tau_{\nu}^{*}(p_{1}, p_{2}) = \mu^{*} \int_{p_{1}}^{p_{2}} \left(\sum_{i=1}^{N} k_{\nu}^{i} \omega^{i} \right) dp$$
(14)

where N is the number of different molecule species involved in the absorption. For a given wave number the monochromatic absorption coefficient of the *i*-th absorber is the sum of the superposition of the individual absorption lines and the continuum absorption coefficient :

$$k_{\nu}^{i}(p,T) = \sum_{j=1}^{N_{B}^{i}} \sum_{k=1}^{N^{i,j}} S_{k}^{i,j}(T) f_{k}^{i,j}(\nu,p,T) + C^{i}(\nu,p,T)$$
(15)

where N_B^i is the number of the vibrational bands, $N^{i,j}$ is the total number of the individual absorption lines belonging to the *j*-th absorption band of the *i*-th molecule type, $S_k^{i,j}$ is the intensity of the k-th line, $f_k^{i,j}$ is the normalized line shape function and C^i is the continuum absorption coefficient.

For further processing, the most convenient expression for the line intensity which fits to the intensity definitions of the spectroscopic data banks is :

$$S_{k}^{i,j}(T) = S_{k}^{i,j}(T_{o})Q_{v}^{i}(T)Q_{r}^{i}(T)exp\left[c_{2}E_{k}^{i,j}\left(\frac{1}{T_{o}}-\frac{1}{T}\right)\right],$$
(16)

where $S_k^{i,j}(T_o)$ is the line intensity at temperature $T_o = 296 \ K, \ Q_v^i$ and Q_r^i are the vibrational and rotational partition functions, and $E_k^{i,j}$ is the lower state energy of the k-th transition in cm^{-1} .

In the HARTCODE we used $atm-cm^{-1}cm^{-1}$ as the unit of the line intensity. The temperature dependences of the partition functions are simple power functions:

$$Q_r^i(T) = \left(\frac{T_o}{T}\right)^{a_r^i} \tag{17}$$

and

$$Q_v^i(T) = a_v^i + b_v^i \left(\frac{T_o}{T}\right)^{c_v^i}$$
(18)

The usual value of a_r^i is 1.0 for linear molecules (like CO_2 , O_2 , and N_2O) and 1.5 for nonlinear molecules (like H_2O , O_3 and CH_4). The numerical values of a_v^i , b_v^i and c_v^i for a few molecules are presented in Table I-1. They were obtained by least-square fitting to the Q_v^i values published by *McClatchey et.al.*^[7].

TABLE I-1

Numerical values of a_v^i , b_v^i and c_v^i that were used to calculate the vibrational partition functions.

i	molecule	a_v^i	b_v^i	c_v^i	
1	H_2O	1.00000	0.00000	0.00000	
2	CO_2	0.99752	0.09310	-3.54915	
3	O_3	0.99852	0.04600	-4.11179	
4	N_2O	1.01819	0.12700	-4.42836	
5	CH_4	1.00000	0.00000	0.00000	
6	СО	0.99935	0.00700	-5.47575	
7	O_2	1.00000	0.00000	0.00000	

The continuum absorption coefficients - although they vary over a wide spectral range - can be regarded as constants within the range of the response function. For the water vapor the HARTCODE uses the digitized values of the H_2O continuum absorption curves published by *Kneizys et.al.*^[8].

The actual values of the self- and foreign- density dependent terms at a given wave number are calculated by the quadratic interpolation of the data presented in Table I-2.

TABLE I-2

wave number	$C_{s}(T_{1})$	$C_{e}(T_{c})$	$C_f(T_c)$
450	2 100 F 23	1.370 F 23	2625E 25
400	2.192E-23 1 270F 22	1.379E-23 8.245F 24	2.025E-25 7 810E 26
550	1.3791-23 8 680F 94	4.020 ± 24	2.576F 26
550 600	0.000E-24 5 462E 94	4.929E-24 2.046E-24	2.370E-20 1 140E 26
650	0.400E-24 4.019E-94	2.940E-24 1.059E-94	1.149E-20 4 405E 97
000 700	4.012E-24 2.659E-24	1.902E-24 1.902E-94	4.400E-27 1.867E-97
700	2.000 E-24 1.761 E.94	1.293E-24 9.570E-25	1.00/E-2/ 9.200E-20
750	1.701E-24 1.002E.94	0.070E-20 5.679E-25	0.320E-20 5 039E 39
800	1.293E-24	0.078E-20 4.170E-25	0.020E-20 2.250E-20
800	9.022E-20 C.075E.05	4.170E-25 2.0COE 25	3.338E-28
900	0.975E-25	3.002E-25	2.(44E-28
950	5.123E-25	2.492E-25	2.480E-28
1000	4.170E-25	1.927E-25	2.609E-28
1050	3.394E-25	1.651E-25	2.609E-28
1100	2.909E-25	1.415E-25	3.035E-28
1150	2.492E-25	1.344E-25	3.714E-28
1200	2.492E-25	1.344E-25	6.152 E-28
1250	$2.624 \text{E}{-}25$	1.490 E- 25	$1.688 \text{E}{-27}$
1300	3.394E-25	2.249E-25	6.936E-27
1350	6.293 E- 25	4.622 E- 25	2.850E-26
1400	1.228E-24	8.570 E- 25	7.819E-26
1450	2.398E-24	1.761E-24	2.145 E- 25
1500	4.223E-24	2.946E-24	3.931E-25
1525	5.463 E- 24	3.619E-24	4.349 E- 25
1550	6.055 E- 24	4.012E-24	4.810 E- 25
1600	4.223E-24	2.525E-24	2.625 E- 25
1612	4.012 E- 24	2.398E-24	2.373E-25
1625	4.012 E- 24	2.398E-24	2.625 E- 25
1650	4.929E-24	3.266E-24	3.931E-25
1675	5.463 E- 24	3.619E-24	4.349E-25
1700	4.681E-24	3.102 E- 24	3.931E-25
1725	4.929E-24	3.266E-24	3.553E-25
1750	2.946E-24	1.952E-24	2.256E-25
1800	1.509E-24	1.000E-24	1.006E-25
1850	8.570E-25	5.678E-25	5.221E-26
1900	4.390E-25	3.062E-25	$2.214\overline{E}$ -26
1950	2.249E-25	1.490E-25	1.149E-26
2000	1.213E-25	8.036E-26	3.785E-27
2050	6.541E-26	3.910E-26	1.688E-27
2100	4.334E-26	2.337E-26	5.562E-28
$\frac{2150}{2150}$	3.351E-26	1.549E-26	3.035E-28
2200	2.337E-26	1.026E-26	2.027E-28
2250	1.630E-26	7.157E-27	1.832E-28
2300	1.260E-26	4.992E-27	1.742E-28
2350	9 746E-27	$3.860E_{-27}$	1.656E-28
2400	8.352E-27	2.984F-27	1.500 ± 20 1.575 ± 28
2450	$6.457E_{-27}$	2.00 ± 1.21 2.420 E-27	$1.575E_{-20}$
2100			

Continuum absorption coefficients in the $450 - 2500 \ cm^{-1}$ spectral region according to *Kneizys et.al.*^[8]. The units are in cm^{-1} and $(cm^{-1} \ molec./cm^2)^{-1}$.

The temperature dependence (at fixed wave number and pressure) is given by the next equation:

$$C^{H_2O}(T) = \left(\frac{\nu}{\rho_a(p_o)}\right) tanh\left[\frac{c_2\nu}{2T}\right] \left(\rho_s(p)C_s(T) + \left[\rho_a(p) - \rho_s(p)\right]C_f\right)$$
(19)

where

$$C_s(T) = C_s(T_o) + \left[C_s(T_o) - C_s(T_1)\right] \frac{T - T_o}{T_o - T_1}.$$
(20)

In Eq. (19) C_f is the foreign broadened term, $\rho_s(p)$ is the H_2O density at pressure p, $\rho_a(p_o)$ is the reference air density at $p_o = 1013.25$ HPa. Eq. (20) is the temperature dependence of the self broadened continuum absorption coefficient where $T_1 = 260$ K. No information are available about the temperature dependence of the foreign broadened term therefore $C_f = C_f(T_o)$.

According to recent measurements made by Billing and $Bolle^{[9]}$ there is an overestimation of the water vapor continuum absorption coefficients in 700-1400 cm^{-1} spectral interval therefore it might be necessary to update the continuum absorption data in Table I-2 .

The incorporation of the nitrogen and oxygen continuum absorption into the HARTCODE is in progress.

6. Line Shape Function

The most problematic term in Eq. (15) is the line shape function which will be discussed in detail in this section. Let us consider a given vibrational band $(f_k^{i,j} = f_k^i)$. Due to the frequent collisions between the gas molecules and to the Doppler-effect the f_k^i function is pressure, temperature and wave number dependent. The adequate line shape function which gives account on both phenomena is the Voigt profile, $f_k^i = V_k^i$, $Armstrong^{[10]}$:

$$V_k^i = \frac{\alpha_k^i}{\pi^{3/2}} \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{(\alpha_k^i)^2 + (\nu - \nu_k - t \ \beta_k^i / \sqrt{\ln 2} \)^2} dt$$
(21)

where

$$\alpha_k^i = \alpha_{k,o}^i \frac{p}{p_o} \left(\frac{T_o}{T}\right)^{\Gamma_k^i} \tag{22}$$

and

$$\beta_k^i = \frac{\nu_k}{c} \sqrt{\frac{2\kappa \ T \ ln \ 2}{m^i}} \tag{23}$$

are the collisional and doppler half widths respectively.

In Eqs. (22) and (23) $\alpha_{k,o}^i = \alpha_k^i(p_o, T_o)$, Γ_k^i is a constant describing the temperature dependence of the collisional half width, c is the speed of the light, κ is the Boltzman constant and m^i is the mass of the molecule of the i-th absorber. The doppler half width may be written in the next form: $\beta_k^i = c_3 \nu_k \sqrt{T/M^i}$, where $c_3 = 3.5811 \times 10^{-7}$ and M^i is the molecular weight.

In the HARTCODE the Voigt profile V_k^i is evaluated by the method developed by $Young^{[11]}$. A faster version of the method with limited accuracy was published by $Drayson^{[12]}$.

Utilizing the characteristics of the Dirac delta function $(\int \triangle(x')dx' = 1 \text{ and } \int \triangle(x-x')f(x')dx' = f(x))$ it is easy to show that at atmospheric pressures smaller than 0.1 *HPa* ($\alpha_k^i \ll \beta_k^i$) or larger than 300 *HPa* ($\alpha_k^i \gg \beta_k^i$) Eq. (21) reduces to its two asymptotic forms:

$$D_k^i = \frac{1}{\beta_k^i} \sqrt{\frac{\ln 2}{\pi}} \exp\left[-\left(\frac{(\nu - \nu_k)\sqrt{\ln 2}}{\beta_k^i}\right)^2\right]$$
(24)

and

$$L_{k}^{i} = \frac{1}{\pi} \frac{\alpha_{k}^{i}}{(\alpha_{k}^{i})^{2} + (\nu - \nu_{k})^{2}}$$
(25)

The first equation is the Doppler line shape and valid in the regions where the doppler effect is the major source of the line broadening.

The second equation is the Lorentz line shape and valid for the collisional broadened lines. Laboratory measurements show that the self and foreign broadened collisional half widths are different $Drayson^{[13]}$. For example in case of CO_2 in the 660 cm^{-1} region the self broadened $\alpha_{k,o}^{CO_2} = 0.1 \ cm^{-1}$ while the foreign (N_2) broadened $\alpha_{k,o}^{CO_2} = 0.064 \ cm^{-1}$. When simulating laboratory measurements where the concentrations of the absorber and the foreign gas are comparable the collisional half width must be a weighted average value by the concentrations. The differences in the self and foreign broadened collisional half widths can be accounted for by introducing an effective pressure $p^{*,i} = p + (b^{*,i} - 1)p^i$ where pis the total pressure, p^i is the partial pressure of the ith absorber and $b^{*,i}$ is an empirical constant. Another problem concerning the collisional half width is that not too much known about the dependence on the rotational quantum numbers.

For the CO_2 the AFGL-82 catalog, Rothman et.al.^[14], uses a simple linear function, due to recent measurements, $Spänkuch^{[4]}$, the dependence is described by two different linear curves one for the small and the other for the large rotational quantum numbers, while Winters et.al.^[15] derived a complicated regression equation containing even a temperature dependence based on Madden's measurements.

The deviations between the different treatments can result more than 30 percent change in the value of $\alpha_{k,o}^i$.

Based on the kinetic theory of gases the number of collisions must be proportional to p/\sqrt{T} , therefore $\Gamma_k^i = 0.5$. Experimental results show significant scatter in the measured values of Γ_k^i . For example, in case of $CO \ \Gamma_k^i = 0.25$ according to Bulanin et.al.^[16] and $\Gamma_k^i = 0.75$ measured by $Varansi^{[17]}$. A detailed set of Γ_k^i were published by Rothman et.al.^[18].

Since very few measurements of α_k^i and Γ_k^i are available most probably they are the least accurately known spectroscopic parameters.

There is a third process (related to the finite lifetime of the exited states of the molecules) which results the natural broadening of the spectrum lines. In the IR region the half width due to the natural broadening is about $10^{-8} \ cm^{-1}$ and completely negligible. For most of the IR active molecules around 1000 $\ cm^{-1} \ \beta_k^i$ is in the order of $10^{-4} \ cm^{-1}$ and $\alpha_{k,o}^i$ is about $10^{-1} \ cm^{-1}$ at STP.

For the rotational water vapor band the Van Vleck Weisskopf (VVW) line shape were successfully used, $Drayson\ et.al.^{[19]}$:

$$W_k^i = \frac{\nu(1 - exp[-c_2\nu/T])}{\nu_k(1 - exp[-c_2\nu_k/T])} \left[L_k^i + \frac{\alpha_k^i}{\pi} \frac{1}{(\nu + \nu_k)^2 + (\alpha_k^i)^2} \right].$$
 (26)

Bulanin et.al.^[16] were using a similar line shape function for the calculations of the CO, N_2O and CO_2 absorption coefficients :

$$W_k^i = 2L_k^i \frac{\nu}{\nu_k} \left(1 + exp[-c_2(\nu - \nu_k)/T]\right)^{-1}.$$
(27)

Another versions of the VVW line shape are temperature independent expressions, $Drayson \ et.al.^{[19]}$:

$$W_{k}^{i} = \left(\frac{\nu}{\nu_{k}}\right)^{2} \left[L_{k}^{i} + \frac{\alpha_{k}^{i}}{\pi} \frac{1}{(\nu + \nu_{k})^{2} + (\alpha_{k}^{i})^{2}} \right],$$
(28)

$$W_{k}^{i} = \left(\frac{\nu}{\nu_{k}}\right) \left[L_{k}^{i} + \frac{\alpha_{k}^{i}}{\pi} \frac{1}{(\nu + \nu_{k})^{2} + (\alpha_{k}^{i})^{2}} \right].$$
 (29)

The common characteristics of these line shapes are: they are not normalized and they are very close to the Lorentz line shape when $\Delta \nu_k = |\nu - \nu_k| \ll 1$. Far from the line centers the conditions under which the VVW line shape was derived are not valid. The last two form may be applied in the microwave region where $c_2\nu_k/T \ll 1.0$.

7. Line Wing and Band Shape

 CO_2 absorption measurements in the ν_3 band around 2349 cm^{-1} performed by Winters et.al.^[15] and Plyler et.al.^[20] indicated that in the pressure broadening region at larger distances from the band center (50-200 cm^{-1}) the measured absorption coefficients are much less than the ones predicted theoretically by using the superposition of pure Lorentzian line shapes. Transmittance measurements using very long path in the ν_2 band of the CO_2 were performed at the Jet Propulsion Laboratory (JPL) showing the same effect, $Taylor^{[21]}$. Bulanin et.al.^[16] obtained similar results by measuring the band shapes of several molecules and vibrational bands.

Although attempts were made for the correct theoretical explanation (see for example $Zuev^{[22]}$, $Armstrong^{[23]}$, $Bulanin et.al.^{[16]}$) the above effect is not fully understood yet. Based on the measurements, however, it is obvious that at the line wings correction must be applied to the Lorentz line shape function. This correction is generally performed by a multiplying function depending only on $\Delta \nu_k$:

$$f_k^i = L_k^i \ F_k^i(\triangle \nu_k).$$

For the CO_2 (i = 2) the next correction functions are commonly used:

$$F_k^2 = \begin{cases} exp \Big[-1.4(\triangle \nu_k - 3.5)^{0.25} \Big], & \text{if } \triangle \nu_k \ge 3.5 \ cm^{-1}; \\ 1, & \text{if } \triangle \nu_k < 3.5 \ cm^{-1}. \end{cases}$$
(30)

This form was originally suggested by $Winters \ et.al.^{[15]}$ and used by T. Aoki and the japanese group during the second ITRA exercise (see $Sp\ddot{a}nkuch^{[4]}$).

$$F_k^2 = \begin{cases} 1, & \text{if } \Delta \nu_k < 0.5 \ cm^{-1}; \\ 1.069 exp[-0.133 \Delta \nu_k], & \text{if } 0.5 \le \Delta \nu_k < 23. \ cm^{-1}; \\ 0.05, & \text{if } 23. \le \Delta \nu_k < 50. \ cm^{-1}; \\ 0.133 exp[-0.0196 \Delta \nu_k], & \text{if } 50. \le \Delta \nu_k < 250. \ cm^{-1}; \\ 0, & \text{if } \Delta \nu_k > 250. \ cm^{-1}. \end{cases}$$
(31)

This stepwise function was published by Susskind and $Searl^{[23]}$. The next function which was applied during the second ITRA exercise by the NOAA group is again a stepwise approximation :

$$F_k^2 = \begin{cases} \left(1 + \frac{2}{11} \triangle \nu_k\right) exp\left[-\frac{2}{11} \triangle \nu_k\right], & \text{if } \triangle \nu_k < 11 \ cm^{-1}; \\ 0, & \text{if } \triangle \nu_k \ge 11 \ cm^{-1} \end{cases}$$
(32)

The simplest $F_k^{i,j}$ function which is the most frequently used in LBL codes is:

$$F_k^{i,j} = \begin{cases} 1, & \text{if } \Delta \nu_k \le R^{i,j}; \\ 0, & \text{if } \Delta \nu_k > R^{i,j}, \end{cases}$$
(33)

where $R^{i,j}$ is the line wing cut-off parameter which depends on the molecule type and vibrational band.

Based on the line-mixing theory Bulanin et.al.^[16] derived a complicated band correction function which seems to be difficult to implement into a LBL code .The problem is that the structure of his correction function is similar to that one of the absorption coefficient itself (ie. it is temperature dependent and contains all the lines being in a given vibrational band). In the simplest case, far from the line centers, the band correction function for the *j*-th vibrational band of the *i*-th molecule type takes the next form:

$$F^{i,j} = \frac{\sum_{k=1}^{N^{i,j}} A_k^{i,j} / (\nu - \nu_k)^2 - \left(\sum_{k=1}^{N^{i,j}} A_k^{i,j} / (\nu - \nu_k)\right)^2}{\sum_{k=1}^{N^{i,j}} A_k^{i,j} (1 - Ak^{i,j}) / (\nu - \nu_k)^2}$$
(34)

where

$$A_{k}^{i,j} = \frac{\nu_{B}^{i,j} S_{k}^{i,j}}{\nu_{k} S_{B}^{i,j}}$$
(35)

is the relative line intensity, $\nu_B^{i,j}$ is the band center and $S_B^{i,j}$ is the band intensity (at a given temperature). In the recent version of the HARTCODE the line interference is not considered although it seems possible to evaluate Eq. (34) simultaneously with Eq. (15) by checking the vibrational quantum identifiers.

Finally let us mention that in the newest version of the HITRAN database Rothman et.al.^[18] a coupling coefficient is introduced to consider the line-mixing effect in the CO_2 fundamental at 668 cm^{-1} and in the two hot bands at 618 and 671 cm^{-1} :

$$F_k = 1 + y_k (\nu - \nu_k) / \alpha_k \tag{36}$$

where y_k is the coupling coefficient. This correction can easily be applied in the HARTCODE whenever the new HITRAN database is available at IMGA. When this report was completed we obtained a copy of the HITRAN database^[34] and we have attempted to apply the correction given by Eq. (36). Unfortunately in the tape at the position of the coupling coefficients we encountered some undefined characters - at 618.024 and 720.7982 cm^{-1} - which made the simple application impossible.

8. Concept of the Line - by - Line Method

The fundamental problem in modeling the atmospheric IR radiation field is

:

How to obtain the average spectral transmittance or absorptance of an atmospheric layer over a given wave number interval.

The relevant mathematical expressions are :

$$\gamma_{\overline{\nu}}(p_1, p_2) = \frac{1}{\delta\nu} \int_{\delta\nu} exp\Big[-\tau_{\nu}^*(p_1, p_2) \Big] d\nu$$
(37)

$$\xi_{\overline{\nu}}(p_1, p_2) = 1 - \gamma_{\overline{\nu}}(p_1, p_2) \tag{38}$$

where $\gamma_{\overline{\nu}}$ and $\xi_{\overline{\nu}}$ are the average spectral transmittance and absorptance subsequently, $\delta\nu$ is the (suitable short) wave number interval and p_1 and p_2 are the pressure values at the lower and upper boundary of the layer subsequently.

To obtain information about $\gamma_{\overline{\nu}}$ and $\xi_{\overline{\nu}}$ there are three possibilities: measurements, calculations using the band model technique or calculations using the line-by-line method.

The limitations of the measurements are obvious. With respect to the variability of the atmosphere in space and time, the cost and time factor do not allow to take large number of measurements under different atmospheric conditions. Moreover, because of the inherent characteristic of the spectrometers the measured data are always weighted with certain type of instrumental response function which poses some difficulties in calculating the true averages.

This study do not intend to discuss critically the band model technique. About the exhausting large number of recently existing band models one may find comprehensive works in the literature, see for example LaRocca and $Turner^{[24]}$, $Anding^{[25]}$. Briefly, the band models are calculating $\gamma_{\overline{\nu}}$ and $\xi_{\overline{\nu}}$ by a more or less closed mathematical expression which is depending on the average spectroscopic parameters normally obtained by laboratory measurements. However, to obtain a mathematically tractable equation for $\gamma_{\overline{\nu}}$ and $\xi_{\overline{\nu}}$ some assumptions must be made on the structure and distribution of the line spacing and line intensities within $\delta\nu$. The problem with the application of the band models is that the spectrum lines in a real absorption band are never placed purely random or purely regular way. With the superposition of the different regular or random bands the accuracy may improve but the complexity of the equations and calculations will approach to that one of the line-by-line method.

By definition the LBL method is the numerical integration of Eq. (37) over the wave number interval $\delta\nu$ considering the real line structure represented by the spectral behavior of the total monochromatic optical thickness. In case of transmittance Eq. (37) may be written in the next form :

$$\gamma_{\overline{\nu}}(p_1, p_2) = \frac{1}{\delta\nu} \sum_{l=1}^{N_{\nu}} w_{\nu}^l exp\Big[-\tau_{\nu^l}^*\Big]$$
(39)

where N_{ν} , w_{ν}^{l} and ν^{l} are the orders, weights and abscissa of the numerical wave number integration subsequently. Further on $\delta\nu$ will be referred as the wave number resolution of the LBL code.

In the HARTCODE the numerical wave number integration is performed over a system of fine subdivisions by Gaussian quadrature of different order. The system of the wave number mesh is generated with respect to the required spectral resolution $\delta\nu$. The length of the sub-intervals are depending on the distance from the line center, the wave number dependent Doppler half width and the pressure range of the input data.

According to Eq. (14) the total monochromatic optical thickness of an atmospheric layer contains the integral of the line shape functions over the pressure range defined by p_1 and p_2 . This integration is only needed when the accuracy of the Curtis-Gudson (CG) approximation is not sufficient, i.e. $(p_2/p_1) >> 1.0$. In the pressure broadening range and close to the line centers the exact pressure integral of the Lorentz line shape may be used (the layer supposed to be isothermal with constant mass mixing ratio) :

$$\int_{p_1}^{p_2} L_k^i dp = \frac{1}{2\pi\alpha^*} ln \left[\frac{(\alpha^* p_2)^2 + \Delta\nu_k^2}{(\alpha^* p_1)^2 + \Delta\nu_k^2} \right]$$
(40)

where $\alpha^* = \alpha_k^i/p$. If the pressure dependence of the mass mixing ratio within the layer is simple power function the product with the Lorentz line shape is still remains integrable. (It is a very crude approximation to assume constant mass mixing ratio in case of H_2O and O_3 within even a relatively thin layer.) In case of the Voigt function the pressure integral might be calculated preceeding the numerical integration with respect t, $Drayson^{[26]}$:

$$\int_{p_1}^{p_2} V_k^i dp = \frac{1}{2\pi^{3/2} \alpha^*} \int_{-\infty}^{\infty} e^{-t^2} ln \left[\frac{(\alpha^* p_2)^2 + (\nu - \nu_k - t\beta_k^i / \sqrt{\ln 2})^2}{(\alpha^* p_1)^2 + (\nu - \nu_k - t\beta_k^i / \sqrt{\ln 2})^2} \right] dt$$
(41)

This equation is useful when 100 HPa > p > 10 HPa and 0.003 $cm^{-1} < \Delta \nu_k < 0.2 \ cm^{-1}$. (For the integration with respect t Drayson applied 20 point Hermite quadrature.)

In the HARTCODE to match the conditions for the CG approximation the secondary layering is an option. In case of several layers $\tau_{\nu_l}^*(p_1, p_{N_L})$ is expressed as the sum of the optical thicknesses of the individual layers :

$$\tau_{\nu_l}^*(p_1, p_{N_L}) = \sum_{m=1}^{N_L - 1} \mu_m^* \int_{p_m}^{p_{m+1}} \left(\sum_{i=1}^N k_{\nu^l}^{i,m} \omega^{i,m} \right) dp$$
(42)

where N_L is the number of levels. If $p_1 = 0.0$ and p_{N_L} is the pressure at the surface Eq. (42) is the total monochromatic optical thickness of the whole atmosphere (which is divided into $N_L - 1$ layers). In the recent version of the code the maximum number of the atmospheric levels is limited to 150. For practical purposes this is sufficient, however, by modifying the declaration statements any kind of layering is possible.

The LBL method requires the pre-calculated set of the basic spectroscopic parameters which is needed for the evaluation of $k_{\nu^l}^i$. Accordingly, when applying efficient numerical methods the accuracy will only depend on the accuracy of the input spectroscopic data.

9. Spectroscopic Data Banks

The frequently mentioned basic spectroscopic data are : resonant wave number, line intensity, air-broadened half width, lower state energy with the corresponding quantum and molecular identifiers and - in special cases - the temperature dependence of the half width and line coupling coefficients. Recently two compilation of the basic spectroscopic data are available :

The first one is the AFGL Atmospheric Line Parameters Compilation, published by *Rothman et al.*^[14,27]. The content of the latest version (edition of October 1982) is divided into two parts. The first one contains information about 176337 transitions of the main absorber (H_2O , CO_2 , O_3 , N_2O , CO, CH_4 , and O_2) in the 0-18000 cm⁻¹ spectral region. The second part with 94682 transitions in the 0-10000 cm⁻¹ region is the trace gas compilation. In the near future the updated version with 348043 transition might be available, see *Rothmanet al.*^[18].

The other compilation is the GEISA line catalog, published by $Chedin^{[28,30]}$ and $Husson \ et \ al.^{[29,31]}$. The 1984 version of the GEISA catalog contains 323554 transitions of 37 different molecules in the spectral range from microwaves to visible.

In this work we are frequently using both compilations. It has been discovered that at some spectral interval the two data significantly differ. The information about how to use the tapes and the details of the differences will be given in the next chapter.

10. Radiance Algorithms

For the radiance calculations we have developed two methods. In both methods the calculation is based on the fact that within a given layer and wave number interval the pressure dependence of the transmittance function can very well be approximated by an exponential-type function. Let us consider now the 'lookingdown' geometry, i.e. the calculation starts at the uppermost layer. Using a transmittance scale factor (or an effective absorption coefficient) for each layer and $\delta\nu$ the transmittance function and weighting function takes the next form:

$$\gamma_{\overline{\nu}}(p') = \gamma^m exp \left[-\frac{p' - p_m}{H^m} \right], \quad p_m < p' < p_{m+1}, \tag{43}$$

$$W_{\overline{\nu}}(p') = -\frac{\gamma_{\overline{\nu}}(p')}{H^m},\tag{44}$$

where H^m is the transmittance scale factor :

$$H^{m} = \frac{p_{m+1} - p_{m}}{\ln(\gamma^{m}/\gamma^{m+1})},$$
(45)

and the superscript m and m + 1 indicate the pressure levels. The accurate transmittances at the m-th level are calculated by Eq. (39), and $\gamma^m = \gamma_{\overline{\nu}}(p_1, p_m)$ where p_1 is the upper boundary pressure. Since within a layer the weighting function is directly proportional to the transmittance function one may calculate a rapidly convergent series of the weighted Planck functions. The temperature profile within the layer is approximated by a third-order polynomial of the pressure, therefore $B_{\overline{\nu}}(T(p')) = B_{\overline{\nu}}(p')$. To obtain the contribution to the radiance from the m-th layer the weighted average Planck function is multiplied with the difference in the transmittances at the upper and lower boundary:

$$B_{\overline{\nu}}^{m}(N_{c}) = \frac{\sum_{n=1}^{N_{c}} B_{\overline{\nu}}(p_{n}') \gamma_{\overline{\nu}}(p_{n}')}{\sum_{n=1}^{N_{c}} \gamma_{\overline{\nu}}(p_{n}')} (\gamma^{m} - \gamma^{m+1}), \qquad (46)$$

where $p'_1 = p_m < p'_{N_c} = p_{m+1}$ and $N_c \ge 2$ is the number of iterations depending on a predetermined accuracy limit. (Even for extreme transmittance and temperature profiles $N_c = 2$ gives good results.)

Another method to obtain accurate radiance is to approximate 1/T(p') (within the given layer) with a linear pressure function and expand the Planck function into a four or five term series :

$$B_{\overline{\nu}}(p') = c_1 \overline{\nu}^3 \left[\frac{e^{-B_2^m p'}}{B_1^m} + \frac{e^{-2B_2^m p'}}{(B_1^m)^2} + \cdots \right], \tag{47}$$

where

$$B_1^m = exp \left[\frac{c_2 \overline{\nu}}{p_{m+1} - p_m} \left(\frac{p_{m+1}}{T^m} - \frac{p_m}{T^{m+1}} \right) \right], \tag{48}$$

and

$$B_2^m = \frac{c_2 \overline{\nu}}{p_{m+1} - p_m} \left(\frac{1}{T^{m+1}} - \frac{1}{T^m} \right).$$
(49)

With not too high temperature differences and above 500 cm^{-1} the approximations are always satisfactory. The product of the Planck function, Eq. (47), and transmission function, Eq. (43), can easily be integrated (with respect the pressure p') giving an analytical formula for the radiance contribution of the layer:

$$B_{\overline{\nu}}^{m}(N_{d}) = c_{1}\overline{\nu}^{3} \sum_{n=1}^{N_{d}} \frac{\gamma^{m+1}exp(-nB_{2}^{m}p_{m+1}) - \gamma^{m}exp(-nB_{2}^{m}p_{m})}{(B_{1}^{m})^{n}(nB_{2}^{m}H^{m} + 1)}, \quad (50)$$

where $N_d \ge 2$ is the number of terms to be considered in the expansion given in Eq. (47).

The above two methods are practically giving the same results. In the HART-CODE both methods are applied and the related algorithms are installed.

Further analysis of the accuracy of other radiance algorithms (including the ones that were used in the second ITRA exercise) showed that the highest accuracy (about 10^{-4} percent relative error) can be achieved by applying 2nd order Gaussian quadrature over a given layer where the transmittance is approximated by Eq. (43) and the temperature is a simple power function. In the next version of the HARTCODE we shall introduce this method.

11. Spherical Refractive Atmosphere

At large zenith angles when the secant-law is not valid μ_m^* must be specified for each layer. The calculation of μ_m^* is discussed in detail in many papers, see for example *Kneizys at.al.*^[8], *Anding*^[25] and *Duncan*^[32].

In the HARTCODE we have developed a new algorithm which considers the changing curvature of the trajectory from layer to layer. In the next equations θ_m is the local zenith angle at the lower boundary of the *m*-th layer, n_m is the refractive index, h_m is the altitude and r_e is the radius of the Earth. In case of the upward direction for the computation of μ_m^* we have applied the following sequence of equations :

$$Z_m = h_m + r_e \tag{51}$$

$$\theta_m^* = asin\left[\frac{Z_m}{Z_{m+1}}sin(\theta_m)\right] \tag{52}$$

$$s_m = Z_{m+1} cos(\theta_m^*) - Z_m cos(\theta_m)$$
(53)

$$\theta_{m+1} = asin\left[\frac{n_m}{n_{m+1}}sin(\theta_m^*)\right]$$
(54)

$$\theta_{m+1}^{*} = asin\left[\frac{Z_{m+1}}{Z_{m+2}}sin(\theta_{m+1})\right]$$
(55)

$$s_{m+1} = Z_{m+2} \cos(\theta_{m+1}^*) - Z_{m+1} \cos(\theta_{m+1})$$
(56)

$$\delta_m = \pi - \theta_{m+1} + \theta_m^* \tag{57}$$

$$c_m = \sqrt{s_m^2 + s_{m+1}^2 - 2s_m s_{m+1} \cos(\delta_m)} \tag{58}$$

$$S_m = \frac{s_m + s_{m+1} + c_m}{2} \tag{59}$$

$$R_m = \frac{s_m s_{m+1} c_m}{4\sqrt{S_m (S_m - s_m)(S_m - s_{m+1})(S_m - c_m)}}$$
(60)

$$\mu_m^* = \frac{2R_m asin[s_m/(2R_m)]}{Z_{m+1} - Z_m}.$$
(61)

The refractive index of the air (as a function of the ambient pressure, temperature, water vapor partial pressure and wave number) is calculated by an empirical formula obtained by Edlen, $Jursa^{[33]}$, which is valid for a wide spectral range from the UV to the far IR.

In case of downward direction similar sequence is applied except that at the last layer the tangent height H_T - from Eqs. (52) and (54) - is calculated by the next equation :

$$H_T = \frac{Z_m n_m \sin(\theta_m)}{n_{m+1}} - r_e.$$
 (62)

The typical numerical accuracy of the calculated geometrical path length or the tangent height is better than 1 m.

Although for the transmittance and radiance calculations the relative optical air mass of the different kind of absorbers for the whole atmosphere are not needed explicitly, in the HARTCODE the module calculating the trajectory of the refracted beam may be used separately for high accuracy air mass calculations. In this case the relative optical air mass of the i-th absorber is given by the next equation :

$$M^{i}(\theta) = \frac{\sum_{m=1}^{N_{L}-1} \mu_{m}^{*}(\theta) u_{m}^{i} \triangle Z_{m}}{\sum_{m=1}^{N_{L}-1} u_{m}^{i} \triangle Z_{m}},$$
(63)

where u_m^i is the average column density of the *i*-th absorber at the *m*-th layer, ΔZ_m is the thickness of the layer and N_L is the number of levels. As an example in Tables I-3 and I-4 the angular deviation of the beam, geometrical path length and the air mass values are presented for different zenith angles at 0.5 μ without considering the refraction (Table I-3) and with refraction (Table I-4). The effect of the refraction at large zenith angles is about ten percent.

Some results of the HARTCODE high accuracy air mass calculations are presented in Appendix A. These Tables might be very useful at the evaluation of the narrow-band radiance measurements aimed to monitor the amount of the trace absorbers when to increase the sensitivity at the observations large zenith angles are used. If simultaneous radiosonde measurements are available the recalculation of the air mass with the actual profiles might also be necessary.

The first six Tables in Appendix A contain the optical air mass values of the air and the non-uniformly mixed main absorbers for the six standard Lowtran profiles at 15 μ . Table A-6 shows the results obtained for the US Standard Atmosphere 76 at 15 μ . If we compare this results with the ones presented in Table I-4 (same model atmosphere but at 0.5 μ) we can recognise the effect of the decreased refractive index (with increased wave length) on the angular deviation and the other quantities. Table A-7 contains the air mass values calculated for some trace gases and for the US Standard atmosphere 76 using the Lowtran trace gas profiles.

TABLE I-3

Relative optical air mass values for the USST 76 atmosphere with no refraction and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.00000	233.688	1.9932	1.9981	1.9793	1.9938	1.9952	1.9937
62.0	0.00000	247.752	2.1215	2.1276	2.1042	2.1223	2.1241	2.1221
64.0	0.00000	263.853	2.2703	2.2781	2.2483	2.2713	2.2736	2.2711
66.0	0.00000	282.418	2.4445	2.4546	2.4163	2.4459	2.4488	2.4456
68.0	0.00000	303.990	2.6510	2.6642	2.6141	2.6527	2.6566	2.6523
70.0	0.00000	329.278	2.8990	2.9168	2.8497	2.9013	2.9065	2.9008
72.0	0.00000	359.211	3.2018	3.2263	3.1343	3.2050	3.2121	3.2043
74.0	0.00000	395.020	3.5790	3.6139	3.4836	3.5835	3.5936	3.5825
76.0	0.00000	438.354	4.0607	4.1125	3.9206	4.0673	4.0823	4.0657
78.0	0.00000	491.430	4.6950	4.7761	4.4794	4.7052	4.7286	4.7028
80.0	0.00000	557.214	5.5645	5.7008	5.2118	5.5811	5.6204	5.5772
81.0	0.00000	596.054	6.1305	6.3132	5.6664	6.1523	6.2048	6.1471
82.0	0.00000	639.619	6.8212	7.0731	6.1968	6.8504	6.9226	6.8434
83.0	0.00000	688.566	7.6803	8.0397	6.8187	7.7206	7.8229	7.7109
84.0	0.00000	743.604	8.7735	9.3078	7.5492	8.8306	8.9811	8.8168
85.0	0.00000	805.489	10.2028	11.0384	8.4050	10.2863	10.5177	10.2660
86.0	0.00000	874.987	12.1330	13.5255	9.3947	12.2599	12.6347	12.2288
87.0	0.00000	952.832	14.8431	17.3589	10.5061	15.0436	15.6883	14.9941
87.5	0.00000	995.095	16.6322	20.1417	11.0922	16.8881	17.7552	16.8246
88.0	0.00000	1039.681	18.8280	23.8684	11.6830	19.1575	20.3446	19.0754
88.2	0.00000	1058.180	19.8478	25.7260	11.9170	20.2133	21.5662	20.1220
88.4	0.00000	1077.063	20.9630	27.8564	12.1479	21.3691	22.9157	21.2675
88.6	0.00000	1096.334	22.1857	30.3159	12.3745	22.6373	24.4107	22.5241
88.8	0.00000	1115.995	23.5293	33.1756	12.5956	24.0322	26.0719	23.9059
89.0	0.00000	1136.049	25.0092	36.5255	12.8099	25.5700	27.9233	25.4290
89.2	0.00000	1156.497	26.6434	40.4799	13.0164	27.2693	29.9932	27.1117
89.4	0.00000	1177.340	28.4523	45.1849	13.2141	29.1516	32.3148	28.9753
89.6	0.00000	1198.581	30.4595	50.8281	13.4024	31.2415	34.9274	31.0441
89.7	0.00000	1209.351	31.5459	54.0744	13.4927	32.3731	36.3571	32.1642
89.8	0.00000	1220.220	32.6924	57.6506	13.5805	33.5677	37.8776	33.3465
89.9	0.00000	1231.188	33.9031	61.5978	13.6657	34.8294	39.4961	34.5952
90.0	0.00000	1242.256	35.1824	65.9625	13.7482	36.1628	41.2205	35.9149

TABLE I-4

Relative optical air mass values for the USST 76 atmosphere at 0.5μ wavelength and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.02751	233.856	1.9939	1.9984	1.9807	1.9945	1.9958	1.9944
62.0	0.02985	247.960	2.1224	2.1280	2.1060	2.1232	2.1248	2.1230
64.0	0.03251	264.114	2.2715	2.2786	2.2506	2.2724	2.2745	2.2722
66.0	0.03558	282.748	2.4461	2.4552	2.4192	2.4473	2.4500	2.4470
68.0	0.03916	304.414	2.6530	2.6650	2.6179	2.6547	2.6582	2.6543
70.0	0.04340	329.830	2.9017	2.9178	2.8547	2.9039	2.9086	2.9034
72.0	0.04851	359.945	3.2055	3.2277	3.1411	3.2085	3.2150	3.2078
74.0	0.05481	396.016	3.5842	3.6160	3.4932	3.5886	3.5978	3.5875
76.0	0.06276	439.742	4.0684	4.1156	3.9345	4.0747	4.0885	4.0732
78.0	0.07314	493.419	4.7071	4.7811	4.5005	4.7168	4.7385	4.7145
80.0	0.08725	560.164	5.5846	5.7093	5.2455	5.6005	5.6370	5.5968
81.0	0.09638	599.700	6.1573	6.3247	5.7100	6.1783	6.2271	6.1733
82.0	0.10749	644.175	6.8578	7.0893	6.2541	6.8861	6.9534	6.8794
83.0	0.12125	694.326	7.7321	8.0634	6.8953	7.7712	7.8671	7.7619
84.0	0.13871	750.989	8.8495	9.3443	7.6537	8.9053	9.0472	8.8919
85.0	0.16144	815.104	10.3195	11.0985	8.5498	10.4018	10.6218	10.3819
86.0	0.19201	887.731	12.3224	13.6334	9.5980	12.4487	12.8094	12.4179
87.0	0.23469	970.098	15.1717	17.5770	10.7923	15.3743	16.0056	15.3244
87.5	0.26274	1015.388	17.0781	20.4702	11.4304	17.3389	18.1979	17.2743
88.0	0.29705	1063.713	19.4464	24.3875	12.0801	19.7862	20.9788	19.7016
88.2	0.31294	1083.953	20.5573	26.3592	12.3394	20.9361	22.3041	20.8416
88.4	0.33030	1104.743	21.7805	28.6359	12.5965	22.2036	23.7782	22.0978
88.6	0.34931	1126.107	23.1314	31.2856	12.8501	23.6047	25.4238	23.4861
88.8	0.37018	1148.070	24.6279	34.3949	13.0987	25.1583	27.2676	25.0252
89.0	0.39314	1170.662	26.2912	38.0759	13.3413	26.8866	29.3417	26.7370
89.2	0.41849	1193.917	28.1462	42.4745	13.5765	28.8156	31.6846	28.6470
89.4	0.44656	1217.872	30.2224	47.7824	13.8037	30.9760	34.3427	30.7860
89.6	0.47775	1242.574	32.5548	54.2529	14.0221	33.4045	37.3728	33.1900
89.7	0.49467	1255.222	33.8299	58.0255	14.1279	34.7328	39.0486	34.5048
89.8	0.51256	1268.079	35.1857	62.2233	14.2315	36.1454	40.8446	35.9028
89.9	0.53152	1281.154	36.6287	66.9065	14.3328	37.6492	42.7724	37.3912
90.0	0.55163	1294.458	38.1665	72.1449	14.4319	39.2521	44.8447	38.9775

II. STRUCTURE AND OPERATION OF THE HARTCODE

1. General Structure

In this chapter, after a short summary, the operation of the individual modules is discussed. The HARTCODE is basically a system of three groups of programmes written in Vax-Fortran.

The first group :

DECODA, DECODG, FIND and LIN

is performing the preliminary processing of the input spectroscopic data. Pre-processing does not necessarily mean neglecting absorption lines. For a particular wave number interval it is simply not economic to carry all the information given by the data banks. The consideration of the weak absorber or the very weak spectrum lines is always depending on the real conditions. The result of the operation of these modules are two data files containing all spectroscopic information needed by the HART programme.

The second group is the HART programme and its subroutines. These programmes are performing several tasks depending on the input instructions. Since this version of the HARTCODE was used for numerical testing the HART module can work in two different modes.

In <u>test</u> mode the spectroscopic parameters are internally generated and the first group of programmes are not used. Using this mode we can model the most extreme line distributions and check the computational accuracy in special cases.

In <u>line</u> mode HART is computing the spectral values (with the required $\delta \nu$ wave number resolution) of the next monochromatic quantities :

- a. optical depth given by Eq. (14),
- b. transmittance given by Eq. (13),
- c. radiance given by Eqs. (9) and (10)

for any kind of laboratory or atmospheric conditions using the spectroscopic data contained by the output files of the LIN program (lin.dat and farwg.dat). The results of the operation of the HART module are written in two data files for further processing (trao.dat and rad.dat).

The third group consists of three programmes :

SMTH, COMP and CHNL.

These programmes either compute the channel-radiance and weighting functions or apply different kind of smoothing. The outputs of these modules are data files for the plotting routines.

The numbered list of the individual modules are presented in the Appendices C, D and E. Figures II-1, II-2 and II-3 may give some idea about the general structure of the HARTCODE by displaying the block-diagrams of the operation of the three groups of programmes.

Since the programmes are not supplied with comment lines we refer to the location of a particular programme statement by quoting the line number(s) in curly braces. The different program-, subroutine- and function segments and the variables (character, scalar, vector or matrix type) are referred by their names written in capital letters. The variables are enclosed with single quotation mark. The names of the internal data files are written in boldface style. In this version all data files are formatted in order to make easier the interactive use and the trace-back in case of 'emergency'.

The full length of the HARTCODE is 4019 programme lines. In the next list we summarize the length of the individual modules. The locations of the programmes are also given by quoting the proper page numbers (in brackets).

DECODA	68	(120)	HART	1190(140)	SMTH	90	(196)
MIX	41	(122)	LAYERS	188 (167)	COMP	573	(198)
DECODG	41	(123)	MINT	85 (172)	CHNL	357	(211)
FIND	26	(124)	LENGTH	225 (174)	GSC	95	(220)
LIN	156	(125)	MESH	$29 \ (179)$			
STAT	111	(129)	CONT	$37\ (180)$			
FAR	207	(132)	FARWG	59 (181)			
WINGS	42	(137)	GAUSS	106 (183)			
			SHAPE	45 (186)			
			VOIGTY	123 (187)			
			VOIGTD	82 (190)			
			WING	43 (192)			



Fig. II-1 : The block-diagram displays the general structure of the first group of programmes performing the pre-processing of the spectroscopic data. Symbols 'o' and '•' are indicating the input and output channels respectively. The internal data files are enclosed in boxes with dashed line. Modules belonging to the same program unit are enclosed with dotted line, except in the case of 'TAPE 1' and 'TAPE 2' where the boxes are indicating the original tapes of the data banks.



Fig. II-2 : The structure of the second group of programmes. In the HART block the numbers are indicating the different phase of processing. The first section is the input module. In the second section the required atmospheric layering is established. At the beginning of the third section is the entry point of the wave-number-loop and the fourth section is the extension of the layer-loop.



Fig. II-3 : Post-processing of the results. Modules SMTH and COMP perform different kind of smoothing. CHNL computes the channel transmittance, weighting functions and radiance for selected wave numbers. The output data files may be used directly in plotting routines.

2. Pre-processing of the Spectroscopic Data

DECODA and MIX

The basic task of these units is to produce a data file by extracting the necessary information from the AFGL-82 compilation. The parameters to be extracted are : line positions, line intensities, collisional half widths, lower state energies, molecular and quantum identification codes.

The data in the AFGL-82 tape are coded and blocked with variable block size . After every 100 cm^{-1} there is an end-of-file mark. As we mentioned before, the data of the main absorber and of the trace gases are separated. The first 179 files contain the data of the main absorber and the data in the last 100 files belong to the trace gases.

The AFGL-82 tape also contains supplementary information about the transitions. This information - which was located by a zero molecular identification code - is stored in the file **remarks.dat**. The unassigned transitions are supplied with a negative lower state energy value. These transitions were rejected although they were copied into the file **remarks.dat**.

The task of the module MIX is to produce one file by mixing the data of the main and trace absorber (files **afglm.dat** and **afglt.dat**) and unify the molecular identification codes, i.e. to change the id. to that one used by the GEISA-84 tape. (The isotopic identification remains unchanged.)

Remarks:

- To read the new version of the AFGL tape the 'BLOCKSIZE' and 'RECL' qualifiers must be changed at line {17} in DECODA.
- The input parameter 'IMIX' activates the MIX routine and 'ICHANGE' is the control parameter to change the molecular identification code at lines {23,80} in DECODA.
- The input format specifications were changed after 100 cm^{-1} at lines {37, 38}.
- Line $\{58\}$ is the output format specification.

DECODG

The GEISA-84 tape contains two files written in standard IBM code. (The specifications of the tape are: 6250 BPI, 9 track, no label, odd parity, two files, blocksize 6160, number of blocks 4240, record length 80, coded). The conversion to ASCII code was performed by a VAX system-library routine at line {32}. The two files in the GEISA-82 tape are identical, except that the second file contains the temperature dependence coefficients of the collisional half widths. (At the same position the first file contains some kind of internal reference code.)

FIND

After having the copies of the original data banks in the computer the next step is to extract the information concerning the wave number interval we are interested in. This job has been done by module FIND. The input file **find.inp** contains the wave number limits and the source file identification.('ID' = 0 for the **geisa.dat** and 'ID' = 1 for the **afgl.dat** at lines {18, 19, 20}.) To select the data for a particular band some modification needed, i.e. a string of quantum identifiers must be inserted in the input file and compared with the value of 'QID' after line {32}.

Remarks:

- The output file **select.dat** does not contain any kind of information about the band and isotopic codes.
- At the selection of the wave number limits the possible wing contribution must be considered.

LIN and STAT

The statistical evaluation of spectroscopic data and the preparation of the final input files for the HART module is performed by these programmes. The input parameters in the file **lin.inp** are:

1. Record

'IFAR'	: Control parameter which activates the routine FAR. Possible values are -1, 0 and 1. If 'IFAR' = -1 only the wing contribution is calculated using a previously created lin.dat file. In this case 'NDDD' must be defined. If 'IFAR' = 0 no wing contribution is calculated.
'WNUA'	: Lower wave number limit for routine FAR.
'WNUB'	: Upper wave number limit for routine FAR.
'REG1'	: Wave number limit for routine FAR.
'REG2'	: Wave number limit for routine FAR.
'REG3'	: Wave number limit for routine FAR.
'IP'	: Print status for the system output.
	2. Record
'ISV'	: Control parameter for the wave numbers points where the wing contribution will be calculated. 'ISV' can be 2, 3, 5 or 11 and the corresponding wave number steps are 1, 0.5, 0.25 and $0.1 \ cm^{-1}$.
'ITA'	: Lower temperature limit for routine FAR.

'ITB'	: Upper temperature limit for routine FAR.
'IDT'	: Temperature step for routine FAR.
	3. Record
'NDDD'	: Number of lines contained by lin.dat
'IWI'	: This vector of seven elements contains the line wing identification codes for the different molecules. 'IWI' must be compatible with 'MOLL'. (Ie. a given element of 'IWI' should refer to the molecule type defined by the same element of 'MOLL'.)
	4. Record
'TRLIM'	: Lines having larger transmittance at the line center than 'TRLIM' are neglected.
'TRLIMS'	: Lines having larger transmittance at the line center than 'TRLIMS' are supplied with a code.
'SRATIO'	: If the (line intensity)/(maximum line intensity) ratio in a given wave number interval is less than 'SRATIO' the line is neglected.
'WNU1A'	: Lower wave number limit in modules LINE and STAT.
'WNU2B'	: Upper wave number limit in modules LINE and STAT.
	5. Record
'IOUT'	: Control parameter. Possible values are 0 and 1. Files lin.dat and farwg.dat are not created if 'IOUT'=0.
'IDI'	: This parameter defines the wave number step. Possible values are 1, 2, 3 and 4 and the corresponding wave number steps are 1, 3, 5 and 10 cm^{-1} .
'LAA'	: This parameter is an option for the STAT subroutine. In case of 'LAA'=0 at each wave number interval and for each molecule type the cumulative number of the spectrum lines is calculated.
'MOLL'	: This is a vector of seven elements containing the molecular identification codes.

For each wave number interval defined by 'IDI' the output file **stat.dat** contains the usual statistical information about the line intensity, collisional half width, ground state energy, and also the histograms of the line intensities and line spacings. As an example of the application of the STAT routine we have compared the CO_2 line intensity histograms of the AFGL-82, GEISA-84 and HITRAN-86 data banks. In the 650 - 700 cm^{-1} spectral region with 1 cm^{-1} wave number steps the differences in the line intensity histograms have been plotted in Fig. II-4 and Fig II-5. The line intensity cells are indicated by the position and widths of the curves. (The thickest curve on the left side belongs to the first intensity cell containing the strongest lines.)

The total number of the CO_2 lines contained by the 600 - 800 cm^{-1} spectral region and included in the GEISA-84, AFGL-82 and HITRAN-86 catalogs are 14797, 14433 and 14801 respectively. The summary of the line intensity histograms for the whole region is included in Table II-1. As we can see the large differences are generally concerned to the very weak lines and they have no noticeable effect on the transmittance calculations.

TABLE II-1

Summary of the CO_2 line intensity histograms of the 600- 800 cm^{-1} spectral region. The ranges of the intensity cells are indicated by the tenth power of the intensity limits measured in $(atm-cm)^{-1}cm^{-1}$.

intensity cells	$0,\!1$	-1,0	-2,-1	-3,-2	-4,-3	-5,-4	-6,-5	-7,-6	-8,-7
GEISA-84 AFGL-82 HITRAN	57 55 57	$118 \\ 115 \\ 115$	336 332 336	$\begin{array}{c} 688 \\ 660 \\ 684 \end{array}$	$1487 \\ 1453 \\ 1488$	$2541 \\ 2477 \\ 2544$	$4040 \\ 3947 \\ 4036$	$5331 \\ 5198 \\ 5342$	$199 \\ 196 \\ 199$

However, there are some very strong lines missing in either the AFGL-82 or the HITRAN-86 catalog which might have serious effect on the accuracy of the calculated high resolution transmittance or radiance spectra. We shall return to this question at the validation of the HARTCODE in chapter III.


Fig. II-4 : Differences in the CO_2 line intensity histograms in the 650 - 700 cm^{-1} spectral region. Positive numbers on the vertical axes are indicating the number of the "missing" lines in the AFGL-82 data bank and the negative ones are the lines missing in the GEISA-84 catalog. The intensity cell is indicated by the width of the curve (see the text).



Fig. II-5 : Differences in the CO_2 line intensity histograms in the 650 - 700 cm^{-1} spectral region. Positive numbers on the vertical axes are indicating the number of the "missing" lines in the HITRAN-86 data bank and the negative ones are the lines missing in the GEISA-84 catalog. The intensity cell is indicated by the width of the curve (see the text).

Remarks:

- The number of the different kind of absorber having lines within 'WNU1A' and 'WNU2B' is limited to 7. It is very rare that we have to consider more than seven molecular species within a short wave number interval.
- For atmospheric applications the line intensity limits corresponding to the transmittance limits were determined by using the US Standard Atmosphere 1976 and nadir viewing geometry. For the seven major absorber the absorber amount, effective temperature and pressure are included in Table II-2.
- Table II-2 also contains the line intensity limits for 'TRLIM'=0.999999.
- The effect of 'SRATIO' on the number of lines within 1 cm⁻¹ is presented in Fig. II-6 and in Table II-3. No lines are neglected by setting 'TRLIM'=1, 'TRLIMS'=1 and 'SRATIO'=0.
- At line {85} in module LIN the unit of the line intensity is converted from $(molec./cm^2)^{-1}cm^{-1}$ into $(atm-cm)^{-1}cm^{-1}$.

TABLE II-2

The total amounts of absorber u^i in atm -cm, effective pressures p_e^i in HPa and the effective temperatures T_e^i in K for the seven major absorber calculated for the US Standard Atmosphere 76 and nadir viewing geometry. Intensity limits S_{lim}^i in (atm-cm)⁻¹cm⁻¹ and calculated for 'TRLIM'=.99999 are also indicated.

i	molecule	u^i	p_e^i	T_e^i	S^i_{lim}	
1	H_2O	1768.0	803.0	275.0	0.1479E-7	
2	CO_2	263.80	506.0	250.0	0.6553E-7	
3	O_3	0.3467	90.30	225.0	0.9380E-5	
4	N_2O	0.2453	525.0	251.0	0.7298E-4	
5	CH_4	0.0885	599.0	258.0	0.2276E-3	
6	CO	1.3170	520.0	251.0	0.1346E-4	
7	O_2	1.671E + 5	506.0	250.0	0.1035E-9	

TABLE II-3

The dependence of the total number of the CO_2 lines in the	$600-800 \ cm^{-1}$
spectral region on 'SRATIO', ('IDI'=1).	

'SRATIO'	0.0	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	
GEISA-84 AFGL-82 HITRAN-86	$14797 \\ 14433 \\ 14801$	$14170 \\ 13850 \\ 14160$	12229 12039 12201	8886 8722 9003	$5798 \\ 5686 \\ 5847$	$3215 \\ 3154 \\ 3242$	

FAR and WINGS

These two routines are activated by the 'IFAR' parameter. When 'IFAR' is set to 1 or -1 a set of continuum type absorption coefficients are calculated between 'WNUA' and 'WNUB' for each 1 cm^{-1} wave number step. The number of wave number mesh points are controlled by 'ISV'. The absorption coefficients are calculated at each mesh point for the temperature values defined by 'ITA', 'ITB' and 'IDT'. The wave number interval from which the absorption lines are contributing is defined by 'REG2' and 'REG3'. (Only those lines are considered for which 'REG2' $\leq \Delta \nu_k <$ 'REG3'.) The line shape function can be specified for the different types of molecules by the vector 'IWI'. If the line shape identifier is 0, 1, 2, 3, 4, 5, 6 or 7 the line shape function is given by Eqs. (25), (30), (31), (32), (26), (28), (29), or (27) respectively. (In the program we use the asymptotic form of the above equations for conditions where $\Delta \nu_k >> \alpha_k^i$.)



Fig. II-6 : The CO_2 absorption line number distribution in the 600-800 cm^{-1} wave number interval (solid line). The dotted and dashed lines indicate the number of absorption lines to be neglected in case of 'SRATIO'=10⁻⁶ and 'SRATIO'=10⁻⁴ respectively.

3. Module HART

This programme - together with its 9 subroutines and 2 function segments - is the kernel of the HARTCODE. There are 16 records in the **hart.inp** file containing the input parameters. Some examples of typical input sequences are given at the end of the list of the HART programme in Appendix D.

As we have mentioned before this version of the HARTCODE were used for numerical testing accordingly the input structure is a little bit complicated but allows us a higher degree of freedom in selecting the proper combination of the input parameters to obtain the required accuracy. (For example the order of the Gaussian quadrature for the calculation of the wave number integral at Eq. (37) is not fixed and even the generation of the wave number mesh points is an option.)

In the next section we summarize the function of each control parameter. When it is necessary the possible values (or functions) are also indicated within the \langle and \rangle signs.

1. Record

: Wave number resolution, $\delta \nu$ in Eq. (37). 'RESL'< 0.1, 0.05, 0.01, 0.005 >
: Wave number step. 'DELV' $>$ 'RESL' and 'DELV'/'RESL' $<$ 200.
: 'ITRN'< 1, $2 > \rightarrow < optical \ depth$, transmittance >.
: 'IRAD'< 0, $1 > \rightarrow < no \ radiance$, radiance >.
: The file trao.dat is created only if 'IOTR'=1 .
: The file $\mathbf{rad.dat}$ is created only if 'IORD'=1.
: The file prnew.dat is not created if 'IOPR'= 0 . This file contains the data of the input profiles after layering.
2. Record
: Print status for the system output.
3. Record
: Control parameter to establish the wave number mesh. 'ISBN'< $1, 2 > \rightarrow < subdivisions$, no subdivisions > If 'ISBN'=2 the gaussian quadrature is applied over $\delta \nu$.
: Order of gaussian quadrature, 'IGNU'< 1, 2, \cdots 10 >.
If 'IGNU'=0 the calculation of Eq. (39) are repeated with increasing order of gaussian quadrature until the results of the subsequent iterations satisfy an accuracy limit.

'EPSN'	: Accuracy limit for the calculation of Eq. (39) .
'ICCH'	: Control parameter to change the default values of the pressure and $ \Delta \nu $ limits for the line shape calculations.
'PDLR'	: Pressure limit for the Doppler line shape in HPa .
'PLNZ'	: Pressure limit for the Lorentz line shape in HPa .
'VDLR'	: Wave number limit for the Doppler line shape in cm^{-1} .
'VLNZ'	: Wave number limit for the Lorentz line shape in cm^{-1} .
	4. Record
'IINT'	: Control parameter to establish a limit for $ \Delta \nu_k $ as the function of the pressure.
'AINT'	: Scale factor. At a given pressure and $ \Delta \nu_k $ only those lines are considered which satisfy the next condition:
	$ \Delta \nu_k \leq \text{REG1} \cdot \text{VPR}^{\text{AINT}} + \text{REG2}(1 - \text{VPR}^{\text{AINT}}),$
	where VPR is the Voigt parameter, 'REG1' and 'REG2' are wave number limits. If 'IINT'=0 the above condition is ignored.
'IVPF'	: If 'IVPF' =1 the vibrational partition functions are computed.
'IRPF'	: If 'IRPF' $=1$ the rotational partition functions are computed.
'KSHP'	: If 'KSHP'=0 the line shape function is controlled (uniformly for each molecular type) by 'PDLR', 'PLNZ', 'VDLR' and 'VLNZ'. If 'KSHP'=1 the line shape function is controlled by 'LMOD'.
'IVDY'	: Determines the method of the calculation of the Voigt function. 'IVDY'< 0,1 > \rightarrow < $Drayson's\ method,\ Young's\ method >$
	5. Record
'MODL'	: Number of molecule types for which different line shape functions will be used.
'IDEN' 'LMOD'	: Molecular ID. code. : Line shape code.
	6. Record
'MODA'	: Number of molecule types for which the collisional half width will be modified.
'IDEN' 'AMOD'	: Molecular ID. code. : Modifying factor.
	7. Record
'MODS'	: Parameter to change the line intensities, $S_{k,i}^{i}(T_{o})$.
'IDEN'	: Molecular ID. code.
'SMOD'	: Vector of seven element containing the modifying factors.

8. Record

'MODR'	: Number of molecule types for which the line wing cut-off parameter will be modified.
'IDEN'	: Molecular ID. code.
'RMOD'	: Modifying factor.
	9. Record
'WNU1'	: Lower wave number limit, cm^{-1} .
'WNU2'	: Upper wave number limit, cm^{-1} .
'REG0'	: Wave number limit for the weak lines. If $ \Delta \nu_k $ for a given weak line is greater than 'REG0' the contribution of the line is neglected.
'REG1'	: If $ \triangle \nu_k $ <'REG1' the line is considered without any condition.
'REG2'	: If 'REG1'< $ \Delta \nu_k $ <'REG2' the consideration of the line will depend on the actual pressure (ie. on the Voigt parameter). If $ \Delta \nu_k $ >'REG2' the contribution is treated as far wing absorption.
	10. Record
'IPSC'	: Control parameter to identify the type of the calculation.
	If 'IPSC'=0 HART evaluates laboratory measurements.
	If $PSC = 4$ HART performs the calculations for model atmospheres.
'IHOM'	: Option for homogeneous atmosphere (with effective pressure,
	temperature and total optical mass).
'IARM'	: Molecular ID. for air mass calculations.
'ASCL'	: Controls the layering with respect the altitude. If 'ASCL' < 0 exponential layering, if 'ASCL' > 0 polynomial layering.
	11. Record
'IPOF'	: Atmospheric model identifier. In a separate data file
	(modatm.dat) the Lowtran Model Atmospheres are available.
	'IPOF' = 0 User defined profil. 'IPOF' = 1, 2, 3, 4, 5 or 6 Standard Lowtran 6 Profiles:
	1 : Tropical
	2 : Midlatitude Summer
	3 : Midlatitude Winter
	4 : Subarctic Summer 5 : Subarctic Winter
	6 : USST 76
'LVEL'	: Number of levels of the input profile (ie. the number of the input records in the files profil.dat or modatm.dat).

'NBND' 'MOLE'	Number of molecular species involved in the calculations.Vector of seven element containing the molecular ID codes.
	12. Record
'LVL1'	: Serial number of the first level where the calculation starts.
'LVL2'	: Serial number of the last level.
'TSKN'	: Temperature at the boundary in K . If 'TSKN' > 0 the skin temperature equal to 'TSKN'. If 'TSKN' = 0 the radiative contribution of the ground (or the boundary layer) is ignored.
'EMIS'	: Emissivity of the boundary layer.
	13. Record
'IDIR'	: Direction of the beam. 'IDIR' < 1, 0, $-1 > \rightarrow < upward$, horizontal, downward > In case of horizontal direction only short path is considered.
'TETA'	: Zenith angle.(In case of air mass calculations the initial zenith angle.)
'TETB'	: Last zenith angle.
'DTET'	: Zenith angle step. If 'DTET' not equal to zero the program stops at the air mass calculations.
	14. Record
'LVEN'	: Number of the layers between 'ALT1' and 'ALT2'.
'ALT1'	: Upper altitude of the trajectory.
'ALT2'	: Lower altitude of the trajectory.
'PATH'	: Length of the trajectory in km ('IDIR'=0).
	15. Record
'MODU'	: Number of the mixing ratio profiles to be modified.
'IDEN'	: Molecular ID.
'UMOD'	: Modifying factor.
	16. Record
'ILIN'	: Selects the source of the spectral input data. If 'ILIN'=1 the spectral parameters are internally generated. If 'ILIN'=2 the spectral input data are in the lin.dat file.
'ILIM'	: Maximum number of the spectrum lines in the lin.dat file.
'ICON'	: If 'ICON'=1 the H_2O continuum absorption is computed.
'IFAR'	: If 'IFAR'=1 the far wing absorption is computed.
'JREF'	: If 'JREF'=1 the refraction is computed.

When HART is evaluating laboratory measurements ('IPSC'=0) the input structure is different from the 10th record. In this case the 10th record contains an integer qualifier which specifies the number of data sets (or the number of the records to be read). The 11th and the subsequent records contains the pressure (HPa), temperature (K), molecular ID. and optical mass (atm-cm) as they are specified in the experiment. The last record will be equivalent with 16th record, ('ILIN' must be equal to 2).

When HART is performing test calculations for selected pressure and temperature ranges ('IPSC'=1, 2 or 3) the 11th record specifies the minimum, maximum and the step of the pressure and temperature. In this case the pressure scale is defined by 'IPSC':

'IPPS'<1, 2, $3 > \rightarrow < linear, log, log-lin >.$

The 12th record contains the number of different kind of absorber, the molecular IDs and the optical masses. The 13th record will be equal to the 16th record.

If one wants to use simulated spectral data 'ILIN' should be set to 1. In this case after the last record the band parameters should be specified by the total number of the lines, central wave number of the band, width of the band, relative position, average line intensity, and ground state energy for each band in separate records.

LAYERS and MINT

These two routines perform the calculation of the relative optical air masses for each layer. The result of the operation is the value of μ_m^* contained by the 'BMU' vector. (See lines {84} and {172} in module LAYERS.) Depending on the viewing geometry these modules are also calculating the next quantities: tangent height, local zenith angles at each level, total geometrical path length of the trajectory and the angular deflection of the beam. MINIT is an auxiliary routine determining the profile-variables by polynomial interpolation or using exponential scale factors.

LENGTH and MESH

If 'ISBN'= 1 LENGTH and MESH set up a system of wave number mesh points within $\delta\nu$. The wave number mesh points are generated at increasing distances from the line centers. The position of the mesh points are depending on the wave number and actually determined by a simple linear transformation using the average doppler half-width. It might happen that the minimum pressure in the input data is still in the Lorentzian range then it worth to apply another transformation to the subpoints with respect the average voigt parameter . For example subpoints 0.001, 0.0015, 0.0025, 0.005, 0.01, 0.025, 0.05, 0.1, 0.25, 0.5, 1.0, 2.5 and 5.0 cm⁻¹ are valid for the CO_2 at 250 K and 700 cm⁻¹ when α_D is about 0.0006 cm^{-1} . For a given wave number the generated subpoints are stored in the 'AGA' vector.

CONT and FARWG

The actual contribution of the H_2O continuum and the far wing absorption to the monochromatic absorption coefficient is calculated by the above routines using the data files **cont.dat** and **farwg.dat**. The continuum absorption coefficient of a layer is evaluated by Eqs. (19) and (20) at each 1 cm^{-1} wave number interval applying parabolic interpolation over the data given in Table I.2, see lines {34} and {44} in module CONT. To obtain the far wing contribution to the total optical depth also interpolation is applied over both the wave number and temperature intervals in subroutine FARWG . Having 11 wave number mesh point in 1 cm^{-1} and ten temperature values between 140 and 320 K with 20 K steps a simple linear interpolation is sufficient. According to test runs line files created with 'SRATIO'= 10^{-2} or 'SRATIO'= 10^{-3} give satisfactory results. The far wing contribution to the total monochromatic optical depth is recalculated at each new $\delta\nu$ wave number interval and is taken into account in the routine GAUSS at line {52}. If the 'ICON' and 'IFAR' qualifiers are not equal to 1 no continuum and far wing contribution is calculated.

GAUSS

This unit performs the wave number integration over the subinterval given by the 'AGA' vector. The order of the gaussian quadrature is defined by 'IGNU'. The vector 'OUTSS' contains the monochromatic optical depth or transmittance belonging to a given gauss abscissa. The dimension of this vector should be equal to the dimension of 'AGA' times 'IGNU' accordingly this is the largest block in the program having 14000 elements.

SHAPE, VOIGT and WING

In the SHAPE module the Lorentz, Doppler and Voigt line shapes are calculated. In case of 'IVDY'=0 the Voigt function is computed by Drayson's subroutine in the VOIGTD module. If 'IDVY'=1 the more accurate (but considerably slower) method of Young is used in module VOIGTY. If in the vector 'LMOD' different line shape is specified the routine WING is activated. When 'IFAR'=1 the vector 'IVI' should be compatible with 'LMOD' (ie. once for a particular molecule the line shape is selected then the far wing contribution should be calculated using the same line shape). The program WING and WINGS are similar, they contain the same line shape functions, Eqs. (25), - (32), except that in the WING routine we do not apply any approximations concerning to the dependence on the distances from the line centers.

4. Post-processing of the Results

These last three programmes are not strictly belonging to the HARTCODE although all the results presented in the next chapter were obtained by applying them. For a particular post-processing of the data contained by the basic result files (**trao.dat** and **rad.dat**) the users can shape their own programmes according to their own needs.

SMTH

If we are interested in a wider spectral range the SMTH routine may be used. This is applying a rectangular or triangular response function for smoothing the data contained by either the **trao.dat** or the **rad.dat** file. The output file **smth.dat** contains the wave number dependence of the smoothed optical depth (absorption coefficient), transmittance or radiance and is ready to use for making graphs.

CHNL and GSC

This program evaluates the channel transmittance and radiance or calculates the weighting functions, (Eqs. (6) and (12)) using the **trao.dat** input file which contains the average transmittance given by Eq. (37). (The **profil.dat** file must be the same than the one was used in the HART program.) Module GSC has similar function than GAUSS has in the HART programme. The output files **twchn.dat** and **rchn.dat** are prepared for immediate use in the plotting routines. They contain the pressure dependence of the channel transmittance and weighting functions or the radiative contributions of the layers.

COMP

This program is designed to make easy comparisons between the calculated and measured radiance. File **hcom.dat** contains the measured data pairs (ie. wave number and radiance in free format). The output file **scom.dat** contains the usual statistical information (average, standard deviation ect.) and **comp.dat** is a file for a plotting program.

III. VALIDATION OF THE HARTCODE

1. Homogeneous Transmittance Calculations

When the functional testing of the individual modules were completed and the HARTCODE as a system of several programme units were running we have conducted extended accuracy and sensitivity tests. Unfortunately, it is impossible to reproduce the detailed results of the early testing procedures within this report. The original aim that the numerical accuracy should be sufficient to evaluate the most recent spectral radiance measurements was achieved. In this chapter joining to the ITRA first experiment we compare the calculated and measured homogeneous CO_2 transmittance spectra. The experimental conditions of the selected spectra are summarized in Table III-1. In case of Gryvnak's measurements only the numerical values of the dependence of the equivalent width on the wave number was available while in Bulanin's case we could compare the direct transmittance spectra.

TABLE III-1

Two set of selected CO_2 transmittance spectra for homogeneous calculations, after $Chedin^{[3]}$. ID is the identification number of the data set, T is the temperature in K, l is the path length in cm, r_v is the volume mixing ratio, p is the pressure in atm and u is the absorber amount in $molec./cm^2$.

Gryvnak's measurements							
ID	T	l	r_v	p	u		
1	310	3291	0.0385	0.123684	3.712E + 20		
2	274	1648	0.005	0.25	5.521E + 19		
3	274	826	0.00125	0.5	1.384E + 19		
4	244	3291	0.153	0.059737	$9.053E{+}20$		
5	245	1648	0.00125	0.25	1.544E + 19		
		Bulanin	's measurem	ents			
ID	T	l	r_v	p	u		
6	213	497	0.01	0.198	3.393E + 19		
7	253	1470	0.01	0.502	2.142E + 20		
8	293	4874	0.01	1.003	1.225E + 21		
9	213	4874	0.01	1.003	1.685E + 21		
10	293	4874	0.01	0.01	$1.222E{+}19$		

To obtain the synthetic spectra the HARTCODE transmittance were calculated with 0.05 cm^{-1} resolution (using the Voigt line shape and four point gaussian quadrature for the wave number integration) and smoothed according to the proper instrumental response functions. For the first set of measurements we used a simple triangular response function with a half width ($\Delta \nu_i$) given by the next equation:

$$\Delta \nu_i = 1.2 + (\nu_i - 500)0.008,$$

where ν_i is the wave number in cm^{-1} . The equivalent width as a function of the wave number is :

$$A(\nu_n) = \sum_{i=1}^n \xi_{\overline{\nu_i}} \delta\nu_i$$

where $\delta \nu$ is the resolution and ξ is the spectral absorptance from Eq. (38).

For the second set we applied a Gaussian-type response function with variable half width:

$$\Phi_{\nu_i}(\nu) = \frac{1.439}{\Delta\nu_i} exp \left[-\left(\frac{0.832(\nu-\nu_i)}{\Delta\nu_i}\right)^2 \right],$$

where $\Delta \nu_i = 0.00537 \nu_i - 1.64$ if $\nu_i < 637 \ cm^{-1}$ and $\Delta \nu_i = 0.00402 \nu_i - 1.345$ if $\nu_i > 637 \ cm^{-1}$. In this case the averaging interval was $6\Delta \nu_i$.

The numerical accuracy of the computed transmittance were better than six significant figures and we did not apply any kind of preselection to the original spectroscopic data. Using the GEISA-84 database the calculations were repeated for several line wing cut-off conditions.

In Fig. III-1 the computed synthetic spectra are presented for the first data set. The line wing cut-off parameter was set to $3.5 \ cm^{-1}$ (solid lines), and $25 \ cm^{-1}$ (dashed lines). Only very slight changes in the transmittance were observed in the vicinity of the centre of the Q branch. When the pressure is low (curves 1 and 4) the effect is smaller. Applying exponential line wings - Eqs. (30), (31), and (32) - the effect disappears.

In Fig. III-2 for the same data set the equivalent widths are compared. The solid lines are the measurements. The dashed and dotted lines were obtained with 3.5 cm^{-1} and 25 cm^{-1} wing cut-off parameter subsequently. In case of weak absorption - curves 2, 3 and 5 - the agreement with the measurements is good and similar results were obtained by the ITRA participants^[35]. In case of stronger absorption - curve 1 and 4 - because of the magnitude and opposite tendency the deviations can not be explained by different line shapes or line wing cut-off parameters. Most probably the real reason is the improper temperature dependence of the line intensity and line half width.

In Fig. III-3 the transmittance spectra are compared with the second set of measurements. The solid lines and the dashed lines are the synthetic spectra using 3.5 and 25 cm^{-1} wing cut-off parameters subsequently and the symbols are the measured values. These results again suggest the same conclusion i.e. no manipulation with the line shape and line wing can compensate the discrepancies at 600-620 and 720-740 cm^{-1} .

In Fig. III-4 the synthetic spectra obtained by using the GEISA-84 (solid line) and HITRAN-86 (dashed line) database and the second set of measurements are compared. The symbols indicate the measured values. The significant differences in the two database - especially in the two problematic spectral interval - are obvious. In general using the HITRAN-86 database at longer wave length the absorption is always larger while on the other side of the band around 720 cm^{-1} the absorption is always less. Under certain experimental (curve 8) condition this difference improves the agreement with the experimental data while at low temperature measurement (curve 9) the discrepancies around 720 cm^{-1} are increased.

In Fig. III-5 a high resolution transmittance spectra calculated for the second set of measurements are presented. In this case the resolution is $0.5 \ cm^{-1}$ with triangular slit function. To identify the reasons of the above mentioned deviations and to apply proper corrections to the spectroscopic data bases further comparisons are needed with experimental data obtained at least with this spectral resolution.

In Fig. III-6 the effect of the pre-selection of the spectroscopic data are presented. Using the GEISA-84 catalog and 'SRATIO'= 10^{-5} the differences in the transmittance spectra are compared for measurements 8 and 9. The results clearly indicate that - although there is a considerable gain in computing time - when working with high resolution laboratory measurements no this kind of pre-selection is allowed.

Concerning the homogeneous calculations our opinion is that the ITRA exercises should continue with continuous improvement of the data banks until satisfactory agreement with the experimental spectra is achieved.



Fig. III-1 : Synthetic transmittance spectra for Gryvnak's measurements. The numbers are the identifiers for the experiment, see Table III-1. Solid lines: $3.5 \ cm^{-1}$ wing cut-off, dashed lines $25 \ cm^{-1}$ wing cut-off.



Fig. III-2 : Equivalent widths vs. wave number for Gryvnak's measurements. The numbers are the identifiers for the experiment, see Table III-1. Solid lines: measurements, dashed lines : $3.5 \ cm^{-1}$ wing cut-off, dotted lines : $25 \ cm^{-1}$ wing cut-off.



Fig. III-3 : Synthetic transmittance spectra for Bulanin's measurements. The numbers are the identifiers for the experiment, see Table III-1. Symbols : measured values, solid lines : $3.5 \ cm^{-1}$ wing cut-off, dashed lines : $25 \ cm^{-1}$ wing cut-off.



Fig. III-4 : Synthetic transmittance spectra for Bulanin's measurements. The numbers are the identifiers for the experiment, see Table III-1. The line wing cut-off parameter is $25 \ cm^{-1}$. Symbols : measured values, solid lines : GEISA-84 database, dashed lines : HITRAN-86 database.



Fig. III-5 : Synthetic high resolution transmittance spectra for Bulanin's measurements. The numbers are the identifiers for the experiment, see Table III-1. The line wing cut-off parameter is $25 \ cm^{-1}$. Triangular slit function with 0.5 cm^{-1} half width.



Fig. III-6 : Effect of neglecting the weak absorption lines on the transmittance. Solid lines : differences in the high resolution synthetic spectra when 'SRATIO'=0 and 'SRATIO'= 10^{-5} . The numbers are the identifiers for the experiment, see Table III-1. The line wing cut-off parameter is $25 \ cm^{-1}$. Triangular slit function with 0.5 cm^{-1} half width.

2. Calculations for Model Atmospheres

In this chapter, joining to the second ITRA exercise, the channel transmittance, weighting functions and radiance calculated for the USST 76 Atmosphere and for the seven HIRS/2 channels are compared. Unfortunately in the ITRA report the documentation of the codes of the ITRA participants were not complete and it was difficult to trace back the real reasons of some differences in the results. Moreover, there were no conclusions about the numerical accuracies of the codes. Therefore, instead of comparing the HARTCODE results with the results of the individual codes we made comparisons with the average ITRA results.

TABLEIII-2

Average CO2 transmittance calculated for the seven HIRS/2 channels by the ITRA participants, $Sp\ddot{a}nkuch^{[4]}$. (USST-76 atmosphere and nadir viewing.) P is the pressure in HPa and ν_i is the central wave number of the i-th channel in cm^{-1} .

	ν_1	ν_2	ν_3	$ u_4$	ν_5	ν_6	ν_7
P	668	679	691	704	716	732	748
0.1	.9700	.9963	.9974	.9985	.9986	.9996	.9999
0.3	.9401	.9923	.9945	.9967	.9967	.9983	.9992
0.5	.9156	.9888	.9919	.9955	.9956	.9976	.9987
0.7	.8921	.9856	.9892	.9940	.9945	.9968	.9985
1.0	.8613	.9810	.9860	.9926	.9930	.9964	.9982
3.0	.6933	.9522	.9656	.9832	.9859	.9925	.9961
5.0	.5949	.9253	.9477	.9758	.9804	.9895	.9948
7.0	.5314	.8984	.9307	.9687	.9747	.9863	.9933
10.0	.4582	.8567	.9048	.9567	.9663	.9815	.9915
20.0	.3098	.7337	.8266	.9279	.9429	.9686	.9863
30.0	.2169	.6253	.7546	.8929	.9218	.9570	.9813
50.0	.1128	.4477	.6267	.8338	.8853	.9361	.9720
70.0	.0550	.3147	.5171	.7791	.8530	.9170	.9632
100.0	.0192	.1762	.3818	.7014	.8083	.8893	.9498
150.0	.0028	.0564	.2246	.5855	.7387	.8452	.9270
200.0	.0002	.0138	.1303	.4862	.6739	.8020	.9062
250.0	.0000	.0022	.0760	.4038	.6150	.7610	.8820
300.0	.0000	.0003	.0429	.3283	.5532	.7165	.8562
400.0	.0000	.0000	.0122	.2041	.4295	.6198	.7941
500.0	.0000	.0000	.0029	.1204	.3216	.5221	.7256
700.0	.0000	.0000	.0001	.0386	.1675	.3436	.5841
850.0	.0000	.0000	.0000	.0161	.0990	.2361	.4856
1000.0	.0000	.0000	.0000	.0068	.0568	.1535	.3966

The average ITRA transmittance data set which was also used for the calculation of the weighting functions is reproduced in Table III-2, after *Spänkuch*^[4]. The averages were calculated from the results of the following three groups: Meteorological Research Institute, Japan; Infrared Physics Branch, Optical Physics Division AFGL, USA; Laboratoire de Meteorologie Dynamique du CNRS, France.

To identify the reasons of the large differences between the results of the individual codes several HARTCODE simulations were performed with the most different line shape and line wing cut-off conditions. It turned out that not even significant changes in the parameters above can produce an effect of the magnitude of the differences observed.

In Fig. III-7 and III-8 the ITRA-averages (dashed lines) and HARTCODE (solid lines) transmittance and weighting functions computed for the selected HIRS/2 channels are compared subsequently. For this comparisons we used the GEISA-84 data (no pre-selection was applied), Voigt line shape, $6.5 \ cm^{-1}$ wing cut-off, 0.01 $\ cm^{-1}$ spectral resolution, USST 76 Standard Atmosphere with the original layering and nadir viewing . As it can be seen the general agreement is good. The differences between the HARTCODE results and the ITRA-averages are less than the differences between the results of the individual ITRA codes . The channel radiance are compared in Table III-3.

TABLE III-3

Comparisons of channel radiance computed for the USST 76 Standard Atmosphere by the ITRA participants and by the HARTCODE. The radiance are in $mW/(m^2sr\ cm^{-1})$. ν_i is the central wave of the HIRS/2 channels, \overline{ITRA} is the average radiance obtained by the ITRA participants, ΔR_I and ΔR_H are the maximum differences between the ITRA results and the differences between the ITRA average and the HARTCODE results subsequently, R, R_1 and R_2 are the HARTCODE radiance obtained by using an accurate numerical integration, Eq. (46) and Eq. (49) subsequently.

$ u_i$	\overline{ITRA}	$\triangle R_I$	$ riangle R_H$	R	R_1	R_2
668	62.502	2.10	0.03	62.528	62.642	62.452
679	47.342	1.17	0.19	47.149	47.211	47.202
691	45.575	0.72	0.36	45.217	45.226	45.253
704	52.985	0.61	0.28	52.702	52.600	52.692
716	65.388	1.08	0.51	64.877	64.741	64.823
732	77.527	0.78	0.41	77.118	76.995	77.045
748	93.032	0.95	0.29	93.331	93.245	93.267



Fig. III-7 : Comparisons of the ITRA and HARTCODE transmittance calculated for the USST 76 Standard Atmosphere. ν is the central wave number of the selected HIRS/2 channels (see Table III-3), solid lines are the HARTCODE transmittance and the dashed lines are the ITRA averages.



Fig. III-8 : Comparisons of the ITRA and HARTCODE weighting functions calculated for the USST 76 Standard Atmosphere. ν is the central wave number of the selected HIRS/2 channels (see Table III-3), solid lines are the HARTCODE transmittance and the dashed lines are the ITRA averages.

The main conclusion of the comparisons above is that the differences between the HARTCODE results are well within the range of the differences between the results of the different ITRA codes and also that the magnitude of the differences are still too large compared with the accuracy requirements of the evaluation of recent high resolution radiance measurements.

In Fig. III-9 the weighting functions are compared when the weak absorption lines being in the vicinity of the strong lines are neglected. (Solid lines are indicating the results obtained with considering also the weak lines and the dashed ones were obtained with 'SRATO' = 10^{-3} .) It is interesting to note that no significant changes in the weighting functions occurred although the number of the absorption lines were reduced from 14797 to 3215 (see Table II-3). These slight changes in the weighting functions result only about 0.2 $mW/(m^2sr \ cm^{-1})$ changes in the channel radiance therefore they can not explain the differences being larger by one magnitude.

In Fig. III-10 and III-11 the weighting functions obtained by using the different spectroscopic data are compared. In this case the **lin.dat** files were created with 'TRLIM' = 'TRLIMS' = 1 and 'SRATIO' = 10^{-3} . Fig. III-10 shows the comparisons between the GEISA-84 (solid lines) and AFGL-82 (dashed lines) data while in Fig. III-11 the GEISA-84 (solid lines) and HITRAN-86 (dashed lines) weighting functions are compared. The corresponding channel radiance are included in Table III-4. (The differences between R in Table III-3 and R_G in Table III-4 are due to the indicated pre-selection of the absorption lines.)

TABLE III-4

Comparisons of channel radiance computed for the USST 76 Standard Atmosphere by the ITRA participants and by the HARTCODE. The radiance are in $mW/(m^2sr\ cm^{-1})$. ν_i is the central wave of the HIRS/2 channels, R_G , R_A and R_H are the radiance computed using the GEISA-84, AFGL-82 and HITRAN-86 databases subsequently, $\Delta R_{GA} = R_G - R_A$ and $\Delta R_{GH} = R_G - R_H$

$ u_i$	R_G	R_A	R_H	$\triangle R_{GA}$	$\triangle R_{GH}$
668	62.353	62.120	62.570	0.23	-0.21
679	46.995	46.609	47.141	0.39	-0.15
691	45.109	45.061	45.170	0.05	-0.06
704	52.730	52.877	53.457	-0.15	-0.72
716	64.838	65.000	66.335	-0.16	-1.49
732	77.013	77.114	79.365	-0.10	-2.35
748	93.134	93.192	95.250	-0.06	-2.12

The results presented above show that the magnitude of the deviations between the basic spectroscopic data do not allows us to derive unique explanations for the observed deviations by the ITRA participants and especially not for the effect of the changes in some particular code- parameter. On the other hand using exactly the same spectroscopic input data and correct numerical procedures one has to obtain the same result (within certain accuracy limit). The main sense of comparing calculations for model atmospheres is to find the required accuracy limits and to identify the significant parameters and the most effective computational methods for a particular application. The second ITRA exercise proved again the existing fundamental differences of the spectroscopic data. Once a code reached the stage of development of precisely predictable accuracy further comparisons with real atmospheric and high accuracy laboratory measurements will decide about the quality of the data and most probably not about the accuracy of a given code.



Fig. III-9 : Effect of the weak absorption lines on the weighting functions. Solid lines were obtained with 'SRATIO'= 0 and the dashed ones with 'SRATIO'= 10^{-3} .



Fig. III-10 : HIRS/2 weighting functions computed by using the GEISA-84 catalog (solid lines) and the AFGL-82 data (dashed lines).



Fig. III-11 : HIRS/2 weighting functions computed by using the GEISA-84 catalog (solid lines) and the HITRAN-86 data (dashed lines).



Fig. III-12 : HARTCODE radiance and brightness temperatures in the 615 - 625 cm^{-1} wave number interval (solid lines).

3. Simulation of the Atmospheric Radiance Spectra and Comparisons with the HIS Measurements

To improve the accuracy of the IR remote sensing in the future the operative satellites are going to be supplied with the new generation of IR spectrometers which spectral resolution is about ten or twenty times higher than the one of the HIRS/2 sounder. The High-resolution Interferometer Sounder (HIS) Aircraft Instrument is one of these new devices. For experimental testing the HIS instrument was mounted on the NASA high altitude aircraft and several measurements were performed with different viewing geometry. HIS has $0.5 \ cm^{-1}$ and $1.0 \ cm^{-1}$ spectral resolution in the 600-1000 $\ cm^{-1}$ and 1100-2600 $\ cm^{-1}$ wave number intervals respectively with an absolute radiometric accuracy of 1 K and an RMS reproducibility of 0.1 K, Clough et al^[38], Revercomb et al^[37].

In this section and in the Appendix B we compare the measured radiance spectra with the calculated ones by the HARTCODE and FASCODE high resolution radiance computer codes.

We are very thankful to W. L. Smith who made available two measured spectra and the FASCODE simulations together with the data of the simultaneous radiosonde measurements, $Smith^{[2]}$. In both cases the measured spectra were obtained during the flights over California Coast and Tucson/Kitt Peak area at 56 HPa flight level. The simultaneous radiosonde data are presented in Table III-5. The sounding data were supplemented with the other six major absorber's concentration profiles taken from the USST 76 Standard Atmosphere. At this simulation the effect of the trace gases were ignored. For atmospheric layering the pressure levels of the original sounding data were adopted without changing.

For the HARTCODE runs at the beginning the AFGL-82 tape was used but after discovering some deficiencies of that line catalog (see *Miskolczi et al*^[36]) we changed for the GEISA-84 data. The input **lin.dat** file were created with 'TRLIM'=.9999, 'TRLIMS'=.99 and 'SRATIO' = 10^{-5} . The line wing cut-off parameter was set to 6.5 cm^{-1} . Only the Voigt line shape function was used and no far wing absorption was taken into account. The wave number integration was performed by applying 2nd order Gaussian quadrature and the spectral resolution was set to 0.005 cm^{-1} . The details of the other input parameters can be found at the end of the HART programme in Appendix D.

A part of the high resolution HARTCODE radiance spectra (solid line) is presented in Fig. III-12. In the upper plot (A) different kind of triangular smoothing functions were applied to the original data. (Dotted line : smoothed with the HIRS response function, dashed line : smoothed with the HIS response function.)

In the lower graph (B) the brightness temperature is plotted in the same spectral interval. Together with the HARTCODE results (solid line) the HIS measurements (full circles) the FASCODE results (empty circles) and the upper and lower boundary temperatures (dashed lines) are also presented. (The HIS and FASCODE results were given at discrete wave numbers therefor at the final comparisons the HARTCODE radiance were computed exactly at the same wave numbers). According to this graph in the 615 - 625 cm^{-1} region there is a good general agreement between the measurement and the theoretical spectra.

Figures showing the detailed results of the comparisons for the whole 500 - 1800 cm^{-1} interval are included in Appendix B. They are similar to Fig. III-12 (B) except that the differences between the measured and theoretical spectra are also plotted in a smaller temperature range inside a "window". After the Figures the numerical values of the statistics of the comparisons are also given for every 10 cm^{-1} in Tables B-1B-12. Within this report we do not want to give a full account on the analysis of the comparison - at some spectral interval the analysis is still in progress - but let us mention some interesting features.

Like in the case of the homogeneous calculations in the two hot CO_2 bands (around 618 and 720 cm^{-1}) there are sharp increase in the differences between the measured and synthetic radiance spectra which can not be accounted for by any line shape and line wing consideration. (In both cases the FASCODE produced the same results.)

At 668 cm^{-1} wave length because of the large CO_2 optical thickness the measurements should reproduce the upper boundary temperature accordingly the observed larger error might be caused by noise of the HIS interferometer.

Despite the smaller line wing cut-off parameter in the window region the HARTCOD gives better agreement with the measurements than the FASCODE. (Moreover in the HARTCODE only the seven major absorber was considered.) The magnitude of the deviations is generally within the accuracy limit of the instrument except the vicinity of the strong H_2O absorption lines.

In Fig. B-5 the results in the 1042 cm^{-1} ozone band are presented. Excellent agreement was achieved by setting the total ozone amount properly to minimize the differences between the observed and theoretical curve. Still the errors are larger than 1 - 2 K indicating that the measurements might contain information about the vertical structure of the ozone distribution being under the flight level.

In Fig. B-7 around 1270 - 1320 cm^{-1} the larger errors are due to the N_2O and CH_4 absorption. In this case we did not try to fit the absorber amount to obtain a better agreement.

In Fig. B-9 and B-10 (from 1400 to 1600 cm^{-1}) there is a constant difference between the measured and calculated spectra which might be explained by the errors in the H_2O continuum absorption coefficients.

Beside the good overall agreement in the future using more measured spectra for the corrections of the spectroscopic data better results could be obtained. Concerning the HARTCODE after implementing the routines for the computation of the nitrogen and oxygen continuum and the trace gas absorption we shall continue the validation and complete the HIS evaluation in the Band-III (2070-2750 cm^{-1}).

TABLE III-5

Ra in K, P i	diosonde ol s the press	Distributions used for the transmission of transmission of the transmission of transm	for the HIS evaluat s the water vapor	tion. T is the mixing ratio	The temperature of in g/kg .			
	case 1			case 2				
California	a Coast, 14-	-04-86	Tucson/H	Kitt Peak, 1	5-04-86			
Surface e	levation :	65 m	Surface e	levation :	789 m			
Skin tem	perature : 2	287.5 K	Skin tem	perature : 3	$309.0 \ K$			
Р	T	M	Р	Т	M			
56.00	212.70	0.0010	56.00	209.00	0.0010			
60.00	212.60	0.0010	60.00	207.80	0.0010			
70.00	212.40	0.0010	70.00	209.00	0.0010			
85.00	212.80	0.0010	85.00	209.90	0.0010			
100.00	211.30	0.0010	100.00	208.70	0.0010			
115.00	211.10	0.0020	115.00	208.80	0.0010			
135.00	213.30	0.0030	135.00	209.00	0.0010			
150.00	213.70	0.0030	150.00	206.20	0.0010			
200.00	211.50	0.0020	200.00	211.20	0.0010			
250.00	220.20	0.0030	250.00	222.40	0.0010			
300.00	229.70	0.0080	300.00	232.80	0.0030			
350.00	237.90	0.0990	350.00	240.90	0.0630			
400.00	244.70	0.1980	400.00	247.90	0.0960			
430.00	248.40	0.5360	430.00	250.60	0.3070			
475.00	253.60	1.0510	475.00	255.10	0.8810			
500.00	256.10	0.7450	500.00	257.90	1.2740			
570.00	263.00	1.4660	570.00	265.90	2.1880			
620.00	267.00	1.5220	620.00	271.10	2.8470			
670.00	271.00	1.5000	670.00	275.90	3.3710			
700.00	273.40	1.5160	700.00	278.60	3.5160			
780.00	278.60	0.8660	780.00	285.90	3.4090			
850.00	282.20	1.3430	850.00	291.90	3.3330			
920.00	284.60	2.4540	920.00	294.30	4.2330			
950.00	285.20	4.1460	924.00	294.35	4.3450			
1000.00	286.90	6.2470						
1006.00	287.35	6.5620						

IV. CONCLUSIONS

Although from the results of the validation of the HARTCODE one can draw several other conclusions the most important one is that the code is able to compute the absorption optical depth, transmittance and radiance spectra with an accuracy which proved to be resonable to evaluate the data obtained by laboratory, field, aircraft or satellite spectral measurements.

Considering the rather complicated input structure of the HARTCODE the recent version is designed for research and not for operational use. The fine "tuning" of the code with respect the computational efficiency and the incorporation of the most up-to-date spectroscopic data still left to be done. Once we have the optimized version the task of setting up a transmittance compilation - i.e. the calculation and collection of accurate transmittance profiles for selected model atmospheres for further parameterization or remote sensing purposes - will be the matter of a routine operation.

In view of the first results of application of the HARTCODE let us mention some further conclusions:

In case of carbon dioxide according to the homogeneous calculations it seems that no manipulations with the line shape and line wing contribution can eliminate the discrepancies between the measured and computed transmittance spectra. The revision of other line parameters belonging to the particular bands might be necessary.

To overcome the problem of the band shapes really high precision laboratory measurements of the line shape function needed in many spectral intervals including the two hot bands of the CO_2 at 618 and 721 cm^{-1} where the discrepancies are the largest and several bands of the H_2O from 800 cm^{-1} . If we accept the line mixing problem as it is treated mathematically by Bulanin at al. it is plain that the original formulation is not adequate for application in LBL codes. Our opinion is that any kind of line wing consideration is justified - as far as they improve the agreement with laboratory measurements - until no better theoretical model is available.

The role of the weak CO_2 lines in the neighbourhood of the ν_2 fundamental is obvious as they can significantly change the position of the peak of the weighting functions. The line wing absorption - even when using Lorentzian line shape has less importance and completely negligible above $6.5 \ cm^{-1}$. Within a given wave number interval the consideration of several hundreds of very weak lines and the careful wave number integration is more vital. However it is true that more economic to compensate the weak line absorption with a more or less constant strong line wing absorption. When comparing the numerical accuracies of the different codes strictly the same spectroscopic input data should be used. The comparisons of the sensitivities of the individual codes to the slight changes in the different input parameters might also be useful.

When validating a code using real atmospheric measurements more care should be taken to monitor the condition of the measurements. Simultaneous ozone sounding and other trace gas measurements might also be necessary. In case of air-born measurements having the measured data of the same trajectory from different altitudes might to reduce the uncertainties in the skin temperatures.

Another important conclusion is that the HIS (or similar instrument) can monitor the amount of ozone and other trace gases being under the flight level. Also there might be a better chance to retrieve some characteristics of the vertical ozone distribution from the radiance spectra using nadir viewing geometry.

Compared with the FASCOD/2 in most spectral regions the HARTCODE can simulate the emission spectrum of the Earth-atmosphere system with a better accuracy.

In the field of the IR atmospheric radiative transfer a high-resolution transmittance/radiance code is always considered as a basic research tool and its application is not restricted to the area of IR remote sensing. In the further development of the HARTCODE the problems arising at the flux-divergence calculations and parameterization will also be considered.
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APPENDIX A

Relative Optical Air Mass Tables for Model Atmospheres

TABLE A-1

Relative optical air mass values for *TROPICAL* atmosphere at 15μ wavelength and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, *L* is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.02576	233.845	1.9936	1.9985	1.9781	1.9943	1.9956	1.9941
62.0	0.02795	247.946	2.1220	2.1282	2.1027	2.1228	2.1246	2.1227
64.0	0.03045	264.096	2.2710	2.2788	2.2465	2.2720	2.2742	2.2718
66.0	0.03332	282.726	2.4455	2.4555	2.4139	2.4468	2.4496	2.4465
68.0	0.03667	304.385	2.6522	2.6654	2.6110	2.6539	2.6577	2.6535
70.0	0.04064	329.793	2.9006	2.9183	2.8455	2.9029	2.9079	2.9024
72.0	0.04542	359.895	3.2040	3.2285	3.1285	3.2072	3.2141	3.2064
74.0	0.05130	395.949	3.5822	3.6170	3.4756	3.5866	3.5965	3.5856
76.0	0.05873	439.648	4.0654	4.1171	3.9089	4.0719	4.0866	4.0703
78.0	0.06841	493.283	4.7023	4.7836	4.4617	4.7123	4.7354	4.7099
80.0	0.08156	559.960	5.5767	5.7135	5.1836	5.5930	5.6319	5.5891
81.0	0.09007	599.445	6.1466	6.3305	5.6301	6.1682	6.2203	6.1630
82.0	0.10039	643.854	6.8432	7.0975	6.1493	6.8722	6.9440	6.8653
83.0	0.11317	693.916	7.7113	8.0754	6.7555	7.7515	7.8536	7.7418
84.0	0.12933	750.456	8.8188	9.3629	7.4643	8.8761	9.0271	8.8622
85.0	0.15031	814.395	10.2720	11.1292	8.2899	10.3564	10.5903	10.3357
86.0	0.17842	886.766	12.2446	13.6892	9.2404	12.3740	12.7568	12.3420
87.0	0.21746	968.742	15.0356	17.6912	10.3079	15.2428	15.9110	15.1911
87.5	0.24300	1013.759	16.8930	20.6438	10.8760	17.1595	18.0667	17.0926
88.0	0.27413	1061.735	19.1898	24.6646	11.4584	19.5363	20.7922	19.4489
88.2	0.28851	1081.808	20.2632	26.6982	11.6938	20.6493	22.0877	20.5516
88.4	0.30419	1102.413	21.4423	29.0547	11.9298	21.8732	23.5262	21.7640
88.6	0.32133	1123.571	22.7412	31.8076	12.1662	23.2228	25.1288	23.1005
88.8	0.34010	1145.303	24.1763	35.0517	12.4026	24.7154	26.9209	24.5782
89.0	0.36072	1167.634	25.7667	38.9099	12.6390	26.3712	28.9321	26.2171
89.2	0.38342	1190.595	27.5349	43.5428	12.8755	28.2136	31.1984	28.0403
89.4	0.40847	1214.215	29.5074	49.1624	13.1123	30.2705	33.7625	30.0754
89.6	0.43621	1238.533	31.7156	56.0500	13.3499	32.5747	36.6766	32.3547
89.7	0.45121	1250.968	32.9195	60.0828	13.4692	33.8315	38.2843	33.5978
89.8	0.46704	1263.596	34.1968	64.5835	13.5890	35.1654	40.0043	34.9171
89.9	0.48377	1276.424	35.5537	69.6204	13.7092	36.5826	41.8471	36.3186
90.0	0.50148	1289.460	36.9964	75.2727	13.8301	38.0899	43.8240	37.8092

TABLE A-2

Relative optical air mass values for *MIDLATITUDE SUMMER* atmosphere at 15μ wavelength and for a path from 0.0 to $120 \ km$ altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.02628	233.848	1.9937	1.9985	1.9801	1.9947	1.9957	1.9945
62.0	0.02852	247.950	2.1221	2.1282	2.1052	2.1234	2.1247	2.1231
64.0	0.03106	264.102	2.2711	2.2788	2.2496	2.2727	2.2744	2.2724
66.0	0.03399	282.732	2.4456	2.4555	2.4180	2.4477	2.4498	2.4472
68.0	0.03741	304.394	2.6523	2.6654	2.6163	2.6552	2.6579	2.6545
70.0	0.04146	329.805	2.9008	2.9183	2.8526	2.9045	2.9083	2.9037
72.0	0.04634	359.910	3.2043	3.2284	3.1382	3.2094	3.2146	3.2082
74.0	0.05234	395.970	3.5825	3.6169	3.4892	3.5898	3.5972	3.5881
76.0	0.05993	439.677	4.0659	4.1170	3.9288	4.0766	4.0875	4.0741
78.0	0.06983	493.325	4.7032	4.7834	4.4919	4.7197	4.7368	4.7159
80.0	0.08328	560.024	5.5781	5.7132	5.2322	5.6053	5.6342	5.5990
81.0	0.09197	599.525	6.1486	6.3301	5.6931	6.1846	6.2234	6.1763
82.0	0.10255	643.955	6.8460	7.0969	6.2326	6.8946	6.9482	6.8834
83.0	0.11564	694.047	7.7155	8.0746	6.8677	7.7829	7.8596	7.7676
84.0	0.13223	750.627	8.8253	9.3618	7.6182	8.9219	9.0359	8.9001
85.0	0.15381	814.627	10.2826	11.1276	8.5048	10.4260	10.6040	10.3942
86.0	0.18279	887.090	12.2633	13.6870	9.5438	12.4851	12.7795	12.4373
87.0	0.22322	969.217	15.0715	17.6896	10.7349	15.4305	15.9522	15.3568
87.5	0.24979	1014.347	16.9444	20.6449	11.3778	17.4094	18.1244	17.3175
88.0	0.28233	1062.478	19.2654	24.6747	12.0401	19.8748	20.8758	19.7602
88.2	0.29743	1082.631	20.3521	26.7161	12.3074	21.0334	22.1858	20.9084
88.4	0.31394	1103.328	21.5475	29.0849	12.5744	22.3104	23.6419	22.1741
88.6	0.33206	1124.593	22.8662	31.8574	12.8400	23.7221	25.2665	23.5739
88.8	0.35199	1146.453	24.3258	35.1330	13.1030	25.2876	27.0859	25.1266
89.0	0.37399	1168.939	25.9468	39.0420	13.3622	27.0293	29.1317	26.8548
89.2	0.39837	1192.086	27.7533	43.7575	13.6163	28.9737	31.4420	28.7850
89.4	0.42548	1215.935	29.7744	49.5114	13.8646	31.1523	34.0630	30.9486
89.6	0.45576	1240.536	32.0447	56.6168	14.1061	33.6027	37.0515	33.3835
89.7	0.47225	1253.137	33.2861	60.8041	14.2241	34.9438	38.7047	34.7165
89.8	0.48975	1265.950	34.6062	65.5001	14.3404	36.3707	40.4772	36.1351
89.9	0.50833	1278.984	36.0118	70.7830	14.4548	37.8907	42.3805	37.6465
90.0	0.52811	1292.250	37.5103	76.7438	14.5675	39.5119	44.4276	39.2588

TABLE A-3

Relative optical air mass values for *MIDLATITUDE WINTER* atmosphere at 15μ wavelength and for a path from 0.0 to $120 \ km$ altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.02862	233.863	1.9941	1.9985	1.9821	1.9950	1.9959	1.9948
62.0	0.03106	247.969	2.1227	2.1281	2.1076	2.1238	2.1249	2.1236
64.0	0.03384	264.126	2.2718	2.2787	2.2527	2.2732	2.2747	2.2729
66.0	0.03704	282.763	2.4465	2.4554	2.4220	2.4484	2.4502	2.4480
68.0	0.04077	304.433	2.6536	2.6653	2.6215	2.6560	2.6584	2.6555
70.0	0.04518	329.856	2.9024	2.9181	2.8595	2.9057	2.9089	2.9050
72.0	0.05051	359.978	3.2065	3.2282	3.1476	3.2110	3.2155	3.2101
74.0	0.05708	396.063	3.5857	3.6166	3.5023	3.5921	3.5985	3.5907
76.0	0.06538	439.807	4.0706	4.1166	3.9478	4.0800	4.0896	4.0780
78.0	0.07622	493.513	4.7105	4.7826	4.5207	4.7250	4.7402	4.7219
80.0	0.09098	560.307	5.5903	5.7119	5.2779	5.6143	5.6400	5.6092
81.0	0.10056	599.878	6.1650	6.3283	5.7520	6.1966	6.2313	6.1899
82.0	0.11222	644.402	6.8684	7.0944	6.3096	6.9112	6.9594	6.9023
83.0	0.12672	694.621	7.7472	8.0708	6.9700	7.8068	7.8760	7.7944
84.0	0.14515	751.379	8.8720	9.3557	7.7562	8.9575	9.0612	8.9400
85.0	0.16927	815.636	10.3547	11.1170	8.6929	10.4821	10.6451	10.4566
86.0	0.20193	888.485	12.3812	13.6663	9.8004	12.5793	12.8512	12.5409
87.0	0.24805	971.226	15.2785	17.6417	11.0779	15.6015	16.0882	15.5424
87.5	0.27875	1016.807	17.2278	20.5653	11.7666	17.6480	18.3194	17.5745
88.0	0.31676	1065.540	19.6630	24.5328	12.4704	20.2168	21.1638	20.1256
88.2	0.33457	1085.991	20.8109	26.5330	12.7515	21.4316	22.5255	21.3324
88.4	0.35417	1107.030	22.0792	28.8453	13.0297	22.7763	24.0449	22.6686
88.6	0.37582	1128.687	23.4856	31.5393	13.3033	24.2700	25.7475	24.1535
88.8	0.39983	1150.999	25.0511	34.7043	13.5705	25.9355	27.6636	25.8096
89.0	0.42656	1174.009	26.8007	38.4557	13.8294	27.7997	29.8301	27.6642
89.2	0.45645	1197.768	28.7644	42.9441	14.0787	29.8952	32.2924	29.7499
89.4	0.49004	1222.337	30.9789	48.3680	14.3172	32.2614	35.1060	32.1061
89.6	0.52799	1247.790	33.4890	54.9917	14.5449	34.9464	38.3406	34.7811
89.7	0.54884	1260.875	34.8718	58.8603	14.6548	36.4266	40.1423	36.2563
89.8	0.57110	1274.218	36.3502	63.1714	14.7625	38.0099	42.0839	37.8345
89.9	0.59490	1287.832	37.9335	67.9900	14.8683	39.7061	44.1801	39.5256
90.0	0.62041	1301.735	39.6319	73.3921	14.9726	41.5264	46.4478	41.3407

TABLE A-4

Relative optical air mass values for SUBARCTIC SUMMER atmosphere at 15μ wavelength and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.02687	233.852	1.9938	1.9984	1.9811	1.9950	1.9958	1.9947
62.0	0.02916	247.955	2.1223	2.1280	2.1064	2.1238	2.1248	2.1234
64.0	0.03177	264.108	2.2713	2.2786	2.2512	2.2732	2.2745	2.2727
66.0	0.03477	282.740	2.4459	2.4553	2.4200	2.4483	2.4500	2.4476
68.0	0.03827	304.404	2.6527	2.6651	2.6189	2.6559	2.6582	2.6551
70.0	0.04241	329.818	2.9013	2.9179	2.8561	2.9055	2.9086	2.9044
72.0	0.04740	359.928	3.2050	3.2279	3.1430	3.2108	3.2151	3.2093
74.0	0.05355	395.994	3.5836	3.6162	3.4959	3.5918	3.5979	3.5896
76.0	0.06132	439.711	4.0674	4.1159	3.9385	4.0795	4.0886	4.0763
78.0	0.07146	493.374	4.7055	4.7816	4.5067	4.7242	4.7386	4.7194
80.0	0.08525	560.098	5.5821	5.7101	5.2557	5.6130	5.6371	5.6049
81.0	0.09418	599.617	6.1540	6.3259	5.7235	6.1948	6.2273	6.1841
82.0	0.10504	644.072	6.8535	7.0909	6.2725	6.9089	6.9536	6.8942
83.0	0.11850	694.198	7.7261	8.0658	6.9210	7.8034	7.8673	7.7828
84.0	0.13557	750.825	8.8411	9.3479	7.6906	8.9527	9.0475	8.9226
85.0	0.15782	814.893	10.3073	11.1041	8.6044	10.4748	10.6221	10.4291
86.0	0.18777	887.458	12.3041	13.6433	9.6813	12.5676	12.8099	12.4943
87.0	0.22967	969.743	15.1438	17.5960	10.9213	15.5816	16.0069	15.4561
87.5	0.25727	1014.985	17.0435	20.4979	11.5907	17.6208	18.2004	17.4520
88.0	0.29111	1063.260	19.4039	24.4300	12.2773	20.1778	20.9839	19.9461
88.2	0.30682	1083.480	20.5113	26.4105	12.5526	21.3856	22.3111	21.1210
88.4	0.32402	1104.252	21.7310	28.6990	12.8260	22.7212	23.7877	22.4180
88.6	0.34287	1125.600	23.0785	31.3646	13.0957	24.2030	25.4368	23.8544
88.8	0.36362	1147.550	24.5720	34.4963	13.3598	25.8522	27.2856	25.4502
89.0	0.38651	1170.134	26.2329	38.2103	13.6164	27.6940	29.3666	27.2289
89.2	0.41183	1193.386	28.0866	42.6599	13.8634	29.7579	31.7191	29.2185
89.4	0.43996	1217.348	30.1634	48.0504	14.0987	32.0790	34.3909	31.4519
89.6	0.47130	1242.067	32.4992	54.6605	14.3201	34.6988	37.4401	33.9686
89.7	0.48834	1254.729	33.7776	58.5377	14.4249	36.1361	39.1281	35.3476
89.8	0.50639	1267.603	35.1379	62.8743	14.5253	37.6676	40.9388	36.8161
89.9	0.52554	1280.700	36.5871	67.7419	14.6212	39.3013	42.8839	38.3815
90.0	0.54590	1294.031	38.1329	73.2252	14.7120	41.0460	44.9767	40.0524

TABLE A-5

Relative optical air mass values for *SUBARCTIC WINTER* atmosphere at 15μ wavelength and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.03017	233.874	1.9944	1.9984	1.9828	1.9952	1.9959	1.9951
62.0	0.03274	247.982	2.1230	2.1280	2.1085	2.1241	2.1250	2.1239
64.0	0.03567	264.142	2.2722	2.2785	2.2538	2.2736	2.2747	2.2734
66.0	0.03904	282.783	2.4470	2.4552	2.4234	2.4488	2.4502	2.4485
68.0	0.04297	304.459	2.6543	2.6650	2.6233	2.6566	2.6585	2.6562
70.0	0.04764	329.890	2.9034	2.9178	2.8619	2.9065	2.9090	2.9059
72.0	0.05326	360.024	3.2078	3.2277	3.1509	3.2121	3.2157	3.2114
74.0	0.06019	396.124	3.5876	3.6160	3.5069	3.5936	3.5988	3.5926
76.0	0.06897	439.894	4.0733	4.1155	3.9544	4.0823	4.0900	4.0808
78.0	0.08044	493.639	4.7148	4.7810	4.5306	4.7286	4.7409	4.7263
80.0	0.09609	560.496	5.5976	5.7091	5.2934	5.6203	5.6414	5.6166
81.0	0.10625	600.115	6.1747	6.3245	5.7720	6.2047	6.2334	6.1998
82.0	0.11865	644.703	6.8818	7.0889	6.3356	6.9225	6.9626	6.9160
83.0	0.13409	695.009	7.7662	8.0628	7.0042	7.8229	7.8812	7.8140
84.0	0.15379	751.890	8.9002	9.3431	7.8018	8.9816	9.0700	8.9692
85.0	0.17968	816.326	10.3985	11.0959	8.7540	10.5201	10.6610	10.5023
86.0	0.21496	889.452	12.4537	13.6272	9.8814	12.6433	12.8824	12.6173
87.0	0.26532	972.651	15.4087	17.5575	11.1810	15.7189	16.1554	15.6807
87.5	0.29922	1018.584	17.4088	20.4319	11.8788	17.8135	18.4223	17.7677
88.0	0.34174	1067.813	19.9228	24.3058	12.5873	20.4580	21.3272	20.4040
88.2	0.36188	1088.523	21.1142	26.2457	12.8679	21.7150	22.7244	21.6579
88.4	0.38425	1109.867	22.4358	28.4758	13.1439	23.1118	24.2890	23.0517
88.6	0.40921	1131.891	23.9081	31.0558	13.4131	24.6705	26.0496	24.6078
88.8	0.43724	1154.650	25.5559	34.0596	13.6729	26.4177	28.0412	26.3530
89.0	0.46895	1178.213	27.4099	37.5779	13.9210	28.3864	30.3074	28.3206
89.2	0.50511	1202.669	29.5083	41.7214	14.1551	30.6176	32.9033	30.5518
89.4	0.54677	1228.134	31.8995	46.6214	14.3731	33.1632	35.8998	33.0990
89.6	0.59529	1254.762	34.6462	52.4277	14.5737	36.0903	39.3892	36.0293
89.7	0.62266	1268.572	36.1774	55.7201	14.6671	37.7231	41.3553	37.6645
89.8	0.65244	1282.750	37.8299	59.2976	14.7558	39.4860	43.4934	39.4304
89.9	0.68493	1297.330	39.6181	63.1777	14.8400	41.3942	45.8251	41.3423
90.0	0.72044	1312.346	41.5583	67.3750	14.9197	43.4653	48.3756	43.4177

TABLE A-6

Relative optical air mass values for the USST 76 atmosphere at 15μ wavelength and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree, $\Delta \theta$ is the angular deviation of the beam in degree, L is the geometrical path length in km. The accuracies of the air mass values are better then 10^{-3} percent.

θ	riangle heta	L	AIR	H_2O	O_3	N_2O	CO	CH_4
60.0	0.02688	233.852	1.9939	1.9984	1.9807	1.9945	1.9958	1.9944
62.0	0.02917	247.955	2.1224	2.1280	2.1059	2.1232	2.1248	2.1230
64.0	0.03177	264.108	2.2714	2.2785	2.2506	2.2724	2.2745	2.2722
66.0	0.03477	282.740	2.4460	2.4552	2.4192	2.4473	2.4500	2.4470
68.0	0.03827	304.404	2.6529	2.6650	2.6178	2.6546	2.6581	2.6542
70.0	0.04241	329.818	2.9016	2.9178	2.8546	2.9038	2.9086	2.9033
72.0	0.04741	359.928	3.2054	3.2277	3.1410	3.2084	3.2150	3.2077
74.0	0.05355	395.994	3.5841	3.6159	3.4930	3.5884	3.5978	3.5874
76.0	0.06132	439.710	4.0682	4.1155	3.9342	4.0745	4.0884	4.0731
78.0	0.07146	493.373	4.7068	4.7810	4.5000	4.7165	4.7382	4.7142
80.0	0.08525	560.097	5.5841	5.7091	5.2447	5.6001	5.6366	5.5963
81.0	0.09417	599.616	6.1566	6.3244	5.7089	6.1777	6.2266	6.1727
82.0	0.10502	644.070	6.8570	7.0889	6.2528	6.8853	6.9527	6.8785
83.0	0.11847	694.193	7.7309	8.0629	6.8935	7.7700	7.8660	7.7607
84.0	0.13552	750.818	8.8478	9.3435	7.6512	8.9036	9.0456	8.8902
85.0	0.15772	814.880	10.3168	11.0971	8.5464	10.3991	10.6194	10.3792
86.0	0.18755	887.433	12.3179	13.6309	9.5932	12.4443	12.8053	12.4135
87.0	0.22921	969.691	15.1639	17.5719	10.7855	15.3664	15.9981	15.3165
87.5	0.25658	1014.907	17.0674	20.4624	11.4223	17.3281	18.1873	17.2635
88.0	0.29004	1063.139	19.4315	24.3751	12.0706	19.7710	20.9635	19.6864
88.2	0.30553	1083.336	20.5401	26.3440	12.3293	20.9186	22.2862	20.8241
88.4	0.32246	1104.078	21.7606	28.6171	12.5857	22.1832	23.7572	22.0776
88.6	0.34099	1125.389	23.1082	31.2620	12.8386	23.5810	25.3989	23.4626
88.8	0.36132	1147.294	24.6008	34.3650	13.0865	25.1306	27.2381	24.9976
89.0	0.38370	1169.821	26.2594	38.0376	13.3283	26.8539	29.3065	26.7045
89.2	0.40839	1193.002	28.1087	42.4249	13.5629	28.7769	31.6423	28.6087
89.4	0.43572	1216.876	30.1778	47.7171	13.7892	30.9300	34.2916	30.7404
89.6	0.46608	1241.486	32.5016	54.1658	14.0068	33.3496	37.3106	33.1355
89.7	0.48255	1254.083	33.7717	57.9243	14.1123	34.6726	38.9797	34.4450
89.8	0.49996	1266.886	35.1218	62.1054	14.2154	36.0792	40.7684	35.8373
89.9	0.51840	1279.904	36.5585	66.7686	14.3163	37.5765	42.6877	37.3191
90.0	0.53796	1293.147	38.0892	71.9831	14.4150	39.1720	44.7505	38.8981

TABLE A-7

Relative optical air mass values of some trace gases for the USST 76 atmosphere at 15μ wavelength and for a path from 0.0 to 120 km altitude. θ is the zenith angle in degree. The accuracies of the air mass values are better then 10^{-3} percent.

θ	NO	SO_2	NO_2	NH_3	PH_3	HNO_3	OH
60.0	1.9868	1.9968	1.9789	1.9979	1.9939	1.9837	1.9555
62.0	2.1136	2.1260	2.1037	2.1274	2.1224	2.1097	2.0745
64.0	2.2603	2.2761	2.2477	2.2779	2.2714	2.2553	2.2110
66.0	2.4317	2.4520	2.4156	2.4543	2.4460	2.4253	2.3688
68.0	2.6343	2.6608	2.6131	2.6638	2.6529	2.6258	2.5525
70.0	2.8769	2.9121	2.8483	2.9162	2.9016	2.8652	2.7684
72.0	3.1717	3.2199	3.1324	3.2255	3.2054	3.1554	3.0248
74.0	3.5369	3.6047	3.4809	3.6128	3.5841	3.5133	3.3324
76.0	3.9997	4.0988	3.9166	4.1108	4.0682	3.9637	3.7056
78.0	4.6029	4.7547	4.4731	4.7734	4.7068	4.5447	4.1629
80.0	5.4180	5.6646	5.2015	5.6962	5.5841	5.3162	4.7273
81.0	5.9413	6.2644	5.6528	6.3069	6.1566	5.8015	5.0573
82.0	6.5726	7.0055	6.1785	7.0642	6.8570	6.3749	5.4225
83.0	7.3472	7.9427	6.7936	8.0265	7.7309	7.0578	5.8239
84.0	8.3177	9.1625	7.5142	9.2873	8.8478	7.8771	6.2594
85.0	9.5650	10.8086	8.3556	11.0040	10.3168	8.8639	6.7221
86.0	11.2206	13.1371	9.3259	13.4625	12.3179	10.0501	7.1973
87.0	13.5120	16.6441	10.4158	17.2269	15.1639	11.4580	7.6600
87.5	15.0155	19.1332	10.9950	19.9372	17.0674	12.2447	7.8761
88.0	16.8608	22.4014	11.5878	23.5328	19.4315	13.0806	8.0758
88.2	17.7198	24.0056	11.8271	25.3092	20.5401	13.4267	8.1500
88.4	18.6619	25.8269	12.0671	27.3322	21.7606	13.7785	8.2207
88.6	19.6984	27.9071	12.3076	29.6482	23.1082	14.1351	8.2876
88.8	20.8427	30.2979	12.5488	32.3130	24.6008	14.4954	8.3507
89.0	22.1106	33.0637	12.7909	35.3943	26.2594	14.8584	8.4097
89.2	23.5206	36.2846	13.0349	38.9730	28.1087	15.2228	8.4648
89.4	25.0948	40.0604	13.2821	43.1443	30.1778	15.5870	8.5161
89.6	26.8594	44.5148	13.5346	48.0188	32.5016	15.9493	8.5637
89.7	27.8227	47.0432	13.6638	50.7581	33.7717	16.1290	8.5864
89.8	28.8459	49.8012	13.7955	53.7210	35.1218	16.3073	8.6082
89.9	29.9341	52.8140	13.9302	56.9250	36.5585	16.4837	8.6294
90.0	31.0928	56.1091	14.0687	60.3883	38.0892	16.6579	8.6501

APPENDIX B

Results of the HIS Evaluations

The next 12 Figures and Tables contain the detailed results of the HART-CODE simulations and the HIS measurements. Because of the large amount of information to be displayed the plots are complex. For the more comfortable scaling of the graphs the comparisons were based on the brightness temperatures.

Thick curves in the main plots are the HIS measurements and the thin ones are the HARTCODE results.

The dashed liens in the main plots (if there are any) indicate the upper or lower boundary temperatures.

Each plot contain a small "window" where the differences between the measured and simulated brightness temperatures have been plotted in different scale. (Solid lines : HIS - HARTCODE, dotted lines : HIS - FASCODE). In the vertical axes (in the right) one division is always one degree and only the reference value (zero degree) is indicated.

The bars just above the wave number axes indicate the spectral intervals where the average error of HARTCODE is less than the one of the FASCODE.

The numerical results are summarized in the Tables following the Figures. For a given Figure the corresponding Table is marked with the same number.





Fig. B-1 : HARTCODE simulations in the 600-700 cm^{-1} spectral region.

Appendix B



Fig. B-1 : Cont.





Fig. B-2 : HARTCODE simulations in the 700-800 cm^{-1} spectral region.



Fig. B-2 : Cont.

Appendix B



Fig. B-3 : HARTCODE simulations in the 800-900 cm^{-1} spectral region.

Appendix B



Fig. B-3 : Cont.

Appendix B



Fig. B-4 : HARTCODE simulations in the 900-1000 cm^{-1} spectral region.

Appendix B



Fig. B-4 : Cont.

Appendix B



Fig. B-5 : HARTCODE simulations in the 1000-1100 cm^{-1} spectral region.



Fig. B-6 : HARTCODE simulations in the 1100-1200 cm^{-1} spectral region.

Appendix B



Fig. B-6 : Cont.



Fig. B-7 : HARTCODE simulations in the 1200-1300 cm^{-1} spectral region.

Appendix B



Fig. B-7 : Cont.



Fig. B-8 : HARTCODE simulations in the 1300-1400 cm^{-1} spectral region.

Appendix B



Fig. B-8 : Cont.



Fig. B-9 : HARTCODE simulations in the 1400-1500 cm^{-1} spectral region.

Appendix B



Fig. B-9 : Cont.



Fig. B-10 : HARTCODE simulations in the 1500-1600 cm^{-1} spectral region.

Appendix B



Fig. B-10 : Cont.



Fig. B-11 : HARTCODE simulations in the 1600-1700 cm^{-1} spectral region.

Appendix B



Fig. B-11 : Cont.



Fig. B-12 : HARTCODE simulations in the 1700-1800 cm^{-1} spectral region.

Appendix B



Fig. B-12 : Cont.

TABLE B-1

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

	case 1 : California Coast, 14-04-86								
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$		
-3.060	-2.710	-5.172	-4.270	1.107	1.263	37	600 - 610		
-0.930	-1.515	8.254	8.052	3.022	3.004	36	610 - 620		
-1.632	-1.813	-3.414	-3.866	1.095	1.008	36	620 - 630		
-0.713	-0.511	-2.144	-1.275	0.626	0.490	36	630 - 640		
-0.015	-0.178	-1.013	-1.221	0.410	0.492	37	640 - 650		
-1.270	-1.345	8.254	8.052	1.252	1.252	182	600 - 650 *		
-0.050	-0.074	-0.724	-0.765	0.313	0.301	36	650 - 660		
-0.110	-0.095	1.800	1.976	0.651	0.672	36	660 - 670		
-0.251	-0.274	-0.806	-0.784	0.306	0.279	37	670 - 680		
-0.008	-0.124	-0.688	-0.711	0.340	0.280	36	680 - 690		
-0.694	-1.100	-2.136	-3.054	0.663	0.971	36	690 - 700		
-0.223	-0.333	-2.136	-3.054	0.455	0.501	181	650 - 700 *		
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86			
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u		
-3.290	-2.483	-5.718	5.930	1.413	1.627	37	600 - 610		
-1.017	-1.645	8.377	7.818	3.355	3.130	36	610 - 620		
-1.644	-2.011	-3.768	-3.901	1.348	1.036	36	620 - 630		
-0.883	-1.046	-2.683	-2.533	0.881	0.767	36	630 - 640		
-0.386	-1.092	-1.825	-2.492	0.574	0.581	37	640 - 650		
-1.444	-1.655	8.377	7.818	1.514	1.428	182	600 - 650 *		
-0.399	-0.933	-1.430	-1.935	0.355	0.311	36	650 - 660		
-0.657	-1.014	-1.965	-1.856	0.521	0.503	36	660 - 670		
-0.597	-1.120	-1.114	-1.608	0.275	0.202	37	670 - 680		
-0.511	-1.181	-1.176	-2.554	0.257	0.403	36	680 - 690		
-1.321	-2.252	-2.199	-3.882	0.577	0.980	36	690 - 700		
-0.697	-1.300	-2.199	-3.882	0.397	0.480	181	650 - 700 *		
Appendix B

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	nia Coast	t, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-1.731	-1.412	-2.524	-2.133	0.513	0.551	37	700 - 710
-0.977	-0.848	-3.020	-2.231	1.079	0.758	36	710 - 720
0.494	-0.016	7.814	7.520	2.751	2.454	36	720 - 730
-0.439	0.013	-1.431	-1.788	0.431	0.564	36	730 - 740
-0.457	-0.076	2.854	2.870	1.089	1.244	37	740 - 750
-0.622	-0.468	7.814	7.520	1.173	1.114	182	700 - 750 *
-0.974	-0.781	-1.707	-1.673	0.347	0.560	36	750 - 760
-1.156	-0.986	-1.518	-1.557	0.262	0.370	36	760 - 770
-1.334	-1.203	-1.612	-1.464	0.161	0.186	37	770 - 780
-1.323	-1.313	-2.419	-2.246	0.253	0.265	36	780 - 790
-1.178	-1.016	-3.108	3.277	1.236	1.420	36	790 - 800
-1.193	-1.060	-3.108	3.277	0.452	0.560	181	750 - 800 *
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-1.963	-1.859	-2.909	-2.655	0.579	0.682	37	700 - 710
-1.126	-0.662	-3.638	-2.703	1.382	0.884	36	710 - 720
0.813	2.077	9.670	8.534	3.374	2.380	36	720 - 730
-0.521	1.788	-1.900	4.430	0.546	1.355	36	730 - 740
-0.699	2.874	-4.872	6.587	1.657	2.078	37	740 - 750
-0.699	0.844	9.670	8.534	1.508	1.476	182	700 - 750 *
-0.851	5.816	-2.901	10.955	1.004	3.273	36	750 - 760
-0.193	9.473	-1.854	11.526	0.578	1.569	36	760 - 770
-1.180	8.555	-3.077	11.380	1.042	3.180	37	770 - 780
-0.683	10.056	-4.338	11.947	1.160	3.278	36	780 - 790
-1.578	6.725	-6.090	12.160	2.574	4.301	36	790 - 800
-0.897	8.125	-6.090	12.160	1.272	3.120	181	750 - 800 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	nia Coast	t, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-0.874	-0.925	-1.244	-1.307	0.278	0.302	36	800 - 810
-0.919	-0.925	-1.083	-1.070	0.106	0.098	37	810 - 820
-0.763	-0.814	-0.898	-0.952	0.158	0.137	36	820 - 830
-0.778	-0.843	-0.962	-0.989	0.053	0.047	36	830 - 840
-1.067	-1.141	-1.535	-1.553	0.165	0.159	37	840 - 850
-0.880	-0.930	-1.535	-1.553	0.152	0.149	182	800 - 850 *
-0.815	-0.895	-1.255	-1.402	0.260	0.239	36	850 - 860
-0.568	-0.633	-0.692	-0.727	0.046	0.036	36	860 - 870
-0.606	-0.676	-1.109	-1.124	0.154	0.137	37	870 - 880
-0.538	-0.620	-0.825	-0.833	0.139	0.104	36	880 - 890
-0.504	-0.560	-0.625	-0.640	0.048	0.047	36	890 - 900
-0.606	-0.677	-1.255	-1.402	0.129	0.112	181	850 - 900 *
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-0.355	9.882	-3.631	12.325	0.987	2.958	36	800 - 810
-0.030	11.397	-2.703	12.543	0.832	2.262	37	810 - 820
0.032	11.577	-1.158	12.537	0.370	1.563	36	820 - 830
-0.047	12.019	-2.227	12.527	0.442	1.208	36	830 - 840
-0.873	10.826	-2.926	11.956	0.714	1.985	37	840 - 850
-0.254	11.140	-3.631	12.543	0.669	1.995	182	800 - 850 *
-1.033	10.053	-4.055	12.360	1.047	2.984	36	850 - 860
-0.251	11.966	-1.548	12.575	0.393	1.208	36	860 - 870
-0.550	11.525	-3.036	12.537	0.772	1.772	37	870 - 880
-0.451	11.310	-2.148	12.454	0.499	1.445	36	880 - 890
-0.196	12.375	-0.682	12.758	0.175	0.422	36	890 - 900
-0.496	11.446	-4.055	12.758	0.577	1.566	181	850 - 900 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	nia Coast	, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-0.491	-0.553	-0.921	-0.918	0.121	0.104	36	900 - 910
-0.650	-0.697	-0.751	-0.768	0.046	0.041	37	910 - 920
-0.686	-0.726	-1.302	-1.376	0.263	0.255	36	920 - 930
-0.452	-0.432	-0.700	-0.729	0.136	0.146	36	930 - 940
-0.299	-0.309	-0.657	-0.656	0.095	0.087	37	940 - 950
-0.516	-0.543	-1.302	-1.376	0.132	0.127	182	900 - 950 *
-0.320	-0.303	-0.645	-0.707	0.121	0.114	36	950 - 960
-0.301	-0.295	-0.428	-0.368	0.067	0.045	36	960 - 970
-0.269	-0.274	-0.596	-0.485	0.146	0.100	37	970 - 980
-0.392	-0.319	-0.438	-0.402	0.030	0.042	36	980 - 990
-0.408	-0.175	-0.559	-0.391	0.051	0.163	36	990 -1000
-0.338	-0.273	-0.645	-0.707	0.083	0.093	181	950 -1000 *
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-0.430	11.832	-2.923	12.770	0.692	1.720	36	900 - 910
-0.517	12.101	-0.907	12.395	0.136	0.397	37	910 - 920
-0.671	11.548	-1.984	12.554	0.470	1.239	36	920 - 930
-0.197	12.644	-0.553	13.040	0.193	0.231	36	930 - 940
-0.161	12.116	-2.241	13.049	0.635	1.402	37	940 - 950
-0.395	12.048	-2.923	13.049	0.425	0.998	182	900 - 950 *
-0.113	12.441	-1.542	13.120	0.433	0.739	36	950 - 960
0.014	12.769	0.298	13.162	0.118	0.303	36	960 - 970
-0.056	12.036	-1.512	12.843	0.450	0.803	37	970 - 980
-0.266	12.767	-0.399	12.958	0.095	0.130	36	980 - 990
-0.487	13.004	-0.747	13.880	0.098	0.371	36	990 -1000
-0.182	12.603	-1.542	13.880	0.239	0.469	181	950 -1000 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	nia Coast	z, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-0.349	0.543	-0.663	1.731	0.126	0.413	36	1000 -1010
-0.184	1.935	-0.786	3.234	0.240	0.623	37	1010 -1020
-0.010	2.838	1.220	3.421	0.450	0.272	36	1020 - 1030
-0.198	3.121	-1.239	4.974	0.409	0.974	36	1030 - 1040
-0.256	2.515	1.355	5.475	0.555	1.818	37	1040 -1050
-0.199	2.191	1.355	5.475	0.356	0.820	182	1000 -1050 *
0.463	4.418	1.952	6.660	0.752	0.827	36	1050 -1060
-0.194	1.289	-1.362	4.335	0.514	1.703	36	1060 - 1070
-0.745	-0.670	-1.573	-1.557	0.234	0.251	36	1070 - 1080
-0.842	-0.658	-1.058	-0.897	0.142	0.192	37	1080 - 1090
-1.019	-0.945	-1.605	-1.598	0.182	0.210	18	1090 -1100
-0.467	0.687	1.952	6.660	0.365	0.636	163	1050 -1100 *
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-0.566	14.139	-1.662	16.297	0.293	0.773	36	1000 -1010
-0.829	15.886	-3.317	18.858	0.773	1.763	37	1010 - 1020
-0.578	17.583	-1.882	18.868	0.583	0.999	36	1020 - 1030
-0.616	18.532	-1.983	22.442	0.747	2.028	36	1030 - 1040
-0.575	17.338	-2.090	23.622	0.736	3.519	37	1040 -1050
-0.633	16.696	-3.317	23.622	0.626	1.817	182	1000 -1050 *
-0.504	19.408	-1.864	23.282	0.836	1.604	36	1050 -1060
-1.291	14.187	-5.458	20.161	1.334	3.874	36	1060 - 1070
-1.647	10.769	-4.407	12.191	0.707	1.546	36	1070 - 1080
-1.568	11.495	-1.924	12.212	0.202	0.380	37	1080 - 1090
-1.817	10.879	-4.100	12.567	0.811	2.197	18	1090 -1100
-1.365	13.348	-5.458	23.282	0.778	1.920	163	1050 -1100 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	nia Coast	, 14-04-8	6	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-0.844	-0.859	-2.060	-2.007	0.395	0.403	21	1100 -1110
-0.450	-0.359	-0.776	-0.676	0.186	0.184	20	1110 -1120
-0.389	-0.268	-1.876	-1.193	0.474	0.402	21	1120 -1130
-0.631	-0.560	-2.806	-2.138	0.681	0.538	21	1130 -1140
-0.458	-0.255	-1.187	-0.836	0.268	0.218	21	1140 - 1150
-0.554	-0.460	-2.806	-2.138	0.401	0.349	104	1100 -1150 *
-0.568	-0.360	-1.090	-0.693	0.229	0.169	20	1150 -1160
-0.667	-0.534	-1.218	-1.037	0.228	0.161	21	1160 - 1170
-0.849	-0.714	-3.521	-3.039	0.880	0.847	21	1170 -1180
-0.667	-0.509	-2.939	-1.950	0.686	0.539	21	1180 -1190
-0.508	-0.479	-2.195	-1.619	0.534	0.448	20	1190 -1200
-0.652	-0.519	-3.521	-3.039	0.512	0.433	103	1150 -1200 *
		case 2 :	Tucson/	'Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-0.680	-1.504	-2.460	-4.038	0.705	1.081	21	1100 -1110
-0.049	-0.310	1.126	-0.774	0.489	0.247	20	1110 -1120
-0.310	-0.498	-3.054	-3.382	0.787	1.110	21	1120 - 1130
-0.162	-0.924	-2.138	-3.768	0.772	1.292	21	1130 - 1140
0.062	-0.072	-1.435	-2.396	0.450	0.797	21	1140 - 1150
-0.228	-0.662	-3.054	-4.038	0.641	0.905	104	1100 -1150 *
0.305	0.068	-1.000	-1.822	0.569	0.799	20	1150 -1160
0.145	-0.213	-1.580	-1.822	0.549	0.625	21	1160 - 1170
0.184	-1.047	-1.561	-4.847	0.644	1.872	21	1170 -1180
0.380	-0.523	-1.811	-3.516	0.692	1.360	21	1180 -1190
0.436	-0.334	-1.589	-2.944	0.660	1.120	20	1190 -1200
0.290	-0.410	-1.811	-4.847	0.623	1.155	103	1150 -1200 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Califor	nia Coast	, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-0.535	-0.505	-0.717	-0.731	0.105	0.104	21	1200 -1210
-0.227	-0.931	-1.207	-1.719	0.507	0.554	21	1210 - 1220
-0.371	-0.622	-1.284	-1.992	0.353	0.601	21	1220 - 1230
-0.614	-0.404	-1.383	-0.693	0.367	0.310	20	1230 - 1240
-0.685	-0.881	-1.837	-2.385	0.649	0.688	21	1240 - 1250
-0.486	-0.668	-1.837	-2.385	0.396	0.451	104	1200 -1250 *
-1.260	-0.444	-2.487	-1.556	0.646	0.449	21	1250 -1260
-2.259	-1.289	-3.748	-4.665	0.923	1.325	21	1260 - 1270
-4.070	-0.874	-6.144	-2.228	1.241	0.663	20	1270 - 1280
-1.236	-0.938	-4.522	-3.270	1.793	1.273	21	1280 - 1290
-3.969	-0.177	-5.775	1.603	1.540	0.683	21	1290 -1300
-2.559	-0.745	-6.144	-4.665	1.228	0.879	104	1250 -1300 *
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
0.202	0.127	0.444	0.425	0.217	0.251	21	1200 -1210
0.444	-1.118	2.445	-3.171	0.991	1.506	21	1210 -1220
0.209	-0.448	2.006	-3.598	0.733	1.532	21	1220 - 1230
0.705	0.973	2.616	1.873	0.723	0.435	20	1230 - 1240
0.341	-0.544	2.969	-3.076	1.058	1.478	21	1240 - 1250
0.380	-0.202	2.969	-3.598	0.745	1.040	104	1200 -1250 *
-0.869	-0.341	-2.255	-2.028	0.851	0.982	21	1250 -1260
-1.894	-1.884	-3.476	-3.749	1.232	1.236	21	1260 - 1270
-4.126	-0.979	-6.763	-2.727	1.601	1.262	20	1270 - 1280
-0.231	-1.288	-4.295	-4.785	2.310	1.640	21	1280 -1290
-3.172	0.135	-5.897	2.645	2.422	1.095	21	1290 -1300
-2.058	-0.871	-6.763	-4.785	1.683	1.243	104	1250 -1300 *

Appendix B

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Califor	nia Coast	, 14-04-8	6	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-2.710	-0.913	-6.163	-2.396	1.657	0.979	21	1300 -1310
1.397	-0.279	4.109	-3.702	1.864	1.541	20	1310 -1320
0.432	0.522	3.873	-2.750	1.226	1.061	21	1320 -1330
1.286	0.195	5.624	-3.737	2.116	1.812	21	1330 - 1340
0.481	0.062	2.972	-3.497	1.522	1.867	20	1340 - 1350
0.177	-0.083	-6.163	-3.737	1.677	1.452	103	1300 -1350 *
2.185	1.359	5.584	3.846	2.123	1.645	21	1350 - 1360
1.754	-0.336	5.036	-3.527	2.223	2.001	21	1360 - 1370
0.705	-1.268	-4.928	-5.893	2.566	2.482	21	1370 - 1380
2.056	0.682	4.422	-3.603	1.886	2.576	20	1380 - 1390
-0.616	-2.957	-5.436	-5.425	2.487	2.008	21	1390 - 1400
1.217	-0.504	5.584	-5.893	2.257	2.143	104	1350 -1400 *
		case 2 :	Tucson/	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-2.982	-1.373	-6.643	-3.911	2.040	1.337	21	1300 -1310
1.911	0.237	3.847	1.809	1.361	0.893	20	1310 -1320
0.241	0.778	3.764	2.999	1.413	1.407	21	1320 - 1330
1.782	1.256	5.523	4.363	2.148	1.418	21	1330 - 1340
0.627	0.152	3.598	3.029	1.670	1.659	20	1340 - 1350
0.316	0.210	-6.643	4.363	1.726	1.343	103	1300 -1350 *
2.267	1.157	5.382	3.242	1.869	1.259	21	1350 - 1360
1.922	0.301	-5.531	-2.535	2.409	1.163	21	1360 - 1370
1.407	-0.052	-4.812	-3.810	2.561	1.645	21	1370 - 1380
2.533	1.316	4.440	2.787	1.870	1.339	20	1380 - 1390
0.240	-0.862	-7.759	-5.098	3.478	1.860	21	1390 -1400
1.674	0.372	-7.759	-5.098	2.437	1.453	104	1350 -1400 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Califorr	nia Coast	, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
1.158	-0.182	-3.591	-4.189	1.999	2.434	21	1400 -1410
0.509	-1.147	-4.009	-5.180	2.541	2.577	21	1410 -1420
-0.709	-2.637	-5.359	-5.497	1.903	1.982	20	1420 - 1430
-1.455	-3.364	-5.223	-6.039	1.808	1.333	21	1430 - 1440
0.007	-0.771	-4.396	-4.528	1.992	2.353	21	1440 - 1450
-0.098	-1.620	-5.359	-6.039	2.049	2.136	104	1400 -1450 *
-2.806	-4.100	-5.048	-6.226	1.783	1.588	21	1450 -1460
-2.872	-4.463	-6.234	-6.958	1.704	1.227	20	1460 - 1470
-3.003	-4.147	-5.839	-6.196	1.970	1.796	21	1470 - 1480
-2.516	-3.265	-5.296	-5.937	1.956	1.973	21	1480 - 1490
-4.055	-4.924	-5.494	-6.895	1.122	1.043	21	1490 - 1500
-3.051	-4.180	-6.234	-6.958	1.707	1.526	104	1450 -1500 *
		case 2 :	Tucson/2	Kitt Pea	k, 15-04-	86	
ε_H	ε_F	ε_{H}^{m}	ε_F^m	σ_H	σ_F	n	riangle u
2.259	0.949	-4.550	-2.793	2.114	1.422	21	1400 -1410
0.492	-0.252	-12.473	-6.920	4.507	2.589	21	1410 -1420
0.816	-0.404	-8.296	-5.577	3.137	1.916	20	1420 - 1430
-0.644	-1.173	-11.613	-6.083	4.413	2.368	21	1430 - 1440
1.462	0.762	-6.739	-4.047	2.607	1.704	21	1440 - 1450
0.877	-0.024	-12.473	-6.920	3.355	2.000	104	1400 -1450 *
-4.530	-3.743	-13.396	-10.266	6.133	4.032	21	1450 -1460
-1.177	-1.570	-13.572	-8.685	4.538	2.829	20	1460 - 1470
-3.703	-3.037	-15.195	-9.843	5.838	3.897	21	1470 - 1480
-1.958	-1.415	-10.838	-8.347	4.625	3.211	21	1480 - 1490
-5.040	-3.721	-12.313	-8.158	4.988	3.218	21	1490 - 1500
-3.282	-2.697	-15.195	-10.266	5.224	3.437	104	1450 -1500 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	nia Coast	t, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-4.893	-4.954	-5.926	-6.767	0.588	1.437	20	1500 - 1510
-4.491	-5.075	-6.365	-6.513	0.788	0.707	21	1510 - 1520
-4.917	-5.002	-6.795	-6.647	0.753	0.995	21	1520 - 1530
-5.372	-4.948	-6.229	-6.675	0.685	1.343	21	1530 - 1540
-5.521	-5.113	-6.477	-6.769	0.478	1.055	20	1540 - 1550
-5.039	-5.018	-6.795	-6.769	0.658	1.107	103	1500 -1550 *
-5.711	-5.038	-6.990	-7.299	1.100	2.057	21	1550 - 1560
-5.504	-5.233	-6.787	-6.997	0.549	1.377	21	1560 - 1570
-5.108	-5.395	-6.591	-7.487	1.029	1.640	21	1570 - 1580
-3.132	-1.945	-4.616	-3.064	0.785	0.601	20	1580 - 1590
-2.943	-3.173	-4.904	-4.455	0.816	0.684	21	1590 - 1600
-4.479	-4.157	-6.990	-7.487	0.856	1.272	104	1550 -1600 *
		case 2 :	Tucson/I	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-8.398	-5.725	-16.602	-10.680	5.949	3.760	20	1500 - 1510
-5.277	-3.506	-14.659	-9.112	4.170	2.671	21	1510 - 1520
-8.817	-6.039	-14.939	-11.187	4.412	3.093	21	1520 - 1530
-8.559	-5.423	-17.347	-11.011	5.702	3.717	21	1530 - 1540
-8.513	-5.528	-16.127	-11.114	5.221	3.874	20	1540 - 1550
-7.913	-5.244	-17.347	-11.187	5.091	3.423	103	1500 - 1550 *
-9.873	-6.316	-15.985	-10.897	4.914	3.141	21	1550 - 1560
-6.872	-4.237	-15.517	-9.313	4.799	2.931	21	1560 - 1570
-5.400	-3.538	-13.654	-8.700	4.952	3.185	21	1570 - 1580
-0.047	0.453	-1.577	0.881	0.586	0.317	20	1580 - 1590
-0.326	-0.458	-4.543	-2.458	1.324	0.575	21	1590 - 1600
-4.503	-2.819	-15.985	-10.897	3.315	2.030	104	1550 -1600 *

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Californ	ia Coas	t, 14-04-8	6	
ε_H	ε_F	ε^m_H	ε_F^m	σ_H	σ_F	n	riangle u
-3.758	-4.267	-5.671	-5.229	1.620	0.650	21	1600 -1610
-4.922	-5.555	-7.966	-7.819	1.869	1.512	20	1610 - 1620
-5.260	-5.895	-7.693	-7.468	1.708	0.742	21	1620 - 1630
-4.853	-5.200	-8.703	-7.294	1.740	1.667	21	1630 - 1640
-4.880	-5.478	-8.138	-7.533	2.133	1.090	21	1640 - 1650
-4.735	-5.279	-8.703	-7.819	1.814	1.132	104	1600 -1650 *
-4.519	-4.809	-7.303	-7.747	2.111	2.426	20	1650 - 1660
-4.169	-4.994	-8.452	-7.366	2.154	1.252	21	1660 - 1670
-4.739	-5.780	-8.055	-7.324	2.153	1.404	21	1670 - 1680
-4.748	-5.505	-7.333	-7.918	1.741	1.744	21	1680 - 1690
-4.204	-4.996	-7.057	-7.085	2.106	2.012	20	1690 - 1700
-4.476	-5.217	-8.452	-7.918	2.053	1.767	103	1650 - 1700 *
		case 2 :	Tucson/I	Kitt Pea	k, 15-04-	86	
ε_H	ε_F	ε_{H}^{m}	ε_F^m	σ_H	σ_F	n	riangle u
-1.689	-1.371	-5.270	-3.480	1.384	1.043	21	1600 -1610
-4.127	-3.151	-13.965	-8.864	4.687	3.103	20	1610 - 1620
-4.834	-3.478	-14.422	-9.740	3.852	2.996	21	1620 - 1630
-5.046	-3.361	-13.583	-9.734	4.961	3.389	21	1630 - 1640
-5.859	-4.212	-16.712	-10.322	5.024	3.445	21	1640 - 1650
-4.311	-3.115	-16.712	-10.322	3.982	2.795	104	1600 -1650 *
-6.031	-3.849	-14.569	-9.575	5.277	3.132	20	1650 - 1660
-3.889	-2.773	-14.526	-8.191	4.502	3.183	21	1660 - 1670
-4.593	-3.376	-9.784	-6.692	3.257	2.346	21	1670 - 1680
-6.633	-4.679	-15.581	-9.871	4.521	2.859	21	1680 - 1690
-5.658	-3.969	-11.570	-7.673	4.211	2.970	20	1690 - 1700
-5.361	-3.729	-15.581	-9.871	4.354	2.898	103	1650 -1700 *

Appendix B

Detailed statistics of the HARTCODE and FASCOD results. ε_H , ε_F , ε_H^m , ε_F^m , σ_H , and σ_F are the average error, maximum error and standard deviation of the computed brightness temperatures (in degrees) subsequently, subscripts H and F stand for the HARTCODE and FASCOD, n indicates the number of data in the wave number interval and $\Delta \nu$ is the wave number interval in cm^{-1} .

		case 1	: Califorr	nia Coast	, 14-04-8	6	
ε_H	ε_F	ε_{H}^{m}	ε_F^m	σ_H	σ_F	n	$\triangle \nu$
-4.169	-4.942	-7.036	-7.395	2.231	2.185	21	1700 -1710
-3.438	-4.996	-6.912	-6.839	2.534	1.317	21	1710 -1720
-1.113	-2.722	-3.243	-4.481	1.003	1.078	21	1720 - 1730
-3.542	-5.219	-6.578	-7.657	2.320	1.722	20	1730 - 1740
-3.142	-5.063	-5.507	-6.155	1.380	0.587	21	1740 - 1750
-3.081	-4.589	-7.036	-7.657	1.894	1.378	104	1700 -1750 *
-0.291	-2.949	-4.028	-5.262	1.507	0.997	21	1750 - 1760
-0.604	-3.135	4.231	-5.563	2.173	1.470	21	1760 - 1770
-2.133	-4.222	-8.049	-7.067	2.991	2.215	20	1770 - 1780
1.242	-1.600	7.184	-3.879	2.257	1.369	21	1780 - 1790
-1.615	-4.173	-6.470	-6.640	2.236	1.222	21	1790 - 1800
-0.680	-3.216	-8.049	-7.067	2.233	1.455	104	1750 -1800 *
		case 2 :	Tucson/2	Kitt Pea	k, 15-04-	86	
ε_H	$arepsilon_F$	ε_{H}^{m}	ε_F^m	σ_H	σ_F	n	riangle u
-5.248	-3.498	-12.501	-7.712	4.051	2.752	21	1700 -1710
-4.773	-3.939	-17.581	-10.999	5.303	3.704	21	1710 - 1720
1.535	0.603	-3.725	-5.243	1.759	1.606	21	1720 - 1730
-3.701	-2.980	-12.076	-6.925	4.043	2.698	20	1730 - 1740
-2.477	-2.143	-7.254	-6.607	2.675	1.909	21	1740 - 1750
-2.933	-2.391	-17.581	-10.999	3.566	2.534	104	1700 -1750 *
1.192	-0.183	3.948	-4.688	2.201	1.785	21	1750 -1760
1.056	-0.297	-6.086	-5.564	2.812	2.122	21	1760 - 1770
-2.535	-2.806	-15.438	-12.423	6.402	4.704	20	1770 - 1780
3.196	1.028	8.919	2.072	2.052	0.775	21	1780 -1790
0.015	-0.748	-6.370	-4.013	2.819	1.576	21	1790 -1800
0.585	-0.601	-15.438	-12.423	3.257	2.192	104	1750 -1800 *

APPENDIX C

Listing of the First Group of Programmes:

DECODA
DECODG
FIND
LIN

```
PROGRAM DECODA
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
3
         CHARACTER*80 A1(41)
         CHARACTER*35 QID
\mathbf{4}
         OPEN (UNIT=1, TYPE='OLD', BLOCKSIZE=3210, RECL=80)
5
         OPEN (UNIT=2, TYPE='NEW', FILE= 'AFGLM.DAT')
6
         OPEN (UNIT=3,TYPE='NEW',FILE= 'AFGLT.DAT')
\overline{7}
         OPEN (UNIT=4, TYPE='NEW', FILE=
                                            'AFGL.DAT')
8
         OPEN (UNIT=7, TYPE='NEW', FILE='REMARKS.DAT')
9
         OPEN (UNIT=8,TYPE='OLD',FILE= 'DECODA.INP')
10
11
         READ(8,*) IMIX, ICHANGE
         IF(IMIX.EQ.-1) THEN
12
                          NMAIN = 176337
13
                          NTRACE = 94682
14
                          GOTO 72
15
16
                          END IF
         IK
               = 0
17
         IREJ = 0
18
         NNLIN = O
19
         IFILE = 2
20
21
     110 READ (1,960,END=120) A1(1)
22
         DECODE (80,990,A1(1)) NLIN
         READ (1,960,END=120) (A1(I+1),I=1,NLIN-1)
23
     960 FORMAT (A80)
24
     969 FORMAT (10X, F10.6, E10.3, F5.4, F10.3, A35)
25
     970 FORMAT (10X,F10.4,E10.3,F5.4,F10.3,A35)
26
     971 FORMAT (3X, I4, I3, 70X)
27
     978 FORMAT (1X,F10.4,E10.3,F5.4,F10.3,I3,2I10)
28
     990 FORMAT (I10,70X)
29
         DO 220 I = 1, NLIN-1
30
         J=I+1
31
                       DECODE(80,970,A1(I)) V,S,A,E,QID
32
33
         IF(V.LT.1D2) DECODE(80,969,A1(I)) V,S,A,E,QID
                       DECODE(80,971,A1(J)) ISOT,II
34
         IF(II.EQ. 0) THEN
35
                       WRITE(7,'(1X,A80)')A1(I),A1(J)
36
                       GOTO 220
37
                       END IF
38
39
         IF(E .LT. 0) THEN
                       IREJ=IREJ+1
40
                       WRITE(7,978)
                                        V,S,A,E,II,NNLIN,IREJ
41
                       GOTO 220
42
                       END IF
43
         NNLIN=NNLIN+1
44
         WRITE (IFILE,10) V,S,A,E,II,NNLIN,ISOT,QID
45
```

```
Appendix \ C
```

46	10	FORMAT (1X,D16	6.8,3D11.4,I4	4,I8,I4,A35)
47	220	CONTINUE		
48		IF(NNLIN-(NNL	IN/500)*500.H	EQ.0)WRITE(6,*)NLIN,NNLIN,V,II
49		GOTO 110		
50	120	IK=IK+1		
51		IF(IK.EQ.179)	THEN	
52			WRITE(7,*)	IK,NLIN,NNLIN
53			NMAIN=NNLIN	
54			NNLIN=0	
55			IFILE=3	
56			GOTO 110	
57			END IF	
58		IF(IK.EQ.279)	GOTO 130	
59		GOTO 110		
60	130	NTRACE=NNLIN		
61			WRITE(7,*)	IK,NLIN,NNLIN
62		REWIND 2		
63		REWIND 3		
64		WRITE(6,*)'NM	AIN=',NMAIN	
65		WRITE(6,*)'NTH	RACE=',NTRACH	3
66	72	IF(IMIX.NE.O)	CALL MIX(NM	AIN,NTRACE,ICHANGE)
67		STOP		
68		END		

```
Appendix C
```

```
SUBROUTINE MIX(N1,N2,IC)
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
3
         DIMENSION MOLA(45)
         CHARACTER*35 QID
4
      10 FORMAT (1X,D16.8,3D11.4,I4,I8,I4,A35)
5
         NALL=0
6
         M1=0
\overline{7}
         M2=0
8
         READ (3,10) V2,S2,A2,E2,I2,L2,IS2,QI2
9
10
         M2=M2+1
     100 IF (M1.GT.N1.AND.M2.GT.N2) GOTO 400
11
         IF (M1.GT.N1) GOTO 200
12
         READ (2,10) V1,S1,A1,E1,I1,L1,IS1,QI1
13
         M1=M1+1
14
         GOTO 300
15
16
    200 IF (M1.GT.N1.AND.M2.GT.N2) GOTO 400
         IF (M2.GT.N2) GOTO 100
17
         READ (3,10) V2,S2,A2,E2,I2,L2,IS2,QI2
18
         M2=M2+1
19
     300 NALL = NALL + 1
20
21
         IF(V1.LE.V2) THEN
                       WRITE (4,10) V1,S1,A1,E1,I1,NALL,IS1,QI1
22
                       GOTO 100
23
                       END IF
24
         IF(V1.GT.V2) THEN
25
                       IF (IC.EQ.0) GOTO 302
26
                       DO 301 I=1,45
27
                       IF(I2.NE.MOLA(I)) GOTO 301
28
                       I2=I
29
                       GOTO 302
30
                       CONTINUE
31
    301
     302
                       WRITE (4,10) V2,S2,A2,E2,I2,NALL,IS2,QI2
32
33
                       GOTO 200
                       END IF
34
    400 WRITE(6,*)'TOTAL NUMBER OF LINES : ', NALL
35
    410 RETURN
36
          DATA MOLA/
37
        * 1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,28,12,13,14,
38
        * 15,16,17,18,19,20,27, 0,26, 0, 0,23, 0, 0, 0,
39
        * 0,21,22,24,25, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0/
40
         END
41
```

```
Appendix C
```

```
PROGRAM DECODG
1
\mathbf{2}
         DIMENSION
                          NSK(10)
3
         CHARACTER*6160 BUFF
         INTEGER
                          FRL, KK*2
4
         EQUIVALENCE
                          (BUFF,KK)
5
         CHARACTER*30
                          NOME, RISP*1
6
         DATA
                          (NSK(I), I=1,10)/1,2,3,4,5,6,7,8,9,10/
7
         PRINT *,
                   'Records IBM a lunghezza variabile? (Y/N):'
8
                   RISP
         READ 10,
9
10
         PRINT *,
                   'Nome file di output:'
11
         READ 10.
                   NOME
         PRINT *, 'RECL-TAPE, NUMBER OF REC/BLOCK-TAPE, RECL-DISC'
12
         READ *,
                   LRL, NRB, MSRL
13
         FRL = NRB*LRL
14
         PRINT *, NOME, NRB, LRL, ' Block length ', FRL, MSRL
15
         OPEN( UNIT=1, NAME=NOME, STATUS='NEW', RECL=MSRL)
16
         OPEN( UNIT=4, NAME='MSAO:', STATUS='OLD', RECL=FRL)
17
         IF(RISP .EQ. 'Y') GOTO 3
18
         NR=0
19
         ISUPDO = FRL/MSRL
20
21
       1 READ(4, 10, END=99) BUFF
         CALL LIB-TRA-EBC-ASC(BUFF, BUFF)
22
         NR=NR+1
23
         PRINT*,' NR = ', NR
24
25
         N2=0
         DO 20 I=1, ISUPDO
26
         N1=N2 + 1
27
         N2=N2 + MSRL
28
      20 WRITE(1,10) BUFF(N1:N2)
29
         GOTO 1
30
       3 CONTINUE
31
32
         L1=IISHFT(KK, -8)
33
         L2=IISHFT(KK,8)
         KK=IOR(L1,L2)
34
         PRINT 11, BUFF(1:2)
35
         PRINT 11,KK
36
         PRINT 12,KK
37
      11 FORMAT(' -',a)
38
39
      12 FORMAT(' ',8z4)
     10 FORMAT(A)
40
     99 END
41
```

Appendix C

```
PROGRAM FIND
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
3
         CHARACTER*35 QID
         OPEN(UNIT=1,TYPE='NEW',FILE='SELECT.DAT')
4
         OPEN(UNIT=4,TYPE='OLD',FILE= 'FIND.INP')
5
         READ(4,*)V1,V2,ID
6
         IF(ID.EQ.0) OPEN(UNIT=2,TYPE='OLD',FILE= 'GEISA.DAT')
\overline{7}
         IF(ID.EQ.1) OPEN(UNIT=3,TYPE='OLD',FILE= 'AFGL.DAT')
8
         NNLIN=0
9
         ITOT =0
10
11
     90 FORMAT(1X,D16.8,3D11.4,I4,I8)
     100 FORMAT(1X,D16.8,3D11.4,I4,I8,I4,A35)
12
     200 FORMAT(F10.5,E10.3,F5.3,F10.3,A35,F3.2,I4,I3)
13
     110 IF(ID.EQ.0) READ(2,200) V,S,A,E,QID,AN,ISOT,II
14
         IF(ID.EQ.1) READ(3,100) V,S,A,E,II,NL,ISOT,QID
15
16
         ITOT=ITOT+1
         IF(II.LE.O) GOTO 110
17
         IF(S.LE.ODO.OR.A.LE.ODO.OR.E.LE.ODO) GOTO 110
18
         IF(V.LT.V1) GOTO 110
19
         IF(V.GT.V2) GOTO 210
20
21
         NNLIN=NNLIN+1
         WRITE(1, 90) V,S,A,E,II,NNLIN
22
         GOTO 110
23
    210 WRITE(6, '(1X, 2F12.2, 2I10)') V1, V2, NNLIN, ITOT
24
         STOP
25
26
         END
```

 $Appendix \ C$

1	PROGRA	M LIN
2	IMPLIC	IT REAL*8(A-H,O-Z)
3	COMMON	/A/ C(5000,4),MSUM,DI,WNU1A,LINE,NOLINE,LAA,IOUT,
4	*	<pre>ISUMS(11),ISUMD(5),IC(5000),SRATIO,</pre>
5	*	<pre>LINALL(7),LINAL(7),LINA(7),SMAX(7),</pre>
6	*	ISTRONG(7),SLIMS(7)
7	COMMON	/B/ MOLL(7),IWI(7),NTOTD
8	DIMENS	ION PE(7),TE(7),U(7),D(4),SLIM(7)
9	OPEN(U	NIT=2,TYPE='OLD',FILE='[.HITRAN]SELECT.DAT')
10	OPEN(U	NIT=4,TYPE='OLD',FILE= 'LIN.INP')
11	NALL=3	00000
12	READ(4	,*) IFAR,WNUA,WNUB,REG1,REG2,REG3,IP
13	READ(4	.,*) ISV,ITA,ITB,IDT
14	READ(4	.,*) NDDD,(IWI(I),I=1,7)
15	READ(4	,*) TRLIM,TRLIMS,SRATIO
16	READ(4	,*) WNU1A,WNU2B
17	READ(4	.,*) IOUT,IDI,LAA,(MOLL(I),I=1,7)
18	IF(IOU	T.NE. 0) OPEN(UNIT=3,TYPE='NEW',FILE= 'LIN.DAT')
19	IF(IFA	R.NE. 0) OPEN(UNIT=8,TYPE='NEW',FILE= 'FARWG.DAT')
20	IF(IFA	R.NE1) OPEN(UNIT=1,TYPE='NEW',FILE= 'STAT.DAT')
21	IF(IFA	R.EQ1)THEN
22		NTOTD=NDDD
23		OPEN(UNIT=3,TYPE='OLD',FILE= 'LIN.DAT')
24		GOTO 83
25		END IF
26	WRITE(6,'(1X,2F10.6,D8.1,2F8.1,5X,2I2,5X,7I3,/)')
27	*TRLIM,	TRLIMS, SRATIO, WNU1A, WNU2B, IDI, LAA, (MOLL(I), I=1,7)
28	WRITE(1,'(1X,2F10.6,D8.1,2F8.1,5X,2I2,5X,7I3,/)')
29	*TRLIM,	TRLIMS, SRATIO, WNU1A, WNU2B, IDI, LAA, (MOLL(I), I=1,7)
30	TR=DLC	G(TRLIM)
31	TRS=DL	OG(TRLIMS)
32	DI=D(I	DI)
33	DO 60	I=1,7
34	IF(MOL	L(I).GT.7) THEN
35		SLIM(I) =ODO
36		SLIMS(I)=ODO
37		GOTO 60
38		END IF
39	SLIM(I) =-3.14D0* TR*PE(I)*DSQRT(296D0/TE(I))/1D3/U(I)
40	SLIMS(I)=-3.14D0*TRS*PE(I)*DSQRT(296D0/TE(I))/1D3/U(I)
41	60 CONTIN	UE
42	WRITE(6,'(1X,7D11.4,/)')(SLIM(I),I=1,7)
43	WRITE(6,'(1X,7D11.4,/)')(SLIMS(I),I=1,7)
44	WRITE(1,'(1X,7D11.4,/)')(SLIM(I),I=1,7)
45	WRITE(1, '(1X,7D11.4,/)')(SLIMS(I),I=1,7)

```
= 0
         LINE
46
         NOLINE = 0
47
         NTOT
                  = 0
48
         NTOTA
                  = 0
49
         NTOTB
                  = 0
50
         NTOTD
                  = 0
51
                  = 0
         MSUM
52
         K = 0
53
         M = 0
54
         L = 0
55
56
         ZC=1D19/0.372195D0
     101 NTOT=NTOT+1
57
         IF(NTOT.GT.NALL) GOTO 200
58
         READ(2,'(1X,D16.8,3D11.4,I4)',ERR=200)
59
        *CC1,CC2,CC3,CC4,ICC
60
61
         IF(CC1.LE.WNU1A)
                              GOTO 101
         IF(CC1.GT.WNU2B)
                              GOTO 200
62
         DO 102 MOL=1,7
63
         IF(MOLL(MOL).EQ.ICC)
                                  GOTO 1101
64
     102 CONTINUE
65
66
         GOTO 101
   1101 NTOTA=NTOTA+1
67
         LINA(MOL)=LINA(MOL)+1
68
         IF(CC2*ZC.LT.SLIM(ICC)) GOTO 101
69
         LINAL(MOL)=LINAL(MOL)+1
70
         NTOTB=NTOTB+1
71
    310 IF(CC1.GT.WNU1A+DI) GOTO 300
72
         M=M+1
73
         IF(M.GT.5000)
                          THEN
74
         WRITE(6,*)'THE DIMENSION OF C AND IC IS TOO SMALL!'
75
                          GOTO 500
76
                           END IF
77
         IC(M)=MOL
78
         C(M,1)=CC1
79
         C(M,2)=CC2*ZC
80
         C(M,3)=CC3
81
         C(M,4)=CC4
82
         GOTO 101
83
84
     300 L=L+1
         K=INT(WNU1A+DI)
85
         IF(M.NE.O) CALL STAT(M,K,L)
86
         IF(M.EQ.0) WRITE(1,'(1X,I5)') K
87
         WNU1A=WNU1A+DI
88
         M=0
89
         GOTO 310
90
```

Appendix C

```
200 L=L+1
91
          K=INT(WNU1A+DI)
 92
93
          IF(M.NE.O) CALL STAT(M,K,L)
          IF(M.EQ.0) WRITE(1,'(1X,I5)') K
94
          M=0
95
     500 CONTINUE
 96
    1002 CONTINUE
97
          INTERV=LINE+NOLINE
98
          WRITE(1,*)
99
          WRITE(1,'(1X,1116,3X,516,3X,516)')(ISUMS(I),I=1,11),
100
         *(ISUMD(I), I=1,5), NALL, MSUM, INTERV, LINE, NOLINE
101
          WRITE(1,'(1X,6I10,/)')NTOTD,NALL,NTOTA,NTOTB,MSUM
102
          WRITE(1, '(1X,718)')(LINA(I), I=1,7)
103
          WRITE(1,*)
104
          WRITE(1, '(1X,718)')(LINAL(I), I=1,7)
105
106
          WRITE(1,*)
          WRITE(1, '(1X,7I8)')(LINALL(I), I=1,7)
107
          WRITE(1,*)
108
          WRITE(1, '(1X,718)')(ISTRONG(I), I=1,7)
109
    3000 CONTINUE
110
111
          IF(IFAR.EQ.O) GOTO 82
112
          REWIND 3
       83 CALL FAR(WNUA, WNUB, REG1, REG2, REG3, ISV, ITA, ITB, IDT, IP)
113
      82 CONTINUE
114
          DATA D/
115
116
         *1.D 0,3.D 0,5.D 0,1.D 1/
          DATA U/
117
         *1768D0,2638D-1,3467D-4,2453D-4,8851D-5,1317D-3,1671D2/
118
          DATA PE/
119
         *803D0, 506D 0, 903D-1, 525D 0, 599D 0, 520D 0, 506D0/
120
          DATA TE/
121
         *275D0, 250D 0, 225D 0, 251D 0, 258D 0, 251D 0, 250D0/
122
```

Appendix C

123	C			-C
124	С	LIN.INP		С
125	С -	-1,2230,2231,1,6.5,100,1	IFAR, WNUA, WNUB, REG1, REG2, REG3, IP	С
126	С	3,140,320,20	ISV,ITA,ITB,IDT	С
127	С	305,0,0,0,0,5,0,0	NDDD, (IWI(I),I=1,7)	С
128	С	1.,1.,0.	TRLIM, TRLIMS, SRATIO	С
129	С	600,800	WNU1A,WNU2B	С
130	С	0,1,1,0,0,0,0,5,0,0	<pre>IOUT,IDI,LAA,(MOLL(I),I=1,7)</pre>	С
131	C			С
132	С	0,0,0,0,0,0,0	IFAR,WNUA,WNUB,REG1,REG2,REG3,IP	С
133	С	0,0,0,0	ISV,ITA,ITB,IDT	С
134	С	0,0,0,0,0,0,0,0	NDDD, (IWI(I),I=1,7)	С
135	С	1,1,0	TRLIM, TRLIMS, SRATIO	С
136	С	600,800	WNU1A,WNU2B	С
137	С	1,1,1, 0,2,0,0,0,0,0	<pre>IOUT,IDI,LAA,(MOLL(I),I=1,7)</pre>	С
138	C			С
139	С	0,0,0,0,0,0,0	IFAR,WNUA,WNUB,REG1,REG2,REG3,IP	С
140	С	0,0,0,0	ISV,ITA,ITB,IDT	С
141	С	0,0,0,0,0,0,0,0	NDDD, (IWI(I),I=1,7)	С
142	С	.9999,.99,1D-5	TRLIM, TRLIMS, SRATIO	С
143	С	500,2500	WNU1A,WNU2B	С
144	С	1,1,1, 1,2,3,4,5,6,7	<pre>IOUT,IDI,LAA,(MOLL(I),I=1,7)</pre>	С
145	C			С
146	С	-1,700,720,1,6.5,20,1	IFAR,WNUA,WNUB,REG1,REG2,REG3,IP	С
147	С	5,160,300,20	ISV,ITA,ITB,IDT	С
148	С	10000,0,0,0,0,0,0,0	NDDD, (IWI(I),I=1,7)	С
149	С	0.99999,1.,0.1	TRLIM, TRLIMS, SRATIO	С
150	С	600,800	WNU1A,WNU2B	С
151	С	0,1,1,1,2,0,0,0,0,0	<pre>IOUT,IDI,LAA,(MOLL(I),I=1,7)</pre>	С
152	С			С
153	С	THIS INPUT STRUCTURE PH	RODUCES THE FAR WING DATA FILE FROM	С
154	С	THE PREVIOUSLY CREATED	LIN.DAT FILE. (H2O, CO2 ONLY)	С
155	C			-C
156		END		

1		SUBROUTINE STAT(MM,KK,LL)
2		IMPLICIT REAL*8(A-H,O-Z)
3		COMMON/A/ C(5000,4), MSUM, DI, WNU1A, LINE, NOLINE, LAA, IOUT,
4	3	<pre>ISUMS(11),ISUMD(5),IC(5000),SRATIO,</pre>
5	;	<pre>k LINALL(7),LINAL(7),LINA(7),SMAX(7),</pre>
6	;	<pre>* ISTRONG(7),SLIMS(7)</pre>
7		COMMON/B/ MOLL(7), IWI(7), NTOTD
8		DIMENSION ISEL(11), IDEL(5), LINAA(7)
9		IF(LAA.NE.O) THEN
10		DO 2000 LA=1,7
11	2000	LINAA(LA)=0
12		END IF
13		K=KK
14		M=MM
15		IU=M
16		LINE=LINE+1
17		FM=FLOAT(M)
18		FK=WNU1A
19		L=LL
20		SMA=0.
21		SMI=1000.
22		SATL=0.
23		ALMA=0.
24		ALMI=1.
25		ALAT=0.
26		EATL=0.
27		D=FK
28		DO 1 I=1,M
29		D=C(I,1)-D
30		S=C(I,2)
31		A=C(I,3)
32		E=C(I,4)
33		MOL=IC(I)
34		IF(I.EQ.1) D=DI-(C(M,1)-C(I,1))
35		IF(ALMA.GT.A) GOTO 8
36		ALMA=A
37	8	IF(ALMI.LT.A) GOTO 9
38		ALMI=A
39	9	IF(SMA.GT.S) GOTO 10
40		SMA=S
41	10	IF(SMI.LT.S) GOTO 20
42		SMI=S
43	20	SATL=SATL+S
44		ALAT=ALAT+S/A
45		EATL=EATL+E*S

```
J=1
46
         DO 11 JJ=1,10
47
         SJ=10.**(2-JJ)
48
         IF(S.GT.SJ) GOTO 12
49
      11 J=J+1
50
      12 ISEL(J)=ISEL(J) +1
51
           J=1
52
           DO 13 JJ=1,4
53
           DJ=10.**(1-JJ)
54
           IF(D.GT.DJ) GOTO 14
55
56
      13
           J=J+1
      14
           IDEL(J)=IDEL(J)+1
57
           D=C(I,1)
58
           IF(SMAX(MOL).LT.S) SMAX(MOL)=S
59
       1 CONTINUE
60
61
         ALAT=SATL/ALAT
         EATL=EATL/SATL
62
         SATL=SATL/FM
63
         IALAT=INT(ALAT*1000.)
64
         IALMA=INT(ALMA*1000.)
65
66
         IALMI=INT(ALMI*1000.)
         IEATL=INT(EATL)
67
         ISMA =INT(DLOG10(SMA)*1.D 1 + 5D-1)
68
         ISMI =INT(DLOG10(SMI)*1.D 1 + 5D-1)
69
         MSUM=MSUM+M
70
         NTOTCC=0
71
         DO 4 I=1,M
72
         S=C(I,2)
73
         MOL=IC(I)
74
         IF(S/SMAX(MOL).LE.SRATIO) GOTO 4
75
         LINAA(MOL)=LINAA(MOL)+1
76
         LINALL(MOL)=LINALL(MOL)+1
77
         NTOTCC=NTOTCC+1
78
         NTOTD=NTOTD+1
79
         NTD=NTOTD
80
         MOLI=MOLL(MOL)
81
         IF(S.LT.SLIMS(MOL)) THEN
82
         ISTRONG(MOL)=ISTRONG(MOL)+1
83
84
         NTD=-NTOTD
         END IF
85
         IF(IOUT.EQ.O) GOTO 4
86
         F=C(I,1)
87
         S=C(I,2)
88
         A=C(I,3)
89
         E=C(I,4)
90
```

 $Appendix \ C$

91		WRITE(3,'(1X,D16.8,3D11.4,I4,I8)')F,S,A,E,MOLI,NTD
92	4	CONTINUE
93		IU=M-NTOTCC
94		WRITE(1,'(1X,I5,I4,I5,I4,E10.3,I4,4I3,I4,11I3,1X,5I3,
95	;	*715)')K,IU,MSUM,M, SATL,ISMI,ISMA, IALMI,IALMA,IALAT,
96	2	<pre>*IEATL,(ISEL(I),I=1,11),(IDEL(I),I=1,5),(LINAA(I),I=1,7)</pre>
97		DO 70 I=1,5000
98		IF(I.GT. 5) GOTO 68
99		ISUMD(I)=ISUMD(I)+IDEL(I)
100		IDEL(I)=0
101	68	IF(I.GT.11) GOTO 69
102		ISUMS(I)=ISUMS(I)+ISEL(I)
103		ISEL(I)=0
104	69	C(I,1)=0.
105		C(I,2)=0.
106		C(I,3)=0.
107		C(I,4)=0.
108		IF(I.LE.7) SMAX(I)=ODO
109	70	CONTINUE
110		RETURN
111		END

Appendix C

```
SUBROUTINE FAR(A1,A2,REGA,REGB,REGC,ISV,ITA,ITB,IDT,IP)
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
         COMMON/B/ MOLL(7), IWI(7), NTOTD
3
         DIMENSION POSA(10000), STRA(10000), ALFA(10000),
\mathbf{4}
                     ENRA(10000), ISIA(10000), IQSW(10000),
        *
5
                     WING(10000), AV(7), BV(7), CV(7), AR(7),
6
        *
        *
                     AL(7),AT(7),QV(7),QR(7),SUM(7,110),II(3,7)
\overline{7}
         V1=A1
8
         V2=A2
9
10
         IST=(ITB-ITA)/IDT+1
11
         DIV=1D0/DFLOAT(ISV-1)
         REG1=REGA
12
         REG2=REGB
13
         REG3=REGC
14
         WRITE(8, '(1X, 1115)')(MOLL(I), I=1,7), ISV, ITA, ITB, IDT
15
16
         IF(IP.NE.0)
        *WRITE(6, '(1X,1115)')(MOLL(I), I=1,7), ISV, ITA, ITB, IDT
17
     207 FORMAT(1X,D16.8,3D11.4,I4,I8)
18
         DO 152 J=1,IST
19
         DO 151 L=1,7
20
21
         T=ITA+(J-1)*IDT
22
         CST1=TTT0/T
         CST2=1.43879*(T-TTT0)/T/TTT0
23
         QV(L) = AV(L) + BV(L) * CST1 * * CV(L)
24
         QR(L) = CST1 * AR(L)
25
26
     151 AT(L)=CST1**AL(L)
         IF(IP.NE.O)
27
        *WRITE(6, '(1X, 12, 4E12.4)')(L, AT(L), QV(L), QR(L), T, L=1,7)
28
     152 CONTINUE
29
         WRITE(6,*)NTOTD
30
         IFILE=0
31
32
         INXY = 0
33
         JLIN =0
34
         DO 1000 POS=V1,V2
         POS1=POS-5D-1
35
         POS2=POS+5D-1
36
         IF(IFILE.EQ.0) GOTO 250
37
         INXY=0
38
39
         DO 210 I=1,INXX
         IF(POSA(I).GE.POS1-REG3) GOTO 220
40
     210 INXY=INXY+1
41
     220 IF(INXY.EQ.0) GOTO 230
42
         DO 240 I=1, INXX-INXY
43
44
         POSA(I)=POSA(I+INXY)
45
         STRA(I)=STRA(I+INXY)
```

46		ALFA(I)=ALFA(I+INXY)
47		ENRA(I)=ENRA(I+INXY)
48		ISIA(I)=ISIA(I+INXY)
49	240	IQSW(I)=IQSW(I+INXY)
50	230	INXY=INXX-INXY
51		IF(Q1.GT.POS2+REG3) GOTO 209
52		INXY=INXY+1
53		POSA(INXY)=Q1
54		STRA(INXY)=Q2
55		ALFA(INXY)=Q3
56		ENRA(INXY)=Q4
57		ISIA(INXY)=IQ
58		IQSW(INXY)=IY
59		GOTO 251
60	250	IFILE=1
61	251	CONTINUE
62	206	IF(IY/NTOTD.NE.O) GOTO 209
63		READ(3,207) Q1,Q2,Q3,Q4,IQ,IY
64		DO 270 ISM=1,7
65		IF(IQ.NE.MOLL(ISM)) GOTO 270
66		IF(IY.GT.O) GOTO 271
67	270	CONTINUE
68		IF(Q1.GT.POS2+REG3) GOTO 209
69		GOTO 206
70	271	IF(Q1.LT.POS1-REG3) GOTO 206
71		IF(Q1.GT.POS2+REG3) GOTO 209
72		JLIN=JLIN+1
73		INXY=INXY+1
74		POSA(INXY)=Q1
75		STRA(INXY)=Q2
76		ALFA(INXY)=Q3
77		ENRA(INXY)=Q4
78		ISIA(INXY)=IQ
79		IQSW(INXY)=IY
80		GOTO 206
81	209	INXX=INXY
82		DO 138 I=1,3
83		DO 138 J=1,7
84	138	II(I,J) =0
85		DO 135 I=1,INXX
86		POL=POSA(I)
87		D3A=POS1-REG3
88		D2A=POS1-REG2
89		D1A=POS1-REG1
90		D1B=P0S2+REG1

```
D2B=POS2+REG2
91
92
          D3B=POS2+REG3
          IF(POL.GE. D3A.AND.POL.LT. D2A) II(3,1)=II(3,1)+1
93
          IF(POL.GE. D2A.AND.POL.LT. D1A) II(3,2)=II(3,2)+1
94
          IF(POL.GE. D1A.AND.POL.LT.POS1) II(3,3)=II(3,3)+1
95
          IF(POL.GE.POS1.AND.POL.LE.POS2) II(3,4)=II(3,4)+1
96
          IF(POL.GT.POS2.AND.POL.LE. D1B) II(3,5)=II(3,5)+1
97
          IF(POL.GT. D1B.AND.POL.LE. D2B) II(3,6)=II(3,6)+1
98
          IF(POL.GT. D2B.AND.POL.LE. D3B) II(3,7)=II(3,7)+1
99
100
     135 CONTINUE
101
          II(1,1)=1
          II(2,1)=II(3,1)
102
          II(1,2)=II(2,1)+1
103
          II(2,2)=II(2,1)+II(3,2)
104
          II(1,3)=II(2,2)+1
105
106
          II(2,3)=II(2,2)+II(3,3)
          II(1,4)=II(2,3)+1
107
          II(2,4)=II(2,3)+II(3,4)
108
          II(1,5)=II(2,4)+1
109
          II(2,5)=II(2,4)+II(3,5)
110
          II(1,6)=II(2,5)+1
111
          II(2,6)=II(2,5)+II(3,6)
112
          II(1,7)=II(2,6)+1
113
          II(2,7)=II(2,6)+II(3,7)
114
          IF(IP.NE.0)WRITE(6, '(1X, I4, 518)')(J,(II(I, J), I=1, 3),
115
         *IQSW(II(1,J)),IQSW(II(2,J)),J=1,7)
116
          I1REG3 =II(1,1)
117
          I2REG3 =II(2,1)
118
          J1REG3 = II(1,7)
119
          J2REG3 = II(2,7)
120
          DO 140 IV=1,ISV
121
          IX=(IV-1)*IST
122
123
          PP=POS-5D-1+(IV-1)*DIV
124
          DO 141 I=I1REG3, I2REG3
          PA = POSA(I)
125
          L = ISIA(I)
126
          IWC=IWI(L)
127
          OUT=1D0
128
129
          IF(IWC.EQ.O.OR.IWC.EQ.4.OR.IWC.EQ.7) GOTO 111
          CALL WINGS(PP,PA,ODO,IWC,OUT)
130
     111 WING(I)=PI*(PA-PP)*(PA-PP)/OUT
131
     141 CONTINUE
132
          DO 142 I=J1REG3, J2REG3
133
          PA =POSA(I)
134
          L = ISIA(I)
135
```

Appendix C

```
136
          IWC=IWI(L)
137
          OUT=1D0
          IF(IWC.EQ.O.OR.IWC.EQ.4.OR.IWC.EQ.7) GOTO 112
138
          CALL WINGS(PP,PA,ODO,IWC,OUT)
139
      112 WING(I)=PI*(PA-PP)*(PA-PP)/OUT
140
      142 CONTINUE
141
          DO 144 J=1,IST
142
          DO 149 L=1,7
143
      149 SUM(L,IX+J)=0D0
144
          Т
              =ITA+(J-1)*IDT
145
146
          CST1=TTT0/T
          CST2=1.43879*(T-TTT0)/T/TTT0
147
          DO 153 L=1,7
148
          QV(L) = AV(L) + BV(L) * CST1 * * CV(L)
149
          QR(L) = CST1 * AR(L)
150
151
          AT(L) = CST1 * AL(L)
      153 CONTINUE
152
          DO 145 I=I1REG3, I2REG3
153
          L = ISIA(I)
154
          WIN=WING(I)
155
          IWC=IWI(L)
156
          IF(IWC.EQ.0) GOTO 113
157
          IF(IWC.EQ.4.OR.IWC.EQ.7) THEN
158
          PA=POSA(I)
159
          CALL WINGS(PP,PA,T,IWC,OUT)
160
          WIN=WIN/OUT
161
          END IF
162
      113 IF(WIN.LT.ODO) GOTO 145
163
          SUM(L,IX+J)=SUM(L,IX+J)+ALFA(I)*AT(L)*
164
         *STRA(I)*QV(L)*QR(L)*DEXP(ENRA(I)*CST2)/WIN
165
      145 CONTINUE
166
          DO 146 I=J1REG3, J2REG3
167
168
          L=ISIA(I)
169
          WIN=WING(I)
          IWC=IWI(L)
170
          IF(IWC.EQ.0) GOTO 114
171
          IF(IWC.EQ.4.OR.IWC.EQ.7) THEN
172
          PA=POSA(I)
173
174
          CALL WINGS(PP,PA,T,IWC,OUT)
          WIN=WIN/OUT
175
          END IF
176
      114 IF(WIN.LT.O) GOTO 146
177
          SUM(L, IX+J) = SUM(L, IX+J) + ALFA(I) * AT(L) *
178
179
         *STRA(I)*QV(L)*QR(L)*DEXP(ENRA(I)*CST2)/WIN
      146 CONTINUE
180
```

```
144 CONTINUE
181
     140 CONTINUE
182
183
          IF(IP.EQ.0) GOTO 900
          WRITE(6, '(1X, F10.1)') POS
184
          DO 147 L=1,7
185
          IF(MOLL(L).EQ.0) GOTO 147
186
          DO 147 IV=1,ISV
187
          IX=(IV-1)*IST
188
          WRITE(6, '(1X, 10F7.6)') (SUM(L, IX+J), J=1, IST)
189
190
     147 CONTINUE
     900 WRITE(8,'(1X,F10.1)') POS
191
          DO 148 L=1,7
192
          IF(MOLL(L).EQ.0) GOTO 148
193
          DO 148 IV=1,ISV
194
          IX=(IV-1)*IST
195
196
          WRITE(8, '(1X, 10E11.4)')(SUM(L, IX+J), J=1, IST)
197
     148 CONTINUE
    1000 CONTINUE
198
          DATA TTTO, PI/296D0,3.14159265D0/
199
          DATA AV, BV, CV/
200
201
         *1D0,.99752D0,.99852D0,1.01819D0,1D0,.99935D0,1D0,
         *0D0,.09310D0,.04600D0, .12700D0,0D0,.00700D0,0D0,
202
         *0D0,-3.54915D0,-4.11179D0,-4.42836D0,0D0,-5.47575D0,0D0/
203
          DATA AR/1.5D0,1.0D0,1.5D0,1.0D0,1.0D0,1.5D0,1.0D0/
204
          DATA AL/0.5D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0,0.5D0/
205
          RETURN
206
          END
207
```

Appendix C

1		SUBROUTINE WINGS(VA,VB,TA,IC,OUT)
2		IMPLICIT REAL*8(A-H,O-Z)
3		DV=DABS(VA-VB)
4		GOTO(10,20,30,40,50,60,70),IC
5	10	IF(DV.GT.3.5D0) GOTO 11
6		OUT=1D0
7		RETURN
8	11	OUT=DEXP(-1.4D0*(DV-3.5D0)**0.25D0)
9		RETURN
10	20	IF(DV.GE.5D-1) GOTO 21
11		OUT=1D0
12		RETURN
13	21	IF(DV.GE.23D0) GOTO 22
14		OUT=1.069*DEXP(-0.133*DV)
15		RETURN
16	22	IF(DV.GE.50D0) GOTO 23
17		OUT=5D-2
18		RETURN
19	23	IF(DV.GE.25D1) GOTO 24
20		OUT=0.133D0*DEXP(-0.0196*DV)
21		RETURN
22	24	OUT=-1D0
23		RETURN
24	30	IF(DV.GE.11DO) GOTO 31
25		OUT=(1D0+2D0*DV/11D0)*DEXP(-2D0*DV/11D0)
26		RETURN
27	31	OUT=-1D0
28		RETURN
29	40	DW=VA+VB
30		DEA=1D0-DEXP(-1.43879D0*VA/TA)
31		DEB=1D0-DEXP(-1.43879D0*VB/TA)
32		OUT=VA*DEA*(1D0+DV*DV/DW/DW)/VB/DEB
33		RETURN
34	50	DW=VA+VB
35		OUT=VA*VA*(1DO+DV*DV/DW/DW)/VB/VB
36		RETURN
37	60	DW=VA+VB
38		OUT=VA*(1DO+DV*DV/DW/DW)/VB
39		RETURN
40	70	OUT=2D0*VA/(1D0+DEXP(-1.43879*DV/TA))/VB
41		RETURN
42		END

APPENDIX D

Listing of the HART Programme

HART LAYERS MINT LENGTH MESH CONT FARWG GAUSS SHAPE VOIGTY VOIGTD WING

Appendix D

1	PROGRAM HART
2	IMPLICIT REAL*8(A-H,O-Z)
3	COMMON/GA/ IPRE,IGNU,EPSN,ERG,ERGB,ITY,IGS,IGI,OUTGS,
4	* NG,OUTSS(14000),H2OC,OFWG,LS1,LS2,ITRN,JSWS
5	COMMON/SH/ IPRF,REGO,IINT,DVPR,PDLR,PLNZ,VDLR,VLNZ,TAV,
6	<pre>* PAV,ALOR(10),AKO(10),XS(10),KSHP,IVDY,</pre>
7	<pre>* LMOD(7),RMOD(7)</pre>
8	COMMON/HA/ POSA(3000),STRA(3000),ENRA(3000),ALFA(3000),
9	*ALFT(3000),CPLG(3000),STRT(3000),ISIA(3000),IQSW(3000)
10	COMMON/LE/ IPRC, IPRG, IWA1, IWB1, AA, BB, ITT, JUMP, IG, IALL,
11	* DZ, AEP(21), ALEN(20), ALENS(20), NLEN, DR, D1,
12	<pre>* KSUB,IALP,ALP,IQQ,IGA(1400),AGA(1400),</pre>
13	* ITYPE(1400)
14	COMMON/CO/ IPRD,ICT,CV(69),CD(3,69),CT(3),SUMH
15	COMMON/FA/ MOLL(7),AMASS(10),IFAR,OFWGS,IVI(7)
16	COMMON/LA/ IPRB,ALT(150),DEY(150),PSTND,TSTND,BMY(150),
17	* CHY(150),TLY(150),PLY(150),AMIY(37,150)
18	DIMENSION
19	<pre>*IIII(3,5),TRABS(150),AMOLE(10),ALORO(10),ALORT(10),</pre>
20	*MOLE(10),SHIFT(10),IBLW(200),IWARN(200),IENDPT(200),
21	*TRAB(200),TRAB1(200),SUMM(200),PLX(150),TLX(150),
22	*AMIX(37,150),CST1(150),CST2(150),TDOPA(150),POS(500),
23	*ISI(500),VPFN(3,7),CS1(7),RPFN(7),DVP(7),VPR(7),
24	*CHX(150),DEX(150),AMIT(150),ADOP(10),UMOD(7),SMOD(7),
25	*AMOD(7),WNBC(10),DWNB(10),NLINE(10),SINT(10),GSEN(10),
26	*PLZ(3000),BMZ(3000),CHZ(3000),TLZ(3000),ALZ(3000),
27	*DEZ(3000),AMZ(3000),TETM(31)
28	EQUIVALENCE
29	*(POSA,PLZ),(STRA,BMZ),(ENRA,TLZ),(ALFA,CHZ),
30	*(ALFT,ALZ),(CPLG,DEZ),(STRT,AMZ)
31 C	
32 C	FIRST SECTION: INPUTS
33 C	
34	UPEN(UNII=9,IYPE='ULD',FILE= 'HARI.INP')
35	READ (9,*) REAL, DELV, IIRN, IRAD, IUIR, IURD, IUPR
36	READ (9,*) IPRA, IPRB, IPRC, IPRD, IPRE, IPRF, IPRG, IPRH
37	$\begin{array}{c} \text{READ} (9,*) \text{ISBN, IGNU, EPSN, ICCH,} \\ \\ \text{(DDD D DINZ VDD D VINZ I-1 ICCU)} \end{array}$
38	$ \begin{array}{c} * \qquad (PDLR, PLNZ, VDLR, VLNZ, I-I, ICCH) \\ PEAD(0, *) \qquad TINT AINT TUDE TDDE KGUD TUDV \\ \end{array} $
39 40	$\frac{1}{2} = \frac{1}{2} = \frac{1}$
40	READ $(9,*)$ MODL, (IDEN, EMOD(IDEN), I-I, MODL) READ $(9,*)$ MODA (IDEN AMOD(IDEN) I-1 MODA)
40	$\mathbf{READ} (\mathbf{\mathcal{F}}, \mathbf{\mathcal{F}}) \mathbf{RODA}, (\mathbf{IDEN}, \mathbf{AROD} (\mathbf{IDEN}), \mathbf{I} = \mathbf{I}, \mathbf{RODA})$
42 13	READ $(9, *)$ MODE (IDEN, SHOD(IDEN), I=1, HODS) READ $(9, *)$ MODE (IDEN RMOD(IDEN) I=1 MODE)
-1J 14	RFAD (9 *) WNII1 WNII2 REGO REG1 REG2
44 45	READ (9 *) TPSC THOM TARM ASCI
40 0	

46	WED = (WNU1 + WNU2)/2
47	JSWS = 1
48	IF(IPSC.EQ.0)THEN
49	READ (9,*) LVEL,NBND,(MOLE(I),I=1,NBND)
50	<pre>READ (9,*)(PLX(I),TLX(I),(AMIX(MOLE(J),I),</pre>
51	* J=1,NBND),I=1,LVEL)
52	GOTO 137
53	END IF
54	IF(IPSC.EQ.4)GOTO 10
55	READ (9,*)PPP1,PPP2,PPPD,TT1,TT2,TTD
56	READ (9,*)NBND,(MOLE(I),AMASS(I),I=1,NBND)
57	GOTO 137
58	10 READ (9,*) IPOF,LVEL,NBND,(MOLE(I),I=1,NBND)
59	READ (9,*) LVL1,LVL2,TSKN,EMIS
60	READ (9,*) IDIR,TETA,TETB,DTET
61	READ (9,*) LVEN,ALT1,ALT2,PATH
62	READ (9,*) MODU, (IDEN, UMOD(IDEN), I=1, MODU)
63	IF(IPOF.EQ.O)THEN
64	OPEN(UNIT= 1,TYPE='OLD',FILE='PROFIL.DAT')
65	READ(1,*)(ALT(I),PLY(I),TLY(I),DEY(I),
66	* (AMIY(J,I),J=1,7),I=1,LVEL)
67	END IF
68	IF(IPOF.NE.O)THEN
69	OPEN(UNIT= 3,TYPE='OLD',FILE='MODATM.DAT')
70	DO 36 K=1,6
71	IF(K.EQ.IPOF) READ(3,*)(ALT(1),PLY(1),
72	* $TLY(1), DEY(1), (AMIY(J,1), J=1, (), I=1, LVEL)$
73	IF(K.NE.IPUF) READ(3,*)(DUM,DUM,DUM,
74	* (DUM, J=1, /), I=1, LVEL)
75	$30 \qquad \qquad$
76	READ(3, (IX, 2EII.4))((DOM, AMIY(J, I), I=I, UVEI) = 1,
77	* $LVEL$, J=0, 3() TE(TDDA EQ 2) UDTTE(6 2(1X TA E11 A 2X
78	IF(IFRA.EQ2) WRIIE(0, (IA, I4, EII.4, 2A, EII.4)) ((IA, IT(I) AMIV(MOLE(I) I) I-1))
79 80	
8U 01	TE LVEL, J-I, NDND/
81 81	LND IF 137 READ (Q *) TIIN TIIM TOON TEAR IREE
02 92	TE(TITN EO 1)THEN
84	$\frac{11}{111111111111111111111111111111111$
85	* SHIFT(I) SINT(I) GSEN(I) I=1 NBND)
86	END IF
87	TF(TI,TN,EQ,2) OPEN(UNIT= 2, TYPE='OLD' FILE= 'LTN DAT')
88	IF(ICON.EQ.1)OPEN(UNIT= 7.TYPE='OLD'.FILE= 'CONT.DAT')
89	IF(IFAR.EQ.1)OPEN(UNIT= 8.TYPE='OLD'.FILE='FARWG.DAT')
90	IF(IOPR.NE.O)OPEN(UNIT=12, TYPE='NEW', FILE='PRNEW.DAT')

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IF(IOTR.EQ.1)OPEN(UNIT=10, TYPE='NEW', FILE= 'TRAO.DAT') 91IF (IORD.EQ.1) OPEN (UNIT=11, TYPE='NEW', FILE= 'RAD.DAT') 92IF(ICON.EQ.1)READ(7,*) (CV(I),(CD(J,I),J=1,3),I=1,69) 93 _____ 94 C-95 C LAYERING 96 C-_____ IF(IPSC.NE.4) GOTO 139 97 RR3 = DEY(LVEL)98 PRMI=1D3 99 100 PRMA=0D0 101 DO 235 L=1,LVEL IF(PLY(L).LT.PRMI) PRMI=PLY(L) 102IF(PLY(L).GT.PRMA) PRMA=PLY(L) 103 CHY(L) = BOLTZ * DEY(L) * AMIY(1,L) * TLY(L) / 1D2104 235 CONTINUE 105106 IF(IPRA.EQ.-2)WRITE(6,'(3X,1HL,5X,3HALT,8X,3HCHY,8X, *3HDEY,8X,3HTLY,/,/(I4,4D11.4))')(L,ALT(L),CHY(L), 107 *DEY(L),TLY(L),L=1,LVEL) 108 109 C----IF(IDIR.EQ.O) THEN 110 CALL MINT (ALT, PLY, 1, LVEL, I, ALT1, PLX(1), IPRB) 111 CALL MINT (ALT, TLY, 3, LVEL, I, ALT1, TLX(1), IPRB) 112CALL MINT (ALT, CHY, 3, LVEL, I, ALT1, CHX(1), IPRB) 113 CALL MINT (ALT, DEY, 1, LVEL, I, ALT1, DEX(1), IPRB) 114DO 179 J=1,NBND 115K=MOLE(J)116DO 177 L=1,LVEL 117177 AMIT(L) = AMIY(K,L)118CALL MINT(ALT, AMIT, 3, LVEL, I, ALT1, AMIX(K, 1), IPRB) 119AMIX(K,1)=DEX(1)*UNIV 120179 AMASS(K)=AMIX(K,1)*PATH 121LVEL=1 122123BMY(1)=1D0124IHOM=0 IPSC=0 125WRITE(6,'(/,1X,14HSHORT PATH AT ,F5.2,11HKM ALTITUDE, 126*/,/,7HTEMP = ,F5.2,8HPRES. = ,F5.2,/,/2X,11HABSORBERS: , 127 *7F8.3,/)')ALT1,TLX(1),PLX(1),(AMASS(M),M=1,NBND) 128129GOTO 49 END IF 130131 C-----LPLUS=0 132IF(LVL1.EQ.0) THEN 133DO 192 I=1,LVEL-1 134IF(ALT1.GT.ALT(I+1)) GOTO 191 135

136	192	CONTINUE
137	191	CALL MINT (ALT, PLY, 1, LVEL, I, ALT1, PLY(I), IPRB)
138		CALL MINT (ALT, DEY, 1, LVEL, I, ALT1, DEY(I), IPRB)
139		CALL MINT (ALT,TLY,2,LVEL,I,ALT1,TLY(I),IPRB)
140		CALL MINT (ALT,CHY,2,LVEL,I,ALT1,CHY(I),IPRB)
141		DO 190 J=1,NBND
142		K=MOLE(J)
143		DO 171 L=1,LVEL
144	171	AMIT(L) = AMIY(K,L)
145	190	CALL MINT(ALT,AMIT,2,LVEL,I,ALT1,AMIY(K,I),IPRA)
146		ALT(I)=ALT1
147		LVL1=I
148		LPLUS=I-1
149		WRITE(6,*)'NEW LVL1 LPLUS AND ALT1 : ',
150	*	LVL1,LPLUS,ALT1
151		END IF
152	IF(]	LVL2.EQ.O) THEN
153		DO 182 I=1,LVEL-1
154		IF(ALT2.GE.ALT(I+1)) GOTO 181
155	182	CONTINUE
156		I = I - 1
157	181	CALL MINT(ALT,PLY,1,LVEL,I,ALT2,PLY(I+1),IPRB)
158		CALL MINT(ALT,DEY,1,LVEL,I,ALT2,DEY(I+1),IPRB)
159		CALL MINT(ALT,TLY,2,LVEL,I,ALT2,TLY(I+1),IPRB)
160		CALL MINT(ALT,CHY,2,LVEL,I,ALT2,CHY(I+1),IPRB)
161		DO 180 J=1,NBND
162		K=MOLE(J)
163		DO 172 L=1,LVEL
164	172	AMIT(L) = AMIY(K,L)
165	180	CALL MINT(ALT,AMIT,2,LVEL,I,ALT2,AMIY(K,I+1),IPRA)
166		ALT(I+1)=ALT2
167		LVL2=I+1
168		WRITE(6,*)'NEW LVL2 AND ALT2 : ',LVL2,ALT2
169		END IF
170	164 IF()	LVEN.GT.2) THEN
171	DSC	=(ALT1-ALT2)/(LVEN-1)
172	DO	197 I=1,LVEN
173	IF()	ASCL.LT.0) ALZ(LVEN-I+1)=ALT2+(ALT1-ALT2)*
174	*(DE)	XP(-ASCL*DSC*(I-1)/(ALT1-ALT2))-1)/(DEXP(-ASCL)-1)
175	IF()	ASCL.GT.0) ALZ(LVEN-I+1)=ALT2+(ALT1-ALT2)*
176	*(DS)	C*(I-1)/(ALT1-ALT2))**ASCL
177	IF(ASCL.EQ.0) ALZ(LVEN-I+1)=ALT2+(ALT1-ALT2)*
178	*DSC	*(1-1)/(ALT1-ALT2)
179	197 CON	TINUE
180	DO	196 I = 1, LVEN

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```
DO 195 J = LVL1, LVL2-1
181
          IF(ALT(J+1).LE.ALZ(I))GOTO 194
182
183
      195 CONTINUE
          J = J - 1
184
      194 CONTINUE
185
          CALL MINT(ALT, PLY, 1, LVEL, J, ALZ(I), PLZ(I), IPRB)
186
          CALL MINT(ALT, DEY, 1, LVEL, J, ALZ(I), DEZ(I), IPRB)
187
          CALL MINT(ALT,TLY,2,LVEL,J,ALZ(I),TLZ(I),IPRB)
188
          CALL MINT(ALT, CHY, 2, LVEL, J, ALZ(I), CHZ(I), IPRB)
189
          DO 173 K=1,NBND
190
191
          M=MOLE(K)
192
          DO 178 L=1,LVEL
      178 AMIT(L)=AMIY(M,L)
193
          CALL MINT(ALT, AMIT, 2, LVEL, J, ALZ(I), AMZ(I), IPRB)
194
          IF(DTET.EQ.ODO)AMIX(M,I)=AMZ(I)
195
196
          IF(DTET.NE.ODO.AND.M.EQ.IABS(IARM))
         *DEZ(I)=DEZ(I)*AMZ(I)*UNIV
197
      173 CONTINUE
198
      196 CONTINUE
199
          LVEL=LVEN
200
201
          LVL1=1
202
          LVL2=LVEL
          LAYER=LVEL-1
203
          END IF
204
205 C----
206
          IF(LVEN.LE.O) THEN
          LVEL=LVL2-LVL1+1
207
208
          LAYER=LVEL-1
          DO 175 L=1,LVEL
209
          ALZ(L) = ALT(LVL1+L-1)
210
          PLZ(L)=PLY(LVL1+L-1)
211
212
          TLZ(L) = TLY(LVL1+L-1)
213
          CHZ(L) = CHY(LVL1+L-1)
214
          DEZ(L) = DEY(LVL1+L-1)
          IF(IARM.NE.O.AND.DTET.NE.ODO)
215
         *DEZ(L)=DEZ(L)*AMIY(IABS(IARM),LVL1+L-1)*UNIV
216
          DO 175 J=1,NBND
217
          AMIX(MOLE(J),L)=AMIY(MOLE(J),LVL1+L-1)
218
219
    175
          CONTINUE
          END IF
220
          IF(IPRA.EQ.1) WRITE(6, '(/,1X,7HLVL1 = ,I3,3X,7HLVL2 = ,
221
         *I3,3X,7HLVEL = ,I3,3X,7HLVEN = ,I3,/,/,2X1HL,7X,3HALZ,
222
         *8X, 3HPLZ, 8X, 3HTLZ, 8X, 3HDEZ, 8X, 3HCHZ, /, /, (1X, I4, 1X,
223
224
         *6E11.4))')LVL1,LVL2,LVEL,LVEN,(L,ALZ(L),PLZ(L),TLZ(L),
         *DEZ(L),CHZ(L),AMZ(L),L=1,LVEL)
225
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Appendix D

226	C	
227	С	SECOND SECTION
228	C	
229		LIMB = 0
230		IF(IPSC.EQ.4.AND.IHOM.EQ.1) JSWS=2
231		WEDD = WED*WED
232		IF (IPSU.NE.4) GUIU 139
233		IF(IPRB.EQ.I) WRITE(6, (/, 3X, 4HIEIA, /X, 5HALFAI, 4X,
234		CALL LAVEDC (UEDD IDEE IDID TETA LUEL ALTO LIMD LUEN)
235		CALL LAIERS (WEDD, JREF, IDIR, IEIA, LVEL, ALIZ, LIMB, LVEN)
236		IF(DIEI.EQ.ODO)WRIIE(0, (IX, / HLIMD - , 15, 4X, / HALII - , 15, 4X, / HALIII - , 15, 4X, / HALII - , 15
231		FI0.0, 4x, MALIZ = FI0.0, 4x, MLVEN = FI0, FID, F
200 220		TE(ITMB EO 1 AND IVEN IT O) THEN
239		AIT1=AIT(IVI1)
240 241		$\Delta I T^2 = \Delta I T (I V FI)$
241		I VEN=-I VEN
243		I.VEL=I.AYER+1
244		GOTO 164
245		END TF
246		IF(DTET.EQ.0) GOTO 176
247		IF(DTET.LT.O) THEN
248		DO 165 I=1,31
249		TET=TETM(I)
250		CALL LAYERS(WEDD, JREF, IDIR, TET, LVEL, ZNEW, LIMB, LVEN)
251	165	CONTINUE
252		GOTO 1000
253		END IF
254		DO 198 TET=TETA+DTET,TETB,DTET
255		CALL LAYERS(WEDD, JREF, IDIR, TET, LVEL, ZNEW, LIMB, LVEN)
256	198	CONTINUE
257		GDTO 1000
258	176	CONTINUE
259		IF(LIMB.EQ.1) THEN
260		DO 151 M=1,NBND
261		K=MOLE(M)
262		DO 152 L=1,LAYER+1
263	152	AMIT(L)=AMIY(K,L)
264		
265	151	CALL MINT(ALT, AMIT, 2, LAYER+1, LOD, ALT2, AMIY(K, LVEL), IPRB)
266		END IF
267		DU 161 LL=1,LVEL
268		
269		
270		PLI(V) = PLI(V)

```
ALT(K) = ALZ(K)
271
272
          PLY(K) = PLZ(K)
273
          TLY(K) = TLZ(K)
          DEY(K) = DEZ(K)
274
          CHY(K) = CHZ(K)
275
276
          DO 162 M=1,NBND
          IF(LL.GE.2.OR.LIMB.EQ.O) AMIY(MOLE(M),K)=AMIX(MOLE(M),K)
277
      162 CONTINUE
278
          IF(LIMB.EQ.0) GOTO 161
279
          BMY(L) = BMZ(K)
280
281
          ALT(L) = ALZ(K)
          PLY(L) = PLZ(K)
282
          TLY(L) = TLZ(K)
283
          DEY(L) = DEZ(K)
284
          CHY(L) = CHZ(K)
285
286
          DO 163 M=1,NBND
          IF(LL.GE.2) AMIY(MOLE(M),L) = AMIX(MOLE(M),K)
287
      163 CONTINUE
288
      161 CONTINUE
289
          IF(LIMB.EQ.1) THEN
290
291
          LVEL=2*LVEL-1
292
          LAYER=LVEL-1
          END IF
293
          IF(IOPR.NE.O) THEN
294
          DO 150 I=1,LVEL
295
      150 WRITE(12, '(1X, 11E11.4)')
296
         *ALT(I), PLY(I), TLY(I), DEY(I), (AMIY(MOLE(J), I), J=1, NBND)
297
          END IF
298
          IF(IPRA.EQ.1)WRITE(6,'(/,1X,7HLVEL = ,15,5X,3H***,/,/,
299
         *3X, HL, 6X, 3HALT, 9X, 3HPLY, 9X, 3HTLY, 9X, 3HDEY, 9X, 3HCHY, 9X,
300
         *3HBMY,/,/,(1X,I3,6D12.4))')LVEL,(L,ALT(L),PLY(L),TLY(L),
301
         *DEY(L),CHY(L),BMY(L),L=1,LVEL)
302
303
          IF(IOPR.EQ.-1) GOTO 1000
304 C----
          DO 34 I=1,NBND
305
          MOO=MOLE(I)
306
          IF(IPRA.EQ.3) WRITE(6, '(/,3X,3HALT,5X,8HPRESSURE,5X,
307
         *4HTEMP,5X,3HPEF,5X,3HTEF,5X,1HU,5X,4HUSUM,/,/)')
308
309
          UUU=0D0
          TFF=0D0
310
          PFF=0D0
311
          IBM=0
312
          DO 34 J=1,LAYER
313
          IF(BMZ(J).LT.DZ) IBM=1
314
          PAV = (PLY(J) + PLY(J+1))/2D0
315
```

Appendix D

```
TAV = (TLY(J) + TLY(J+1))/2D0
316
         DAV=(DEY(J)+DEY(J+1))/2D0
317
         AXA=(AMIY(MOO,J)+AMIY(MOO,J+1))/2D0
318
         USU=AXA*DAV*UNIV*DABS(ALT(J)-ALT(J+1))
319
         UUU=UUU+USU
320
         IF(IHOM.EQ.1) THEN
321
                        IF(I.EQ.NBND)
                                        PLX(J)=PAV
322
                        IF(I.EQ.NBND)
                                        TLX(J)=TAV
323
                AMIX(MOO,J)=USU
324
325
                BMY(J)=BMY(J+IBM)
326
                        END IF
         IF(IHOM.EQ.2) THEN
327
                        PLX(J)=(TFF*UUU+TAV*USU)/(USU+UUU)
328
                        TLX(J) = (PFF*UUU+PAV*USU) / (USU+UUU)
329
                        TFF=TLX(J)
330
331
                        PFF=PLX(J)
                AMIX(MOO,J)=UUU
332
                END IF
333
334 CB----
         IF(IPRA.EQ.3) WRITE(6, '(1X, I3, 6D12.4)')
335
336
        *J,ALT(J),PLX(J),TLX(J),USU,UUU,BMY(J)
      34 CONTINUE
337
         IF(ICON.EQ.1) THEN
338
                  DO 234 L=1,LAYER
339
                  DEX(L) = (DEY(L) + DEY(L+1))/2D0
340
     234
                  CHX(L) = DEX(L) * (AMIY(1,L) + AMIY(1,L+1)) * 5D-7
341
                  END IF
342
         IF(IPRA.EQ.1) WRITE(6, '(/,1X,6HRR3 = ,2X,D15.5,/,/,
343
        *(2X, I5, 3D15.5))') RR3, (L, CHX(L), CHY(L), DEX(L), L=1, LVEL)
344
345 C-----
         GOTO 39
346
347 C-----
                                       _____
348 C
                      END OF LAYERING
349 C-----
                         ------
     139 IF(IPSC.GT.O.AND.IPSC.LT.4) THEN
350
         IPPH=0
351
         LY=0
352
         LSUB=51
353
354
         IPPJ=0
         IPPK=8
355
         IF(IPSC.EQ.3) PSCALE=(DLOG10(PPP1)-DLOG10(PPP2))/PPPD
356
      18 GOTO(21,22,23) ,IPSC
357
      21 PPP=PPP1-PPPD*IPPJ
358
         IF(PPP-PPP2.LT.-DZ) GOTO 41
359
         IPPJ=IPPJ+1
360
```

```
GOTO 40
361
       22 PPP=PPP1*(9-IPPK)/1.D 1**IPPJ
362
363
          IF(PPP-PPP2.LT.-DZ) GOTO 41
          IPPK=IPPK+1
364
          IF(IPPK.GE.9) THEN
365
          IPPK=0
366
          IPPJ=IPPJ+1
367
          END IF
368
          GOTO 40
369
370
       23 PPP=PPP1*1.D 1**(-PSCALE*DFLOAT(IPPJ))
371
          IF(PPP-PPP2.LT.-DZ) GOTO 41
          IPPJ=IPPJ+1
372
373 C-----
       40 ITTJ=0
374
       19 TTT=TTT1+TTTD*ITTJ
375
          IF(TTT.GT.TTT2) GOTO 18
376
          ITTJ=ITTJ+1
377
          LY=LY+1
378
          LSUB=LSUB-1
379
          PLX(LSUB)=PPP
380
          TLX(LSUB)=TTT
381
          DO 13 I=1,NBND
382
       13 AMIX(MOLE(I),LSUB)=AMASS(I)
383
          GOTO 19
384
       41 DO 45 I=1,LY
385
          PLX(I)=PLX(LSUB+I-1)
386
          TLX(I)=TLX(LSUB+I-1)
387
388
          DO 45 J=1,NBND
       45 AMIX(MOLE(J),I)=AMIX(MOLE(J),LSUB+I-1)
389
          LVEL=LY
390
          END IF
391
392 C----
393
       39 CONTINUE
394
          DO 174 I=1,NBND
      174 MOLL(MOLE(I))=MOLE(I)
395
       49 IHOMH=0
396
          IF(IHOM.NE.O) IHOMH=1
397
398 CA----
399
          IF(IPRA.EQ.1) THEN
          WRITE(6,'(3(/,1X,I2,3X),F7.2,/)')
400
         *(I,MOLE(I),MOLL(MOLE(I)),UMOD(MOLE(I)),I=1,NBND)
401
          WRITE(6, '(/,1X,1415,/,/)') IPOF, LAYER, NBND, LY, LSUB, IPSC,
402
         *IHOM, (MOLE(I), I=1, NBND)
403
          DO 42 I=1,LVEL-IHOMH
404
          IF(IPSC.EQ.4)WRITE(6,'(1X,I3,11D11.4)')I,ALT(I),PLX(I),
405
```

```
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```

```
*TLX(I),DEY(I),BMY(I),(AMIX(MOLE(J),I),J=1,NBND)
406
          IF(IPSC.NE.4)WRITE(6,'(1X,I5, 9D11.4)')I,PLX(I),TLX(I),
407
        *(AMIX(MOLE(J),I),J=1,NBND)
408
      42 CONTINUE
409
          END IF
410
411 C----
          DO 33 I=1,LVEL-IHOMH
412
          IF(IPSC.NE.4) BMY(I)=1D0
413
          TDOPA(I)=C3*DSQRT(TLX(I))
414
          CST1(I) = TTTO/TLX(I)
415
          CST2(I) = 1.439*(TLX(I)-TTTO)/TTTO/TLX(I)
416
      33 CONTINUE
417
418 CA---
          IF(IPRA.EQ.1)WRITE(6,'(/,8X,5HTDOPA,17X,4HCST1,17X,
419
        *4HCST2,/,/,(1X,3D20.10))')(TDOPA(I),CST1(I),CST2(I),
420
421
        *I=1,LVEL-IHOMH)
422 C----
423
     199 GOTO(101,102),ILIN
     102 IFILE=1
424
          INXY =0
425
          JLIN =0
426
         MAINXX=0
427
428 C----
     101 CONTINUE
429
430
          IF(IFAR.EQ.1) CALL FARWG(WNU1,0D0,0D0,0FWG,IPRD)
          IF(WED.GT. ODO.AND.WED.LT.50D0) SCLL=1D2
431
          IF(WED.GT. 50D0.AND.WED.LT.500D0) SCLL=1D1
432
433
          IF(WED.GT. 500D0.AND.WED.LT.5000D0) SCLL=1D0
          IF(WED.GT. 5000D0.AND.WED.LT.20000D0) SCLL=1D-1
434
          IF(PRMI.GT.1D2) SCLL=SCLL/5D0
435
          WRITE(6, '(/,1X,7HSCLL = ,F7.2,/)') SCLL
436
         DO 143 I=1,21
437
     143 AEP(I)=AEP(I)/SCLL
438
439
          SUMA=0D0
440
          DO 144 I=1,NLEN
          ALEN(I) = AEP(I+1) - AEP(I)
441
          SUMA=SUMA+ALEN(I)
442
     144 ALENS(I)=SUMA
443
444
          DO 145 I=1,7
     145 RMOD(I)=RMOD(I)*REG2
445
446
          SLOG2=DSQRT(DLOG(2D0))
          SLOG2P=DSQRT(DLOG(2D0)/PI)
447
          SQTTTO=DSQRT(TTTO)
448
          DR
               = RESL
449
          IIR = INT(DELV/DR+DR)
450
```

```
IF(IIR.GT.200) THEN
451
         WRITE(6,*)'REDUCE THE SIZE OF THE WNU. STEP (DELV)'
452
         GOTO 1000
453
         END IF
454
         IWNU=0
455
456 C
       END OF THE SECOND SECTION - WAVE NUMBER LOOP BEGINS
457
   С
458 C-----
                                _____
      17 POS1 = WNU1 + DFLOAT(IWNU)-DELV/2D0
459
         POS2 = POS1 + DELV
460
461
         WNUAV= (POS1+POS2)/2D0
         IF(POS2-WNU2-DELV/2D0.GT.DZ) GOTO 504
462
         IWNU = IWNU+1
463
         ICT=1
464
         IF(IFAR.EQ.2) CALL FARWG(WNUAV,ODO,ODO,OFWG,IPRD)
465
466
         GOTO( 99,91),ILIN
      91 GOTO(250,92), IFILE
467
      92 INXY=0
468
         DO 210 I=1,INXX
469
         IF(POSA(I).GE.POS1-REG2) GOTO 220
470
     210 INXY=INXY+1
471
472
     220 IF(INXY.EQ.0) GOTO 230
         DO 240 I=1, INXX-INXY
473
474
         POSA(I)=POSA(I+INXY)
         STRA(I)=STRA(I+INXY)
475
         ALFA(I)=ALFA(I+INXY)
476
         ENRA(I)=ENRA(I+INXY)
477
478
         ISIA(I)=ISIA(I+INXY)
479
         IQSW(I)=IQSW(I+INXY)
         IF(I.EQ.1)WRITE(6, '(1X, 3I6, 12X, I6, D16.8)')
480
        *INXX,INXY,I,IQSW(I),POSA(I)
481
     240 CONTINUE
482
     230 INXY=INXX-INXY
483
484
         WRITE(6,'(1X,3I6,12X,I6,D16.8)')
        *INXX,INXY,I,IQSW(I),POSA(I)
485
         IF(Q1.GT.POS2+REG2) GOTO 209
486
         INXY=INXY+1
487
         POSA(INXY)
                      = Q1
488
489
         STRA(INXY)
                      = Q2 * SMOD(IQ)
                     = Q3 + AMOD(IQ)
         ALFA(INXY)
490
                      = Q4
         ENRA(INXY)
491
                      =
                         IQ
492
         ISIA(INXY)
                         IΥ
         IQSW(INXY)
                      =
493
         WRITE(6,'(1X,3I6,12X,I6,D16.8)')INXX,INXY,IQ,IY,Q1
494
         GOTO 251
495
```

```
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```

```
250 IFILE=2
496
     251 CONTINUE
497
          WRITE(6,*)
498
          WRITE(6,*)'
                                                     IQSW
                                                                POSA'
499
                        INXX INXY
                                    JLINE
          WRITE(6,*)
500
    206
          IF(IY/ILIM.NE.0) GOTO 209
501
          READ(2,'(1X,D16.8,3D11.4,I4,I8)')Q1,Q2,Q3,Q4,IQ,IY
502
          DO 270 ISM =1, NBND
503
          IF(IQ.NE.MOLE(ISM)) GOTO 270
504
505
          GOTO 271
506
     270 CONTINUE
          GOTO 206
507
     271 IF(Q1.LT.POS1-REG2) GOTO 206
508
          IF(Q1.GT.POS2+REG2) GOTO 209
509
          JLIN=JLIN+1
510
511
          INXY=INXY+1
          POSA(INXY) = Q1
512
                       = Q2 * SMOD(IQ)
513
          STRA(INXY)
          ALFA(INXY) = Q3 + AMOD(IQ)
514
          ENRA(INXY) = Q4
515
          ISIA(INXY) = IQ
516
          IQSW(INXY) = IY
517
          GOTO 206
518
     209 INXX=INXY
519
          IF(MAINXX.LT.INXX) MAINXX=INXX
520
          WRITE(6, '(1X,3I6,12X,I6,D16.8,I6,2H==,/)')
521
         *INXX,INXY,JLIN,IQSW(INXX),POSA(INXX),MAINXX
522
523 C·
524 C
                            SET POSITION
   C-----
525
          GOTO(99,98),ILIN
526
      99 DO 100 I=1,NBND
527
          DSHIFT = SHIFT(I)
528
529
          DWNU
                  = DWNB(I)/DFLOAT(NLINE(I))
                  = DWNU/2D0
          DWN
530
          AKURVA = WNBC(I) - DWNB(I)/2.D O
531
          IF(DSHIFT.EQ.1.D 0) THEN
532
          INXX
                    = INXX+1
533
534
          POSA(INXX) = AKURVA
          STRA(INXX)=SINT(I)
535
          ENRA(INXX)=GSEN(I)
536
          ISIA(INXX)=MOLE(I)
537
          ALFA(INXX)=ALORO(MOLE(I))
538
          END IF
539
          DO 100 J=1,NLINE(I)
540
```

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541		INXX=INXX+1
542		POL=AKURVA+(J-1)*DWNU+(1.D O+DSHIFT)*DWN
543		POSA(INXX)=POL
544		STRA(INXX)=SINT(I)
545		ENRA(INXX)=GSEN(I)
546		ISIA(INXX)=MOLE(I)
547		ALFA(INXX)=ALORO(MOLE(I))
548	100	CONTINUE
549	98	ISI1=0
550		ISI2=0
551		JJ1=1
552		JJ2=1
553		INX=1
554		LPLUS=0
555		POS(1)=POS1
556		ISI(1)=ISI1
557		DO 111 I=1,INXX
558		IF(IQSW(I).GT.0) LPLUS=LPLUS+1
559		POL =POSA(I)
560		DZZ1=DABS(POL-POS1)
561		DZZ2=DABS(POL-POS2)
562		IF(DZZ1.LE.DZ) THEN
563		ISI1=ISI1-JJ1*ISIA(I)
564		JJ1=JJ1*10
565		GOTO 111
566		END IF
567		IF(DZZ2.LT.DZ) THEN
568		ISI2=ISI2-JJ2*ISIA(I)
569		JJ2=JJ2*10
570		GOTO 111
571		END IF
572		IF(POL.LT.POS1-DZ.OR.POL.GT.POS2+DZ) GOTO 111
573		INX=INX+1
574		POS(INX)=POL
575		ISI(INX)=ISIA(I)
576	111	CONTINUE
577		ISI(1)=ISI1
578		INX=INX+1
579		ISI(INX)=ISI2
580		POS(INX)=POS2
581		IMAX=INX
582		<pre>WRITE(6, '(/,1X,5I10,3H===,/)') INXX,LPLUS,IMAX,ISI1,ISI2</pre>
583	C	
584	С	REARRANGE
585	C	

```
Appendix D
```

```
130 IF(ILIN.NE.1) GOTO 97
586
          DO 134 I=1, INXX-1
587
          IN=I
588
          CHN =POSA(I)
589
          DO 133 J=I+1, INXX
590
          IF( CHN . LE . POSA(J) ) GOTO 133
591
          IN
               = J
592
          CHN = POSA(J)
593
     133 CONTINUE
594
          IF( IN . EQ . I ) GOTO 134
595
596
          CHNP = POSA(I)
          CHNS = STRA(I)
597
          CHNE = ENRA(I)
598
          CHNI = ISIA(I)
599
          CHNA = ALFA(I)
600
601
          POSA(I) = POSA(IN)
          STRA(I) = STRA(IN)
602
          ENRA(I) = ENRA(IN)
603
          ISIA(I) = ISIA(IN)
604
          ALFA(I) = ALFA(IN)
605
606
          POSA(IN) = CHNP
          STRA(IN) = CHNS
607
          ENRA(IN) = CHNE
608
          ISIA(IN) = CHNI
609
          ALFA(IN) = CHNA
610
     134 CONTINUE
611
612 C-----
613 C
                       LINES IN REG1 AND REG2
614 C-----
      97 CONTINUE
615
          DO 138 I=1,3
616
          DO 138 J=1,5
617
618
     138 IIII(I,J)=0
619
          DO 135 I=1,INXX
          POL = POSA(I)
620
          D2A=POS1-REG2
621
          D1A=POS1-REG1
622
          D1B=POS2+REG1
623
624
          D2B=POS2+REG2
          IF(POL.GE. D2A.AND.POL.LT. D1A) IIII(3,1)=IIII(3,1)+1
625
          IF(POL.GE. D1A.AND.POL.LT.POS1) IIII(3,2)=IIII(3,2)+1
626
          IF(POL.GE.POS1.AND.POL.LE.POS2) IIII(3,3)=IIII(3,3)+1
627
          IF(POL.GT.POS2.AND.POL.LE. D1B) IIII(3,4)=IIII(3,4)+1
628
          IF(POL.GT. D1B.AND.POL.LE. D2B) IIII(3,5)=IIII(3,5)+1
629
          IF(I.EQ.1.OR.I.EQ.INXX) WRITE(6, '(1X, 215, 4D16.8)')
630
```

```
Appendix D
```

```
*I, ISIA(I), POSA(I), STRA(I), ENRA(I), ALFA(I)
631
     135 CONTINUE
632
633
         IIII(1,1)=1
         IIII(2,1)=IIII(3,1)
634
         IIII(1,2)=IIII(2,1)+1
635
         IIII(2,2)=IIII(2,1)+IIII(3,2)
636
         IIII(1,3)=IIII(2,2)+1
637
         IIII(2,3)=IIII(2,2)+IIII(3,3)
638
         IIII(1,4)=IIII(2,3)+1
639
         IIII(2,4)=IIII(2,3)+IIII(3,4)
640
641
         IIII(1,5)=IIII(2,4)+1
         IIII(2,5)=IIII(2,4)+IIII(3,5)
642
         IREG1 = IIII(1,2)
643
         JREG1 = IIII(2,4)
644
         IREG2 = IIII(1,1)
645
646
         JREG2 = IIII(2,5)
         WRITE(6, '(/,5(1X,3I4,2X,/))')((IIII(I,J),I=1,3),J=1,5)
647
              _____
648 C-----
649 C
                         SET
                                ISI(I)=0
650 C-----
651
         ICHG=0
652
     141 DO 114 I=1,IMAX-1
         IN=I
653
         CHN=POS(I)
654
         DO 113 J=I+1, IMAX
655
         IF(CHN.LE.POS(J)) GOTO 113
656
         CHN=POS(J)
657
658
         IN=J
         ICHG=ICHG+1
659
     113 CONTINUE
660
         IF(IN.EQ.I) GOTO 114
661
662
         CHN1=POS(I)
663
         CHN2=ISI(I)
664
         POS(I) = CHN
         ISI(I)=ISI(IN)
665
         POS(IN)=CHN1
666
         ISI(IN)=CHN2
667
     114 CONTINUE
668
669
         IF(ICHG.NE.0) WRITE(6,*)' ICHG = ',ICHG,'
                                                           *****
670 C----
     112 JJ=10
671
         IZ=0
672
         IZZ=1
673
674
         JZZ=0
         IF(ISI2.LT.0) IZZ=0
675
```

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```
DO 115 I=1,IMAX-IZZ
676
        JZ = I + JZZ
677
        DELL=POS(JZ)-POS(I+1)
678
        IF(DABS(DELL).GT.DZ) GOTO 116
679
        WRITE(6,*)'JJ JZ IMAX IZZ',JJ,JZ,IMAX,IZZ,'
                                                    *****
680
        ISI(JZ)=ISI(JZ)+JJ*ISI(I+1)
681
        ISI(I+1)=0
682
        JJ = JJ*10
683
        IZ = IZ+1
684
        JZZ = JZZ-1
685
686
        GOTO 115
     116 JJ = 10
687
        JZZ = 0
688
     115 CONTINUE
689
        WRITE(6, *)
690
691 C-----
                         ------
692 C
                    ELIMINATE ISI(I)=0
693 C-----
        IJ=0
694
        IF(IMAX.LE.3)GOTO 156
695
696
        IF(ISI2.EQ.0) IJ=-1
        DO 117 I=3,IMAX+IJ
697
        IK=I+IJ
698
        IF(ISI(IK).NE.0)GOTO 117
699
700
        IIJ=I+1+IJ
        DO 118 J=IIJ,IMAX+IJ
701
        ISI(IK)=ISI(J)
702
        POS(IK)=POS(J)
703
        IK=IK+1
704
     118 CONTINUE
705
        IJ=IJ-1
706
707
    117 CONTINUE
708
        IMAX=IMAX-IZ
     156 IF(ISI2.NE.0)GOTO 157
709
        POS(IMAX)=POS2
710
        ISI(IMAX)=0
711
        GOTO 158
712
     157 ISI(IMAX)=ISI2
713
714
        POS(IMAX)=POS2
     158 CONTINUE
715
716 C-----
                                             _____
717 C
            SET IBLW(I), IENDPT(I) AND IWARN(I)
718 C-----
719
        POA=DR
        POB=DR
720
```

```
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```

```
IRE1A=IIII(3,2)
721
          IRE1B=IIII(3,4)
722
723
          IF(IRE1A.NE.0) POA=DABS(POS1-POSA(IIII(2,2)))
          IF(IRE1B.NE.0) POB=DABS(POSA(IIII(1,4))-POS2)
724
          IQQ=1
725
          J=2
726
          JJJ=2
727
          IES=0
728
729
          DO 119 I=1,IIR
730
          ENP=I*DR+POS1
731
          IENDPT(I)=0
          IBLW(I)=0
732
          IWARN(I) = 0
733
          JJ=0
734
          IF(JJJ.GT.IMAX-1)GOTO 128
735
736
          DO 120 J=JJJ, IMAX-1
          DELL=ENP-POS(J)
737
          IF(DABS(DELL).LT.DZ) GOTO 122
738
          IF(DELL.GT.ODO) GOTO 123
739
          GOTO 121
740
741
     122 JJ=JJ+1
742
          ISI(J)
                     = -IABS(ISI(J))
          IENDPT(I) = IENDPT(I)+1
743
          IBLW(I) = JJ
744
          JJJ=JJJ+JJ-1
745
746 CA5---
          IF(IPRA.EQ.5)
747
         *WRITE(6, '(/,1X,D15.5,616,/)')DELL,122,I,JJJ,JJ,J,ISI(J)
748
          GOTO 129
749
     121 IBLW(I)=JJ
750
          JJJ=JJJ+JJ
751
752 CA5---
753
          IF(IPRA.EQ.5)
         *WRITE(6,'(/,1X,D15.5,616,/)')DELL,121,I,JJJ,JJ,J,ISI(J)
754
          GOTO 129
755
     123 CONTINUE
756
757 CA5---
          IF(IPRA.EQ.5)
758
759
         *WRITE(6,'(/,1X,D15.5,616,/)')DELL,123,I,JJJ,JJ,J,ISI(J)
     126 CONTINUE
760
     120 JJ=JJ+1
761
          IBLW(I)=JJ
762
          JJJ=JJJ+JJ
763
764
     129 IENDPT(I)=IENDPT(I)+IES
          IES=0
765
```

```
IF(IENDPT(I).EQ.1.OR.IENDPT(I).EQ.3)IES=2
766
     128 IF(I.EQ.1) THEN
767
768
         POAA=POA
         IF(ISI1.EQ.0) GOTO 167
769
         IENDPT(1) = IENDPT(1) + 2
770
         IBLW(1) = IBLW(1) + 1
771
         END IF
772
     127 IF(I.EQ.IIR) THEN
773
         POBB=POB
774
         IF(ISI2.EQ.0) GOTO 168
775
         IENDPT(IIR)=IENDPT(IIR)+1
776
         IBLW(IIR)=IBLW(IIR)+1
777
         END IF
778
     167 POBB=DABS(POS(J)-ENP)
779
     168 IF(IENDPT(I).EQ.3) IWARN(I)=101
780
         IF(IENDPT(I).EQ.2.OR.IENDPT(I).EQ.0) THEN
781
              = POBB
         D1
782
         IG
              = I
783
         ITT = JJJ
784
         IWA1 = J
785
         CALL MESH
786
         IWARN(I)=KSUB+1
787
         END IF
788
         IF(IENDPT(I).EQ.1.OR.IENDPT(I).EQ.0) THEN
789
         D1=POAA
790
         IG=I
791
         ITT=JJJ
792
         IWA1=J
793
         CALL MESH
794
         IWARN(I) = IWARN(I) + (KSUB+1) * 100
795
         END IF
796
         POAA=DABS(ENP-POS(J-1))
797
798
     119 CONTINUE
799 CA6---
         IF(IPRA.EQ.6) THEN
800
                        WRITE(6, '(1X, 415)')(I, IBLW(I), IENDPT(I),
801
                        IWARN(I),I=1,IIR)
802
        *
                        WRITE(6, '(1X, I4, D25.8, I10)')(I, POS(I),
803
804
        *
                        ISI(I),I=1,IMAX)
                        WRITE(6,'(1X,2I10,/)')IZ,IMAX
805
                       END IF
806
807 C-----
                     ._____
                                 _____
                                                       -----
            AA, BB, ITT, IWA1, IWB1, K FOR LENGTH
808 C
809 C-----
         IALL=2
810
```

811		K=1
812		IF(ISI1.EQ.O) K=K+1
813		DO 400 I=1,IIR
814		IWA = IWARN(I)/100
815		IWB = IWARN(I)-IWA*100
816		IWA1= IWA
817		IWB1= IWB
818		EP1 = POS1+ DR*DFLOAT(I-1)
819		EP2 = EP1 + DR
820		IBW = IBLW(I)
821		AA = EP1
822		BB = EP2
823		IT = IENDPT(I)
824		ITT = IT
825		IF(IT.EQ.0.OR.IT.EQ.2) IC=0
826		IF(IT.EQ.1.OR.IT.EQ.3) IC=1
827		IF(IBW.EQ.O) GOTO 410
828		IF(IBW.EQ.1.AND.IT.NE.O) GOTO 410
829		IF(IBW.EQ.2.AND.IT.EQ.3) GOTO 410
830		GOTO(401,402,402,403),ITT+1
831	401	IBP=1
832		GOTO 404
833	402	IBP=0
834		GOTO 404
835	403	IBP=-1
836	404	L=IBW+IBP
837		KK=0
838		IF(IT.EQ.1.OR.IT.EQ.O)KK=-1
839		DO 421 J=1,L
840		JUMP=1
841		KKK=KK+K+J
842		IWA1=1
843		IWB1=1
844		ITT=3
845		BB=POS(KKK)
846		IF(J.EQ.1) GOTO 422
847		IF(J.EQ.L) GOTO 423
848		GOTO 443
849	422	IWA1=IWA
850		IF(IT.EU.1.UK.IT.EU.0)ITT=1
851	400	GUIU 443
852	423	TMR1=TMR
853		RR=FLS
854	404	IF(IT.EU.2.UR.IT.EU.0)ITT=2
855	424	GUTU 443

```
425 AA=BB
856
      421 CONTINUE
857
          GOTO 444
858
     410 JUMP=2
859
     443 IG=I
860
          CALL LENGTH
861
          GOTO(425,444), JUMP
862
      444 K=K+IBW-IC
863
      400 CONTINUE
864
          IALL=IALL-1
865
866
          IALLG=IALL*IGNU
          DO 699 I = 1, IALLG
867
     699 \text{ OUTSS}(I) = 0D0
868
869 C-RAD-
          IF(IRAD.NE.O) THEN
870
          DO 228 I = 1, IIR
871
          TRAB1(I) = 1DO
872
     228 \text{ SUMM}(I) = 0D0
873
          END IF
874
875 C-RAD-
876
          H20C=0D0
          OFWG=ODO
877
          SUMH=ODO
878
          OFWGS=0D0
879
880
   С
                                     _____
881
            END OF THE THIRD SECTION - LAYER LOOP BEGENS
   С
882
   С
                                     _____
          DO 700 LLDIR=1,LVEL-IHOMH
883
          IF(IPSC.NE.4) LL=LLDIR
884
          IF(IDIR.EQ. 1) LL=LLDIR
885
          IF(IDIR.EQ.-1) LL=LVEL-IHOM-LLDIR+1
886
          PAV=PLX(LL)
887
          TAV=TLX(LL)
888
          DVPR = ODO
889
          VPRAV = ODO
890
          DO 701 N = 1,NBND
891
          M = MOLE(N)
892
          AMASS(M) = AMIX(M, LL) * UMOD(M) * BMY(LL)
893
894
          ALOR(M) = PLX(LL)/PPPO*CST1(LL)**ALORT(M)
          ADOP(M) = TDOPA(LL) * WNUAV/DSQRT(AMOLE(M))
895
                    = AMASS(M)*SLOG2P/ADOP(M)
          AKO(M)
896
          XS(M)
                    = SLOG2/ADOP(M)
897
                    = 1D0
          CS1(M)
898
          IF(IRPF.EQ.1) CS1(M)=CS1(M)*CST1(LL)**RPFN(M)
899
          IF(IVPF.EQ.1) CS1(M)=CS1(M)*(VPFN(1,M)+VPFN(2,M)*
900
```

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```
*CST1(LL)**VPFN(3,M))
901
          VPR(M) = ADOP(M) / (ALOR(M) * ALORO(M) + ADOP(M))
902
903
          VPR(M)=VPR(M)**AINT
          DVP(M) = REG1 * VPR(M) + REG2 * (1DO - VPR(M))
904
          VPRAV =VPRAV+VPR(M)/DFLOAT(NBND)
905
          DVPR =DVPR+DVP(M)/DFLOAT(NBND)
906
907 701
          CONTINUE
          LS1=DFLOAT(IREG1)*VPRAV+DFLOAT(IREG2)*(1D0-VPRAV)
908
          LS2=DFLOAT(JREG1)*VPRAV+DFLOAT(JREG2)*(1D0-VPRAV)
909
910 C-----
911
          IF(ICON.EQ.1) THEN
                   DAV = DEX(LL)
912
                   RR1 = CHX(LL)
913
                   RR2 = DAV-RR1
914
                   OM = AMASS(1) * ALOSMT
915
916
                   CALL CONT(WNUAV, TLX(LL), RR1, RR2, RR3, OM, H2OC)
                   END IF
917
918 C-----
          CS2 = CST2(LL)
919
          DO 703 N = LS1, LS2
920
921
          M=ISIA(N)
922
          ENRAM=ENRA(N)*CS2
          STRT(N) = STRA(N) * CS1(M) * DEXP(ENRAM)
923
      703 CONTINUE
924
925 CA----
926
          IF(IPRA.EQ.6) THEN
          WRITE(6, '(1X, I4, 3F15.7, /)')LL, PLX(LL), TLX(LL), WNUAV
927
928
          DO 702 N=1,NBND
          M=MOLE(N)
929
      702 WRITE(6,'(1X,12,7D11.4,/)')M,AMASS(M),ALOR(M),ADOP(M),
930
         *AKO(M),XS(M),VPR(M),DVP(M)
931
932
          WRITE(6,*)
933
          IF(IPRH.EQ.1)
         *WRITE(6,'(1X,2I6,I3,D15.8,D15.4,F15.4,F15.5)')
934
         *(N,IQSW(N),ISIA(N),STRT(N), STRA(N),ENRA(N),POSA(N),
935
         *N=LS1,LS2)
936
          END IF
937
938 C-----
939
          OUTGS
                    = 0D0
          NG
                    = 0
940
          DO 599 I = 1, IIR
941
      599 \text{ TRAB}(I) = 0D0
942
          TRABS(LL) = ODO
943
944 C-----
945
          IF(ISBN.EQ.2) THEN
```

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```
IF(IPRE.NE.O)WRITE(6, '(/,4X,21HNG IGS IGI ITY
                                                            IDAB ,
946
         *5X, 3HGAA, 13X, 4HOUTG, 17X, 5HOUTGS, /)')
947
          GAA=POS1
948
          DO 596 I=1,IIR
949
          GBB
                =
                   GAA+DR
950
          IGS
                   Ι
951
                =
          IGI
                   Ι
952
                =
          ITY
                = -1
953
          GAB = (GAA + GBB) / 2D0
954
          GCC=(GBB-GAA)/2D0
955
956
          IF(IFAR.EQ.3) CALL FARWG(GAB,TLX(LL),PLX(LL),OFWG,IPRD)
          CALL GAUSS (DR, GAB, GCC, OUTG)
957
          GAA=GBB
958
     596 TRAB(I)=TRAB(I)+OUTG/DR
959
          IF(IFAR.EQ.3) IFAR = 2
960
961
          OFWGS=OFWGS/DFLOAT(IIR)
962
          IALLL=IIR
          GOTO 595
963
          ENDIF
964
965 C----
          IF(IPRE.NE.O)WRITE(6, '(/,4X,21HNG IGS IGI ITY
                                                            IDAB ,
966
         *5X, 3HGAA, 13X, 4HOUTG, 17X, 5HOUTGS, /) ')
967
          DO 600 I=1,IALL-1
968
          IGS=I
969
          IGI=IGA(I)
970
          ITY=ITYPE(I)
971
          GAB = (AGA(I+1) + AGA(I))/2DO
972
973
          GCC=(AGA(I+1)-AGA(I))/2DO
          IF(IFAR.EQ.3) CALL FARWG(GAB,TLX(LL),PLX(LL),OFWG,IPRD)
974
          CALL GAUSS (DR, GAB, GCC, OUTG)
975
     600 TRAB(IGI)=TRAB(IGI)+OUTG/DR
976
          OFWGS=OFWGS/DFLOAT(IALL)
977
978
          IF(IFAR.EQ.3) IFAR = 2
979
          IALLL=IALL-1
  C----
980
     595 DO 601 I=1,IIR
981
     601 TRABS(LL)=TRABS(LL)+TRAB(I)*DR
982
983 C-----
                            ______
984 C
                          OUTPUT SECTION
985
   C-
                              _____
                                         _____
          _____
          IF(IOTR.NE.0)
986
                            WRITE(10, *)
                            LL, (TRAB(I), I=1, IIR), TRABS(LL), WNUAV
987
         *
          IF(IGNU.EQ.0) GOTO 602
988
          WRITE(6, '(4X, I2, I5, 2I3, D22.14, F6.1, F10.6, F9.3, 2I5)')
989
         *IGNU, IALLL, LL, ISBN, TRABS(LL), WNUAV, VPRAV, DVPR, LS1, LS2
990
```

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```
GOTO 603
991
      602 WRITE(6, '(414, 4D25.15, /)')
992
          *IGNU, IALLL, ITRN, ISBN, TRABS(LL), ERG, ERGB
993
      603 CONTINUE
994
           IF(IPRA.EQ.5)
995
          *WRITE(6, '(1X, I5, D25.15)')(I, TRAB(I), I=1, IIR)
996
997 C-RAD-
           IF(IRAD.NE.O)THEN
998
           TLY1=TLY(LL)
999
           TLY2=TLY(LL+1)
1000
1001
           DO 229 I=1,IIR
           IF(TRAB1(I).LT.DZ) GOTO 229
1002
           WNUU=WNUAV-5D-1+DR/2DO+(I-1)*DR
1003
           WNUP=C1*WNUU*WNUU*WNUU
1004
           WNUT1=C2*WNUU/TLY1
1005
1006
           WNUT2=C2*WNUU/TLY2
           BP1 =WNUP/(DEXP(WNUT1)-1)
1007
           BP2 =WNUP/(DEXP(WNUT2)-1)
1008
           BPL = (BP1*TRAB1(I)+BP2*TRAB(I))/(TRAB1(I)+TRAB(I))
1009
           SUMM(I) = SUMM(I) + BPL * (TRAB1(I) - TRAB(I))
1010
           IF(IPRH.EQ.2)
1011
          *WRITE(6,'(1X,F8.3,2F15.10)')WNUU,BPL,SUMM(I)
1012
           TRAB1(I)=TRAB(I)
1013
      229 CONTINUE
1014
           END IF
1015
1016 C-RAD-
      700 CONTINUE
1017
1018 C-RAD-
           IF(IRAD.NE. 0) THEN
1019
           IF(TSKN.EQ.ODO) GOTO 226
1020
           DO 227 I=1,IIR
1021
           IF(TRAB(I).LT.DZ) GOTO 227
1022
           WNUU=WNUAV-5D-1+DR/2DO+(I-1)*DR
1023
1024
           WNUP=C1*WNUU*WNUU*WNUU
           WNUT=C2*WNUU/TSKN
1025
           BPL =TRAB(I)*EMIS*WNUP/(DEXP(WNUT)-1)
1026
           SUMM(I)=SUMM(I)+BPL
1027
           IF(IPRH.EQ.2)WRITE(6, '(1X,F8.3,2F15.10)')
1028
1029
          *WNUU, BPL, SUMM(I)
      227 CONTINUE
1030
      226 IF(IORD.EQ.1)WRITE(11, '(1X, F11.3)')
1031
                                                             WNUAV
           IF(IORD.EQ.1)WRITE(11, '(10(1X,E11.6))')(SUMM(I),I=1,IIR)
1032
           END IF
1033
1034 C-RAD-
           GOTO 17
1035
```

1036	504 CONTINUE
1037	DATA MOLE,LMOD,AMOD,SMOD,UMOD,RMOD/17*0,7*0D0,21*1D0/
1038	DATA PDLR,PLNZ,VDLR,VLNZ/1D-2,1D2,1D-3,2D-1/
1039	DATA AEP,NLEN/
1040	*0D0,1D-3,1.5D-3,2.5D-3,5D-3,1D-2,2.5D-2,5D-2,1D-1,2D-1,
1041	*5D-1,1D0,2.5D0,5D0,1D1,2.5D1,5D1,1D2,25D1,50D1,1D3,20/
1042	DATA ALORO/
1043	*1D-1,64D-3,11D-2,8D-2,6D-2,55D-3,6D-2,1D-1,1D-1,1D-1/
1044	DATA ALORT/
1045	*62D-2,75D-2,5D-1,5D-1,5D-1,5D-1,5D-1,5D-1,5D-1,5D-1
1046	DATA AMOLE/
1047	*18.150,44.010,47.998,44.010,28.011,16.043,31.999,
1048	*30.010,64.060,46.010/
1049	DATA RPFN/
1050	<pre>* 1.5D0,1.0D0,1.5D0,1.0D0,1.0D0,1.5D0,1.0D0/</pre>
1051	DATA VPFN/
1052	*1D0,0D0,0D0,0.99752D0,0.09310D0,-3.54915D0,0.99852D0,
1053	*0.04600D0,-4.11179D0,1.01819D0,0.12700D0,-4.42836D0,
1054	*1D0,0D0,0D0,0.99935D0,0.00700D0,-5.47575D0,1D0,0D0,0D0/
1055	DATA PI, PPPO, TTTO, PSTND, TSTND, AVOGAD, ALOSMT, GASCON,
1056	*PLANK,BOLTZ,CLIGH,UNIV,ATMA,DZ,VOLG,C1,C2,C3,
1057	*XAB,WAB,RR3/
1058	*3.14159265358973D0,1013.25D0,296D0,1013.25D0,273.15D0,
1059	*6.022169D26,2.68684D19,8.31432D3,6.62617D-27,
1060	*1.380662D-23,2.997924D8,0.372184D-20,1.660565D-27,
1061	*1D-14,22.24136D0,1.1909596D-5,1.43879,3.58D-7,
1062	*0.577350269189626D0,1D0,0.2548D20/
1063	DATA TETM/
1064	*62D0,64D0,66D0,68D0,70D0,72D0,74D0,76D0,78D0,80D0,
1065	*81D0,82D0,83D0,84D0,85D0,86D0,87D0,87.5D0,88D0,88.2D0,
1066	*88.4D0,88.6D0,88.8D0,89D0,89.2D0,89.4D0,89.6D0,89.7D0,
1067	*89.8D0,89.9D0,90D0/
1068	1000 CONTINUE
1069	END

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1070 C-----INPUTS FOR THE FIRST ITRA EXPERIMENT 1071 C 1072 C------1073 C .05,1,2,0,0,0,0 RESL DELV ITRN IRAD IOTR IORD IOPR 1074 C 0,0,0,0,0,0,0 IPRA IPRB IPRC IPRD IPRE IPRF IPRG IPRH 1075 C 1,2,0,0ISBN IGNU EPSN ICCH PDLR PLNZ VDLR VLNZ1076 C 1,1,1,1IINT AINT IVPF IRPF KSHP IVDY1077 C 0MODL IDEN LMOD(IDEN)... 1078 C O MODA IDEN AMOD(IDEN)... MODS IDEN SMOD(IDEN)... 1079 C O 1080 C O MODR IDEN RMOD(IDEN)... 1081 C 580,780,0.1,1,7 WNU1 WNU2 REGO REG1 REG2
 1082
 C
 0,0,0
 IPPS
 IPPH
 IARM
 ASCL

 1083
 C
 5
 1
 2
 LVEL
 NBND
 MOLE(1)...
 LVEL NBND MOLE(1)...MOLE(NBND) 1084 C 125.13 310 13.81 1085 C 253.31 274 2.054 1086 C 506.62 274 0.5151 1087 C 60.528 244 33.695 1088 C 253.31 245 0.5746 1089 C 2,64222,0,0,0 ILIN ILIM ICON IFAR JREF 1090 C 1091 C-----INPUTS FOR THE SECOND ITRA EXPERIMENT. 1092 C 1093 C------1094 C 0.01,1,2,1,1,1,0 RESL DELV ITRN IRAD IOTR IORD IOPR 1095 C 0,0,0,0,0,0,0,0 IPRA IPRB IPRC IPRD IPRE IPRF IPRG IPRH 1096 C 1,2,0,0,0,0,0,0 ISBN IGNU EPSN ICCH PDLR PLNZ VDLR VLNZ 1097 C 1,1,1,1,0,0 IINT AINT IVPF IRPF KSHP IVDY MODL IDEN LMOD(IDEN)... 1098 C O MODA IDEN AMOD(IDEN)... 1099 C O 1100 C O MODS IDEN SMOD(IDEN)... MODR IDEN RMOD(IDEN)... 1101 C O 1102 C 660,780,.1,1,6.5 WNU1 WNU2 REGO REG1 REG2

 1102 C 0000,780,.1,1,0.5 WN01 WN02 KEGO KEGI KEG2

 1103 C 4,1,0,0
 IPPS IPPH IARM ASCL

 1104 C 6,50,1,2
 IPOF LVEL NBND MOLE(1)....MOLE(NBND)

 1105 C 1,50,288.2,1
 LVL1 LVL2 TSKN EMIS

 1106 C 1,0,0,0
 IDIR TETA TETB DTET

 1107 C 0,0,0,0
 LVLN ALT1 ALT2 PATH

 1108 C 0
 MODU IDEN UMOD(IDEN)...

 1109 C 2,64220,0,0,0
 ILIN ILIM ICON IFAR JREF

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1110 C-----INPUTS FOR THE HIS EVALUATIONS (CASE 2.) 1111 C 1112 C------1113 C 5D-3,1,2,1,0,1,0 RESL DELV ITRN IRAD IOTR IORD IOPR 1114 C 0,0,0,0,0,0,0 IPRA IPRB IPRC IPRD IPRE IPRF IPRG IPRH 1115 C 1,2,0,0,0,0,0,0 ISBN IGNU EPSN ICCH PDLR PLNZ VDLR VLNZ

 1115
 C
 1,2,0,0,0,0,0,0,0,0
 10DN
 10DN
 10DN
 10DN
 10DN
 10DN
 12DN
 12D 1121 C 610,630,.1,1,6.5 WNU1 WNU2 REGO REG1 REG2 1122 C 4,1,0,0 IPPS IPPH IARM ASCL

 1122 C 4,1,0,0
 1115 1111 1Rtt1 RBCL

 1123 C 0,24,4,1,2,3,4
 IPOF LVEL NBND MOLE(1)....MOLE(NBND)

 1124 C 1,24,309,1
 LVL1 LVL2 TSKN EMIS

 1125 C 1,0,0,0
 IDIR TETA TETB DTET

 1126 C 0,0,0,0
 LVLN ALT1 ALT2 PATH

 1127 C 1,3,0.29
 MODU IDEN UMOD(IDEN)...

 1128 C 2,64220,1,0,0
 ILIN ILIM ICON IFAR JREF

 1129 C 1130 C-----_____ INPUT STRUCTURE FOR AIRMASS CALCULATIONS 1131 C 1132 C------1133 C 0.1,1,2,0,0,0,0 RESL DELV ITRN IRAD IOTR IORD IOPR 1134 C 0,1,0,0,0,0,0 IPRA IPRB IPRC IPRD IPRE IPRF IPRG IPRH 1135 C 0,0,0,0,0,0,0,0 ISBN IGNU EPSN ICCH PDLR PLNZ VDLR VLNZ 1136CO,O,O,O,O,OIINTAINTIVPFIRPFKSHPIVDY1137COMODLIDENLMOD(IDEN)...1138COMODAIDENAMOD(IDEN)...1139COMODSIDENSMOD(IDEN)...

 1139 C 0
 MODS IDEN SMOD(IDEN)...

 1140 C 0
 MODR IDEN RMOD(IDEN)...

 1141 C 610,610,0,0,0
 WNU1 WNU2 REGO REG1 REG2

 1142 C 4,1,14,-30
 IPPS IPPH IARM ASCL

 1143 C 6,50,1,14
 IPOF LVEL NBND MOLE(1)....MOLE(NBND)

 1144 C 1,50,0,0
 LVL1 LVL2 TSKN EMIS

 1145 C 1,60,90,-1
 IDIR TETA TETB DTET

 1146 C 3000,120,0,0
 LVLN ALT1 ALT2 PATH

 1147 C 0
 MODU IDEN UMOD(IDEN)...

 1148 C 0,0,0,0,1
 ILIN ILIM ICON IFAR JREF

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1149 C-----INPUT STRUCTURE FOR LIMB GEOMETRY 1150 C 1152 C .1,1,2,0,0,0,1 RESL DELV ITRN IRAD IOTR IORD IOPR 1153 C 1,4,0,0,0,0,0,0 IPRA IPRB IPRC IPRD IPRE IPRF IPRG IPRH 1154 C 1,2,0,0,0,0,0,0 ISBN IGNU EPSN ICCH PDLR PLNZ VDLR VLNZ 1160 C 610,610,.1,.1,.5 WNU1 WNU2 REGO REG1 REG2 1161 C 4,1,0,0 IPPS IPPH IARM ASCL

 1161 C 4,1,0,0
 IFFS IFFN IARM ASCE

 1162 C 6,50,1,1,2,3,4
 IPOF LVEL NBND MOLE(1)...MOLE(NBND)

 1163 C 0,0,309,1
 LVL1 LVL2 TSKN EMIS

 1164 C -1,80,0,0
 IDIR TETA TETB DTET 79.0451206

 1165 C 0,40,0,0
 LVLN ALT1 ALT2 PATH

 1166 C 1,3,0.29
 MODU IDEN UMOD(IDEN)...

 1167 C 2,64220,1,0,1
 ILIN ILIM ICON IFAR JREF

 1168 C 1169 C-----1170 C THIS IS THE CONTROL SEQUENCE FOR LIMB GEOMETRY. AT THE 1171 C INPUT THE TANGENT HEIGHT WAS OBTAINED IN THE PREVIOUS EXAMPLE (UPWARD DIRECTION). 1172 C 1174 C .1,1,2,0,1,0,0 RESL DELV ITRN IRAD IOTR IORD IOPR 1175 C 1,1,0,0,0,0,0,0 IPRA IPRB IPRC IPRD IPRE IPRF IPRG IPRH 1176 C 1,2,0,0,0,0,0,0 ISBN IGNU EPSN ICCH PDLR PLNZ VDLR VLNZ

 1176 C 1,2,0,0,0,0,0,0
 ISBN IGNO EPSN ICCH FDLR FLN2

 1177 C 1,1,1,1,0,0
 IINT AINT IVPF IRPF KSHP IVDY

 1178 C 0
 MODL IDEN LMOD(IDEN)...

 1179 C 1,1,4D-2
 MODA IDEN AMOD(IDEN)...

 1180 C 0
 MODS IDEN SMOD(IDEN)...

 1181 C 0
 MODR IDEN RMOD(IDEN)...

 1182 C 610,610,.1,.1,.5 WNU1 WNU2 REGO REG1 REG2 1183 C 4,1,0,0 IPPS IPPH IARM ASCL 1184 C 6,50,1,1,2,3,4 IPOF LVEL NBND MOLE(1)....MOLE(NBND) 1185C 0,0,309,1LVL1LVL2TSKNEMIS1186C 1,90,0,0IDIRTETATETBDTET 79.0451206 1187 C 0,120,21.4023,0 LVLN ALT1 ALT2 PATH

 1188
 C 1,3,0.29
 MODU IDEN UMOD(IDEN)...

 1189
 C 2,64220,1,0,1
 ILIN ILIM ICON IFAR JREF

 1190 C-----

```
SUBROUTINE LAYERS (WEDD, JREF, IDIR, TETA, LVEL, ZN, LIMB, LVEN)
1
         IMPLICIT REAL*8 (A-H,O-Z)
\mathbf{2}
         COMMON/HA/ POSA(3000), STRA(3000), ENRA(3000), ALFA(3000),
3
        *ALFT(3000), CPLG(3000), STRT(3000), ISIA(3000), IQSW(3000)
\mathbf{4}
         COMMON/LA/ IPRB, ALT(150), DEY(150), PSTND, TSTND, BMY(150),
5
                     CHY(150), TLY(150), PLY(150), AMIY(37, 150)
6
        *
         DIMENSION
\overline{7}
        *PLZ(3000), BMZ(3000), CHZ(3000), TLZ(3000), ALZ(3000),
8
        *DEZ(3000),AMZ(3000)
9
10
         EQUIVALENCE
        *(POSA,PLZ),(STRA,BMZ),(ENRA,TLZ),(ALFA,CHZ),
11
12
        *(ALFT,ALZ),(CPLG,DEZ),(STRT,AMZ)
         LAYER = LVEL-1
13
         DVERT = ODO
14
         DPATH = ODO
15
16
         SLANT = ODO
         GAMAS = ODO
17
         CNST = ODO
18
         COR
                = 1D0
19
20 C-----
21
         DO 38 I=1,LAYER
         IF(IDIR.EQ.-1) GOTO 100
22
         L=LVEL-I
23
         PAV1=(PLZ(L)+PLZ(L+1))/2D0
24
         TAV1=(TLZ(L)+TLZ(L+1))/2D0
25
         HAV1=(CHZ(L)+CHZ(L+1))/2D0
26
         IF(JREF.EQ.-1) HAV1=ODO
27
         ZZ1 = RAE + ALZ(L+1)
28
         ZZ2 = RAE + ALZ(L)
29
         DZZ= ZZ2-ZZ1
30
         AIRMV = DZZ/DLOG(DEZ(L+1)/DEZ(L))*(DEZ(L+1)-DEZ(L))
31
         REF1=((ED1+ED2/(1D0-WEDD/ED4)+ED3/(1D0-WEDD/ED5))*
32
        *(TSTND+15D0)*PAV1/PSTND/TAV1-
33
34
        *(ED6-WEDD/ED7)*HAV1/PSTND)*1D-6+1D0
         IF(L.EQ.LAYER) TETA1=TETA
35
         IF(L.EQ.1) THEN
36
                     REF2=REF1
37
                     GOTO 37
38
39
                     END IF
         ZZ3 = RAE + ALZ(L-1)
40
         PAV2=(PLZ(L)+PLZ(L-1))/2D0
41
         TAV2=(TLZ(L)+TLZ(L-1))/2D0
42
         HAV2=(CHZ(L)+CHZ(L-1))/2D0
43
         IF(JREF.EQ.-1) HAV2=0D0
44
         REF2=((ED1+ED2/(1D0-WEDD/ED4)+ED3/(1D0-WEDD/ED5))*
45
```

Appendix D

46	*(TSTND+15D0)*PAV2/PSTND/TAV2-
47	*(ED6-WEDD/ED7)*HAV2/PSTND)*1D-6+1D0
48	IF(JREF.EQ.0) REF2=REF1
49	37 ALFA1=PIDE*DASIN(DSIN(TETA1*PIRA)*ZZ1/ZZ2)
50	SLANT1=ZZ2*DCOS(ALFA1*PIRA)-ZZ1*DCOS(TETA1*PIRA)
51	GAMA1=TETA1-ALFA1
52	GAMAS=GAMAS+GAMA1
53	IF(L.EQ.1) THEN
54	COR=1D0
55	GOTO 1009
56	END IF
57	TETA2 = DASIN(DSIN(ALFA1*PIRA)*REF1/REF2)
58	ALFA2 = DASIN(DSIN(TETA2)*ZZ2/ZZ3)
59	SLANT2= ZZ3*DCOS(ALFA2)-ZZ2*DCOS(TETA2)
60	DELTA = PI-(TETA2-ALFA1*PIRA)
61	CSIDE = DSQRT(SLANT1*SLANT1+SLANT2*SLANT2
62	<pre>* -2*SLANT1*SLANT2*DCOS(DELTA))</pre>
63	IF(DABS(CSIDE-SLANT1-SLANT2).LT.DZ.OR.JREF.EQ2)THEN
64	COR=1D0
65	GDTD 1009
66	END IF
67	SS = (SLANT1+SLANT2+CSIDE)/2D0
68	SSS = 4D0*DSQRT(SS*(SS-SLANT1)*(SS-SLANT2)*(SS-CSIDE))
69	RDS = SLANT1*SLANT2*CSIDE/SSS
70	COR = RDS*2D0*DASIN(SLANT1/RDS/2D0)/SLANT1
71	1009 CORA = COR-1DO
72	AMU = SLANT1 * COR / DZZ
73	SLANT = SLANT + SLANT1*COR
74	DPATH = DPATH + AMU*AIRMV
75	DVERT = DVERT + AIRMV
76	PATAL = DPATH / DVERT
77	RFI=(-ID0+REFI)*ID6
78	RFZ = (-IDU + REFZ) * IDO $IE(IDDD ED Q) UDITE(C) (EV IA QE10 A QV QEQ0 14)))$
79	Ir(IPRD.EQ.2) WRIIE(0, (5A, 14, 2r10.4, 2A, 2r20.14))
80	*L, π r 1, π 2, λ LANII, \cup URA TE(TODD EO 2) UDTTE(C)(1V TA CE10 A E12 C)) I AMU CLANT
80 80	*PATAI TETA1 ALEA1 CAMAS CNST
02 92	RM7(I) = DABS(AMII)
84	$TFT \Delta 1 = PTDF * TFT \Delta 2$
85	$CNST = RFF2 * 772 * DSTN (TFT \Delta 1 * PTR \Delta)$
86	GULU 38
87	C
88	100 L=I
89	LIMB=0
90	PAV1=(PLZ(L)+PLZ(L+1))/2D0

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```
TAV1=(TLZ(L)+TLZ(L+1))/2D0
91
          HAV1=(CHZ(L)+CHZ(L+1))/2D0
92
          IF(JREF.EQ.-1) HAV1=0D0
93
          ZZ1 = RAE + ALZ(L)
94
          ZZ2 = RAE + ALZ(L+1)
95
          DZZ = ZZ2 - ZZ1
96
          AIRMV = DZZ/DLOG(DEZ(L)/DEZ(L+1)) * (DEZ(L) - DEZ(L+1))
97
         REF1=((ED1+ED2/(1D0-WEDD/ED4)+ED3/(1D0-WEDD/ED5))*
98
         *(TSTND+15D0)*PAV1/PSTND/TAV1-
99
        *(ED6-WEDD/ED7)*HAV1/PSTND)*1D-6+1D0
100
101
          IF(L.EQ.1)
                      THEN
                      ALFA1=TETA
102
                      COR =1D0
103
                      END IF
104
          IF(L.EQ.LAYER) GOTO 1
105
106
          PAV2=( PLZ(L+1)+ PLZ(L+2))/2D0
          TAV2=(TLZ(L+1)+TLZ(L+2))/2D0
107
          HAV2=(CHZ(L+1)+CHZ(L+2))/2D0
108
          IF(JREF.EQ.-1) HAV2=0D0
109
          REF2=((ED1+ED2/(1D0-WEDD/ED4)+ED3/(1D0-WEDD/ED5))*
110
        *(TSTND+15D0)*PAV2/PSTND/TAV2-
111
112
        *(ED6-WEDD/ED7)*HAV2/PSTND)*1D-6+1D0
       1 IF(JREF.EQ.0) REF2=REF1
113
          TEMPA=DSIN(ALFA1*PIRA)*ZZ1/ZZ2
114
          IF(TEMPA-1DO.GT.DZ) THEN
115
         LIMB=1
116
          IF(LVEN.GE.O) GOTO 3
117
118
         LVEL=L+1
         RETURN
119
       3 ZN=ZZ1*DSIN(ALFA1*PIRA)-RAE
120
          LEVL=L+1
121
          CALL MINT(ALZ, DEZ, 1, LVEL, L, ZN, DEYZ, IPRB)
122
          CALL MINT(ALZ, PLZ, 1, LVEL, L, ZN, PLYZ, IPRB)
123
          CALL MINT(ALZ, TLZ, 2, LVEL, L, ZN, TLYZ, IPRB)
124
          CALL MINT(ALZ, CHZ, 2, LVEL, L, ZN, CHYZ, IPRB)
125
          DEZ(LEVL) = DEYZ
126
          PLZ(LEVL) = PLYZ
127
          TLZ(LEVL) = TLYZ
128
129
          CHZ(LEVL) = CHYZ
          ALZ(LEVL) = ZN
130
          ZZ2=ZN+RAE
131
          DZZ=ZZ2-ZZ1
132
                     DZZ / DLOG(DEZ(L)/DEYZ) * (DEZ(L)-DEYZ)
          AIRMV =
133
          REF2=REF1
134
          TEMPA=1D0
135
```

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Appendix D
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136	LVEL = LEVL
137	END IF
138	2 TETA1=PIDE*DASIN(TEMPA)
139	SLANT2=ZZ1*DCOS(ALFA1*PIRA)-ZZ2*DCOS(TETA1*PIRA)
140	GAMA1=TETA1-ALFA1
141	GAMAS=GAMAS+GAMA1
142	IF(L.EQ.1) GOTO 1010
143	CSIDE = DSQRT(SLANT1*SLANT1+SLANT2*SLANT2
144	<pre>* -2*SLANT1*SLANT2*DCOS(DELTA))</pre>
145	IF(DABS(CSIDE-SLANT1-SLANT2).LT.DZ.OR.JREF.EQ2)THEN
146	COR=1D0
147	GOTO 1010
148	END IF
149	SS = (SLANT1+SLANT2+CSIDE)/2D0
150	SSS = 4D0*DSQRT(SS*(SS-SLANT1)*(SS-SLANT2)*(SS-CSIDE))
151	RDS = SLANT1*SLANT2*CSIDE/SSS
152	COR = RDS*2D0*DASIN(SLANT2/RDS/2D0)/SLANT2
153	CORA = COR-1DO
154	C
155	1010 AMU = SLANT2*COR / DZZ
156	SLANT = SLANT + SLANT2*COR
157	DPATH = DPATH + AMU*AIRMV
158	DVERT = DVERT + AIRMV
159	PATAL = DPATH / DVERT
160	RF1=(-1D0+REF1)*1D6
161	RF2=(-1D0+REF2)*1D6
162	IF(IPRB.EQ.2) WRITE(6,'(5X,I4,2F10.4,2X,2F20.14)')
163	*L,RF1,RF2,SLANT2,CORA
164	IF(IPRB.EQ.3)WRITE(6,'(1X,I4,6F10.4,F13.5)')L,AMU,SLANT,
165	*PATAL, TETA1, ALFA1, GAMAS, CNST
166	BMZ(L)=DABS(AMU)
167	ALFA2 = DASIN(DSIN(TETA1*PIRA)*REF1/REF2)
168	DELTA = PI-(TETA1*PIRA-ALFA2)
169	ALFA1=PIDE*ALFA2
170	REF1=REF2
171	SLANT1=SLANT2
172	CNST=REF2*ZZ2*DSIN(ALFA1*PIRA)
173	IF(LIMB.EQ.1) GOTO 4
174	38 CUNTINUE
175	IF(IDIR.EQ. 1) DEFL = ALFA1+GAMAS-TETA
176	4 IF (IDIR.EQ1) DEFL = $-IETA-GAMAS+ALFA1$
177	IF (IPRB.EU.2) WRITE (6, '(/,5X,26HGEUMETRICAL PATH
178	*LENGIH = $F_{20.14}$ SLANT
179	IF(IPKB.EU.I)WKIIE(0, (IX,F5.1,IX,F8.4,2X,F8.5,2X,F8.3,
180	*1X,F8.4,ZH *//)IETA,ALFA1,DEFL,SLANT,PATAL

- 181 IF(LIMB.EQ.1) WRITE(6,'(/,1X,14HLIMB GEOMETRY,,5X,17H
- 182 ***TANGENT HEIGHT = ,F13.8,5X,8HLEVEL = ,I5,/,/)'ZN,LVEL**
- 183 RETURN
- 184 DATA PI, PIRA, PIDE, DZ, RAE, ED1, ED2, ED3, ED4, ED5, ED6, ED7/
- *3.1415926535898D0,1.7453292519943D-2,5.72957795130823D1,
- 186 ***1D-13,6370D0,83.42D0,185.08D0,4.11D0,1.2996D10,**
- *38.9376D8,43.49D0,2.89D8/
- 188 END

Appendix D

1	SUBROUTINE MINT(P,T,ISC,LVEL,LEVIN,ZNEW,OTMN,IPRB)
2	IMPLICIT REAL*8(A-H,O-Z)
3	DIMENSION P(150),T(150)
4	I = LEVIN
5	ZN = ZNEW
6	ITR=0
7	IF(IPRB.EQ.5)WRITE(6,'(1X,2I4,5(D11.4,1X))')
8	*ISC,I,P(I),P(I+1),T(I),T(I+1),ZNEW
9	IF(ISC.LE.1)THEN
10	IF(I.EQ.LVEL) I=I-1
11	HSCAL=ISC*(P(I)-P(I+1))/DLOG(T(I)/T(I+1))
12	OTMN=T(I+1)*DEXP((ZN-P(I+1))/HSCAL)
13	GOTO 10
14	END IF
15	2 IF(ISC.EQ.2)THEN
16	IF(I.EQ.1) K=0
17	IF(I.GE.2) $K=-1$
18	IF(I.EQ.LVEL-1) K=-2
19	PAV=(P(I+K)+P(I+K+1)+P(I+K+2)+P(I+K+3))/4D0
20	TAV = (T(I+K)+T(I+K+1)+T(I+K+2)+T(I+K+3))/4D0
21	C1=P(I+K)/PAV
22	C2=P(I+K+1)/PAV
23	C3=P(I+K+2)/PAV
24	C4=P(I+K+3)/PAV
25	C21=C2-C1
26	C31=C3-C1
27	C41=C4-C1
28	B1=C1*C1
29	B21=C2*C2-B1
30	B31=C3*C3-B1
31	B41=C4*C4-B1
32	A1=C1*C1*C1
33	A21=C2*C2*C2-A1
34	A31=C3*C3+C3-A1
35	A41 = C4 + C4 + C4 - A1
36	T1 = T(I+K) / TAV
37	T21=T(I+K+1)/TAV-T1
38	T31=T(I+K+2)/TAV-T1
39	T41=T(I+K+3)/TAV-T1
40	T3121=T31/C31-T21/C21
41	T4121=T41/C41-T21/C21
42	A3121=A31/C31-A21/C21
43	A4121=A41/C41-A21/C21
44	B3121=B31/C31-B21/C21
45	B4121=B41/C41-B21/C21

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46	A=(T4121*B3121-T3121*B4121)/(A4121*B3121-A3121*B4121)
47	B=(T3121-A*A3121)/B3121
48	C=(T21-A*A21-B*B21)/C21
49	D=T1-A*A1-B*B1-C*C1
50	ZN=ZN/PAV
51	OTMN=((((A*ZN+B)*ZN+C)*ZN+D)*TAV
52	GOTO 10
53	END IF
54	3 IF(ISC.EQ.3)THEN
55	IF(I.LE.LVEL-2) J=I
56	IF(I.EQ.LVEL-1) J=I-1
57	IF(I.EQ.LVEL) J=I-2
58	PAV = (P(J) + P(J+1) + P(J+2))/3D0
59	TAV = (T(J) + T(J+1) + T(J+2))/3D0
60	P1=P(J)/PAV
61	P2=P(J+1)/PAV
62	P3=P(J+2)/PAV
63	T1=T(J)/TAV
64	T2=T(J+1)/TAV
65	T3=T(J+2)/TAV
66	A=T3/(P3-P2)/(P3-P1)+T2/(P2-P1)/(P2-P3)+
67	* T1/(P1-P2)/(P1-P3)
68	B=(T2-T3)/(P2-P3)-A*(P2-P3)
69	C=T2-(A*P2+B)*P2
70	ZN=ZN/PAV
71	OTMN = ((A * ZN + B) * ZN + C) * TAV
72	GOTO 10
73	END IF
74	4 IF(ISC.EQ.4)
75	*OTMN=(T(I)-T(I+1))/(P(I)-P(I+1))*(ZN-P(I))+T(I)
76	10 CONTINUE
77	IF(IPRB.EQ.4)WRITE(6,'(1X,2I4,6(D11.4,1X))')
78	*ISC,I,P(I),P(I+1),T(I),T(I+1),ZNEW,OTMN
79	IF(ISC.LE.1.OR.ISC.EQ.4) GOTO 20
80	IF(T(I).GE.OTMIN.AND.T(I+1).LE.OTMIN) GOTO 20
81	IF(T(I).LE.OTMIN.AND.T(I+1).GE.OTMIN) GOTO 20
82	ITR=ITR+1
83	GOTO(2,2,3,4),ISC+ITR
84	20 RETURN
85	END

```
SUBROUTINE LENGTH
1
         IMPLICIT REAL*8(A-H,O-Z)
\mathbf{2}
         COMMON/LE/ IPRC, IPRG, IWA1, IWB1, AA, BB, ITT, JUMP, IG, IALL,
3
                      DZ, AEP(21), ALEN(20), ALENS(20), NLEN, DR, D1,
        *
\mathbf{4}
                      KSUB, IALP, ALP, IQQ, IGA(1400), AGA(1400),
        *
5
                      ITYPE(1400)
6
        *
         KSU=IALL-1
\overline{7}
         AGA(KSU) = AA
8
         IJUMP=1
9
10
         JJUMP=1
11
         GOTO(1000,2000), JUMP
    2000 DD=DR/2D0
12
         IF(ALEN(IWA1).GE.DR.AND.ALEN(IWB1).GE.DR) GOTO 710
13
         IF(ALEN(IWA1).GE.DD.AND.ALEN(IWB1).GE.DD) GOTO 610
14
         GOTO 1000
15
16
     710 KSU=KSU+1
         AGA(KSU)=BB
17
         ITYPE(KSU-1) = -1
18
         IGA(KSU-1)=IG
19
         GOTO 1001
20
21
     610 DO 611 KG=1,2
22
         KSU=KSU+1
         AGA(KSU) = AGA(KSU-1) + DD
23
         ITYPE(KSU-1) = -2
24
     611 IGA(KSU-1)=IG
25
         GOTO 1001
26
    1000 D0=BB-AA
27
         IF(DO.LE.ALEN(1)) THEN
28
                              KSU=KSU+1
29
                              AGA(KSU) = AGA(KSU-1) + DO
30
                              ITYPE(KSU-1)=0
31
                              IGA(KSU-1)=IG
32
                              GOTO 1001
33
                              END IF
34
         D2=(D0+AEP(IWA1)+AEP(IWB1))/2.D 0
35
         IMI=1
36
         IF(IWA1.LT.IWB1) THEN
37
                      IF(D2-D0-AEP(IWA1).LT.-DZ) GOTO 1
38
39 C-- A ---
                      D1=D0
40
                      IQQ=IWA1
41
                      CALL MESH
42
                      IF(KSUB.EQ.0) GOTO 2
43
                      DO 3 KG=1,KSUB
44
                      KSU=KSU+1
45
```

App	endix	D
p p		_

46		AGA(KSU)=AGA(KSU-1)+ALEN(IWA1+KG-1)
47		ITYPE(KSU-1)=IWA1+KG-1
48	3	IGA(KSU-1)=IG
49		IF(IALP.EQ.0) GOTO 1001
50		IF(ALP.GT.ALEN(IWA1+KG-1)) GOTO 2
51		KSU=KSU-1
52		IMI=0
53	2	KSU=KSU+1
54		AGA(KSU)=AGA(KSU-IMI)+ALP
55		ITYPE(KSU-1)=0
56		IF(IMI.EQ.0) ITYPE(KSU-1)=-(IWA1+KSUB-1)
57		IGA(KSU-1)=IG
58		GOTO 1001
59	C AB-A	
60	1	DPLUS=0D0
61		IF(D2-AEP(IWB1)-ALEN(IWB1).LTDZ) DPLUS=D2-AEP(IWB1)
62		D1=D2-AEP(IWA1)+DPLUS
63		IQQ=IWA1
64		CALL MESH
65		IF(KSUB.EQ.0) GOTO 6
66		DO 5 KG=1,KSUB
67		KSU=KSU+1
68		AGA(KSU)=AGA(KSU-1)+ALEN(IWA1+KG-1)
69		ITYPE(KSU-1)=IWA1+KG-1
70	5	IGA(KSU-1)=IG
71		IF(DPLUS.EQ.O.D 0) GOTO 6
72		IF(IALP.EQ.0) GOTO 1001
73		IF(ALP.LT.ALEN(IWA1+KSUB-1)) GOTO 55
74		KSU=KSU+1
75		AGA(KSU) = AGA(KSU-1) + ALP
76		TTYPE(KSU-1)=0
77		IGA(KSU-1)=IG
78		
79	55	AGA(KSU) = AGA(KSU) + ALP
80		IIIPE(KSU-1) = -IIIPE(KSU-1)
81		GUIU 1001
82	C AB-B	
83	0	DI=DZ-AEP(IWBI)+ALP
84	00	
85		VALL MEDI TE(TAID ED A) COTO 7
80		LE (THEE, EQ. V) GUID (RGII-RGIIT1
87		VCV(RdI) = VCV(RdII - 1) + VID VDO - VDO + I
88		
89		TITE(VOLT) - C
90		

Appendix D

91	7	IF(KSUB.EQ.0) GOTO 1001
92		IF(ALP.GT.ALEN(KSUB+IWB1-1)) GOTO 77
93		KSU=KSU-1
94		IMI=0
95	77	DO 8 KG=1,KSUB
96		KSU=KSU+1
97		AGA(KSU)=AGA(KSU-IMI)+ALEN(KSUB+IWB1-KG)
98		IF(IMI.EQ.1) GOTO 88
99		ITYPE(KSU-1)=-(KSUB+IWB1-KG)
100		IMI=1
101		GOTO 8
102	88	ITYPE(KSU-1)=KSUB+IWB1-KG
103		TGA(KSU-1)=TG
104	8	CONTINUE
105	-	GOTO 1001
106		END IF
107	С В	-
108		IF(IWA1.GT.IWB1) THEN
109		TF(D2-D0-AFP(TWB1), LT, -DZ) GOTO 11
110		D1=D0
111		IQQ=IWB1
112		CALL MESH
113		IF(IALP.EQ.0) GOTO 132
114		KSU=KSU+1
115		AGA(KSU) = AGA(KSU-1) + ALP
116		ITYPE(KSU-1)=0
117		TGA(KSU-1)=TG
118	12	TF(KSUB, EQ, 0) GOTO 1001
119		TF(ALP,GT,ALEN(KSUB+TWB1-1)) GOTO 132
120		KSU=KSU-1
121		TMT=0
122	132	DO 13 KG=1.KSUB
123		KSU=KSU+1
124		AGA(KSU)=AGA(KSU-IMI)+ALEN(KSUB+IWB1-KG)
125		IF(IMI.EQ.1) GOTO 133
126		ITYPE(KSU-1)=-(KSUB+IWB1-KG)
127		IMI=1
128		GOTO 13
129	133	ITYPE(KSU-1)=KSUB+IWB1-KG
130		IGA(KSU-1)=IG
131	13	CONTINUE
132		GOTO 1001
133	C AB-A	
134	11	D1=D2-AEP(IWA1)
135		DPLUS=0D0

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136		IF(D1.GE.ALEN(IWA1)) GOTO 111
137		DPLUS=D1
138		GOTO 16
139	111	
140		CALL MESH
141		TF(KSUB.EQ.0) GOTO 14
142		DO 15 KG=1 KSUB
143		KSII=KSII+1
144		AGA(KSU) = AGA(KSU-1) + ALEN(TWA1 + KG-1)
145		TTYPE(KSU-1) = TWA1 + KG-1
146	15	TGA(KSII-1)=TG
147	10	TE(TALP, EQ. 0) GOTO 16
1/18	14	$DPI IIS = \Delta I P$
140	C	AB-B
150	16	D1=D2-AFP(TWR1)+DPIIIS
151	10	TOO = TWB1
152		CALL MESH
152		TE(TALP ED O) COTO 17
154		
154		ACA(KSII) = ACA(KSII-1) + AIP
156		TTVPF(KGII-1)=0
157		TCA(KSU-1) = TC
157		TE(ALP CT ALEN(KSUB+TWB1-1)) COTO 17
150		KGII=KGII-1
160		TMT=0
161	17	TE(KSUB ED O) COTO 1001
160	11	D0 18 KC=1 KGUB
162		KGII=KGII+1
164		ACA(KGII) = ACA(KGII - TMT) + AI FN(KGIIB + TWB1 - KC)
165		TE(IMI ED 1) COTO 188
166		TTVPF(KSII-1) = -(KSIIB+TWB1-KG)
167		TMT=1
168		GULU 18
169	188	TTYPE(KSII-1) = KSIIB + TWB1 - KG
170	100	TGA(KSU-1)=TG
171	18	
172	10	GUTU 1001
172		FND IF
174	C	AB
175	0	D1 = D0/2D0
176		TOO=TWA1
177		CALL WEGH
178		TE(KSUB ED O) THEN
170		KSII=KSII+1
180		AGA(KSII) = AGA(KSII - 1) + AIP

181		ITYPE(KSU-1)=0		
182		IGA(KSU-1)=IG		
183		KSU=KSU+1		
184		AGA(KSU)=AGA(KSU-1)+ALP		
185		ITYPE(KSU-1)=0		
186		IGA(KSU-1)=IG		
187		GOTO 1001		
188		END IF		
189		DO 23 KG=1,KSUB		
190		KSU=KSU+1		
191		AGA(KSU)=AGA(KSU-1)+ALEN(IWA1+KG-1)		
192		ITYPE(KSU-1)=IWA1+KG-1		
193	23	IGA(KSU-1)=IG		
194		IF(IALP.EQ.O) GOTO 24		
195		IF(ALP.GT.ALEN(IWA1+KSUB-1)) THEN		
196		KSU=KSU+1		
197		AGA(KSU)=AGA(KSU-1)+ALP+ALP		
198		ITYPE(KSU-1)=0		
199		IGA(KSU-1)=IG		
200		GOTO 24		
201		END IF		
202		KSU=KSU-1		
203		IMI=0		
204	22	KSU=KSU+1		
205		AGA(KSU)=AGA(KSU-IMI)+ALP		
206		ITYPE(KSU-1)=-(IWA1+KSUB-1)		
207		IGA(KSU-1)=IG		
208		KSU=KSU+1		
209		AGA(KSU)=AGA(KSU-1)+ALP		
210		ITYPE(KSU-1)=0		
211		IGA(KSU-1)=IG		
212		KSU=KSU-1		
213	24	DO 26 KG=1,KSUB		
214		KSU=KSU+1		
215		AGA(KSU)=AGA(KSU-IMI)+ALEN(KSUB+IWB1-KG)		
216		IF(IMI.EQ.1) GOTO 266		
217		ITYPE(KSU-1)=-(KSUB+IWB1-KG)		
218		IMI=1		
219		GOTO 26		
220	266	ITYPE(KSU-1)=KSUB+IWB1-KG		
221		IGA(KSU-1)=IG		
222	26	CONTINUE		
223	1001	IALL=KSU+1		
224		RETURN		
225		END		

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1	SUBROUTINE	MESH		
2	IMPLICIT REAL*8(A-H,O-Z)			
3	COMMON/LE/	<pre>IPRC,IPRG,IWA1,IWB1,AA,BB,ITT,JUMP,IG,IALL,</pre>		
4	*	DZ,AEP(21),ALEN(20),ALENS(20),NLEN,DR,D1,		
5	*	<pre>KSUB,IALP,ALP,IQQ,IGA(1400),AGA(1400),</pre>		
6	*	ITYPE(1400)		
7	D2=0D0			
8	IALP=0			
9	ALP=ODO			
10	DO 1 LG=IQQ,NLEN			
11	D2=D2+ALEN(LG)			
12	IF(D2-D1.GT.DZ) THEN			
13	IALP=1			
14	ALP=D1-D2+ALEN(LG)			
15	KSUB=LG-IQQ			
16	GOTO 2			
17	END IF			
18	IF(DABS(D2-	-D1).LT.DZ) THEN		
19	KSUB=LG-IQ	↓ +1		
20	GOTO 2			
21	END IF			
22	1 CONTINUE			
23	KSUB=LG-IQ	Q+1		
24	2 CONTINUE			
25	CG			
26	IF(IPRG.EQ	.1) WRITE(6,'(1X,8I5,1X,3F10.7)')		
27	*IG,ITT,IWA1,IWB1,IQQ,LG,KSUB,IALP,ALP,D1,D2			
28	RETURN			
29	END			

Appendix D

```
SUBROUTINE CONT(VI, TP, RS, RF, RO, UH, OUTC)
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
3
         COMMON/CO/ IPRD, ICT, CV(69), CD(3, 69), CT(3), SUMH
         GOTO(40,400),ICT
4
         DO 100 I=1,69
5
      40 IF(VI.GT.CV(I)) GOTO 100
6
         I2=I
\overline{7}
         GOTO 200
8
     100 CONTINUE
9
10
     200 IF(I2.EQ. 1) I2=I2+1
         IF(I2.EQ.69) I2=I2-1
11
         I1=I2-1
12
         I3=I2+1
13
         V1=CV(I1)
14
         V2=CV(I2)
15
16
         V3=CV(I3)
         DO 300 I=1,3
17
         C1=CD(I,I1)
18
         C2=CD(I,I2)
19
         C3=CD(I,I3)
20
21
         A=C3/(V3-V2)/(V3-V1)+C2/(V2-V1)/(V2-V3)+
        * C1/(V1-V2)/(V1-V3)
22
         B=(C2-C3)/(V2-V3)-A*(V2+V3)
23
         C=C2-(A*V2+B)*V2
24
     300 \text{ CT(I)} = (A*VI+B)*VI+C
25
26
         ICT = 2
         IF(IPRD.EQ.1)WRITE(6,'(/,6X,5HCT(1),7X,5HCT(2),7X,
27
        *5HCT(3),8X,2HR0,8X,2HTP,/,/,1X,5D12.3,/,/,7X,2HRS,10X,
28
        *2HRF,10X,2HUH,8X,4HOUTC,8X,4HSUMH,10X,2HAC,/)') CT(1),
29
        *CT(2),CT(3),R0,TP
30
     400 CST=CT(2)+(CT(2)-CT(1))*(TP-296)/36D0
31
         OUTC=UH*DTANH(1.43879*VI/2D0/TP)*VI*(RS*CST+RF*CT(3))/R0
32
         SUMH=SUMH+OUTC
33
         AC=1DO-DEXP(-SUMH)
34
         IF(IPRD.EQ.1)WRITE(6, '(1X,6D12.3)')RS,RF,UH,OUTC,SUMH,AC
35
         RETURN
36
         END
37
```
Appendix D

```
SUBROUTINE FARWG(AABB, TF, PF, OFWG, IPRINT)
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
3
         COMMON/FA/ MOLL(7), AMASS(10), IFAR, OFWGS, IVI(7)
         DIMENSION SUM(7,110)
\mathbf{4}
         OFWG=ODO
5
         GOTO(100,200,500,550), IFAR
6
     100 READ (8, '(1X, 1115)')(IVI(I), I=1,7), ISV, ITA, ITB, IDT
\overline{7}
         WRITE(6, '(1X, 1115)')(IVI(I), I=1,7), ISV, ITA, ITB, IDT
8
         DV=1D0/DFLOAT(ISV-1)
9
10
         IST=(ITB-ITA)/IDT+1
11
         IFAR=2
         RETURN
12
     200 READ (8, '(1X, F10.1)') POS
13
         WRITE(6, '(1X, F10.1)') POS
14
     300 DO 400 L=1,7
15
16
         IF(IVI(L).EQ.0) GOTO 400
         DO 400 IV=1,ISW
17
         IX=(IV-1)*IST
18
         READ(8, '(1X, 10E11.4)') (SUM(L, IX+J), J=1, IST)
19
     400 CONTINUE
20
21
     550 IF(POS.GT.AABB) THEN
22
                           IFAR=4
                           RETURN
23
                           END IF
24
         IF(POS.EQ.AABB) THEN
25
                           IFAR=3
26
                           RETURN
27
                           END IF
28
         GOTO 200
29
     500 DO 610 I=1, ISV-1
30
         V1=POS-5D-1+(IV-1)*DV
31
32
         V2=V1+DV
         IF(AABB.GE.V1.AND.AABB.LE.V2) GOTO 620
33
     610 CONTINUE
34
     620 DO 630 J=1,IST-1
35
         T1=ITA+(J-1)*IDT
36
         T2=TA1+IDT
37
         IF(TF.LT.T1) GOTO 640
38
39
         IF(TF.GE.TA1.AND.TF.LE.TA2) GOTO 640
     630 CONTINUE
40
         J=IST-1
41
     640 CONTINUE
42
         DO 700 M=1,7
43
44
         IF( IVI(M).EQ.0) GOTO 700
         IF(MOLL(M).EQ.0) GOTO 700
45
```

```
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```

```
46 I1=(I-1)*IST+J
```

- 47 I2=I1+1
- 48 J1=I1+IST
- 49 J2=I2+IST
- 50 SI=(SUM(M,I2)-SUM(M,I1))*(TF-T1)/(T2-T1)+SUM(M,I1)
- 51 SJ=(SUM(M,J2)-SUM(M,J1))*(TF-T1)/(T2-T1)+SUM(M,J1)
- 52 SUV=(SI-SJ)*(AABB-PA1)/(V2-V1)+SI
- 53 700 OFWG=OFWG+SUV*AMASS(M)*PF
- 54 C 700 OFWG=OFWG+SUV
- 55 OFWGS=OFWGS+OFWG
- 56 IF(IPRINT.EQ.1)
- 57 *WRITE(6,'(1X,4I5,E10.5)')I1,I2,J1,J2,OFWG,OFWGS
- 58 RETURN
- 59 END

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```
SUBROUTINE GAUSS (DRR, GAB, GCC, OUTG)
1
         IMPLICIT REAL*8(A-H,O-Z)
\mathbf{2}
         COMMON/GA/ IPRE, IGNU, EPSN, ERG, ERGB, ITY, IGS, IGI, OUTGS,
3
        *
                      NG, OUTSS(14000), H2OC, OFWG, LS1, LS2, ITRN, JSWS
\mathbf{4}
         DIMENSION
                     XG(25), WG(29), XXG(55), WWG(55)
5
         GOTO(500,600), JUMPG
6
     500 OUTG= ODO
\overline{7}
         ER = ODO
8
         Ν
              = IGNU-1
9
     501 \text{ N1} = \text{N+1}
10
         IF(N1.GT.10) GOTO 508
11
         F=0D0
12
         K=N*N1/2
13
         DO 504 I=1,N1
14
         L = K+I
15
16
         VGA = GCC * XXG(L) + GAB
         GOTO(503,502), JSWS
17
     502 INY=(IGS-1)*N1+I
18
         OUT=OUTSS(INY)
19
         IF(ITRN.EQ.2.AND.OUT.GT.2D1) GOTO 504
20
21
         IF(IGNU.GT.1)CALL SHAPE(LS1,LS2,VGA,OUTS)
         OUT=OUT+OUTS+H2OC+OFWG
22
         IF(ITRN.EQ.1)
                            F=F+WWG(L)*OUT
23
         IF(ITRN.EQ.2)
                            F=F+WWG(L)*DEXP(-OUT)
24
         OUTSS(INY)=OUT
25
         GOTO 504
26
     503 IF(IGNU.GT.1)CALL SHAPE(LS1,LS2,VGA,OUTS)
27
         IF(ITRN.EQ.2.AND.OUTS.GT.2D1) GOTO 504
28
         IF(ITRN.EQ.1) F=F+WWG(L)*OUTS
29
         IF(ITRN.EQ.2) F=F+WWG(L)*DEXP(-OUTS)
30
     504 CONTINUE
31
         F=F*GCC
32
         IF(IGNU.NE. 0) GOTO 509
33
                 .EQ.-1) GOTO 507
34
         IF(N
         IF(DABS(F).GT.1D-30) GOTO 505
35
         ER=0D0
36
         GOTO 508
37
     505 ER=DABS(F-FR)/F
38
39
     506 IF(ER.LT.EPSN) GOTO 508
     507 FR=F
40
         N=N+1
41
         IF(IPRE.EQ.2)WRITE(6, '(1X,2I8,2D15.8)')IGI,N1,F,ER
42
         GOTO 501
43
44
     508 ERG=ER
         ERGB=ER*F
45
```

```
509 OUTG=F
46
         IF(IPRE.LT.1) GOTO 510
47
         NG = NG+N1
48
         IDAB=INT(1D-5+GCC*2D5)
49
         GAA =GAB-GCC
50
         OUTGS=OUTGS + OUTG
51
         WRITE(6, '(1X, I5, 3I4, I6, F12.5, 2D22.14)')
52
        *NG, IGS, IGI, ITY, IDAB, GAA, OUTG, OUTGS
53
     510 RETURN
54
     600 DO 604 I=1,9
55
         INXG=I*(I+1)/2
56
         J=(I+1)/2
57
         IF(I-(I/2)*2.EQ.0) GOTO 601
58
         GOTO 602
59
     601 KKW=KKW+1
60
         XXG(INXG+J+1)=ODO
61
         WWG(INXG+J+1)=WG(KKW)
62
     602 DO 603 K=1,J
63
         KK=I-K+2
64
         KX=KKX+J-K+1
65
66
         KW=KKW+J-K+1
         XXG(INXG+KK) = XG(KX)
67
         XXG(INXG+ K) = -XG(KX)
68
         WWG(INXG+KK) = WG(KW)
69
         WWG(INXG+ K) = WG(KW)
70
71
     603 CONTINUE
         KKX=KKX+J
72
         KKW=KKW+J
73
     604 CONTINUE
74
         JUMPG=1
75
         GOTO 500
76
```

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77	DATA	XXG(1),KKX,XG/OD0,0,5.77350269189626D-1,
78	*	7.74596669241483D-1,3.39981043584856D-1,
79	*	8.61136311594053D-1,5.38469310105683D-1,
80	*	9.06179845938664D-1,2.38619186083197D-1,
81	*	6.61209386466265D-1,9.32469514203152D-1,
82	*	4.05845151377397D-1, 7.41531185599394D-1,
83	*	9.49107912342759D-1, 1.83434642495650D-1,
84	*	5.25532409916329D-1, 7.96666477413627D-1,
85	*	9.60289856497536D-1,3.24253423403809D-1,
86	*	6.13371432700590D-1,8.36031107326636D-1,
87	*	9.68160239507626D-1,1.48874338981631D-1,
88	*	4.33395394129247D-1, 6.79409568299024D-1,
89	*	8.65063366688985D-1,9.73906528517172D-1/
90	DATA	WWG(1),KKW,WG/2D0,0,1.0000000000000 0,
91	*	8.8888888888889D-1,5.5555555555556D-1,
92	*	6.52145154862546D-1, 3.47854845137454D-1,
93	*	5.68888888888889D-1, 4.78628670499366D-1,
94	*	2.36926885056189D-1, 4.67913934572691D-1,
95	*	3.60761573048139D-1,1.71324492379170D-1,
96	*	4.17959183673469D-1,3.81830050505119D-1,
97	*	2.79705391489277D-1,1.29484966168870D-1,
98	*	3.62683783378362D-1,3.13706645877887D-1,
99	*	2.22381034453374D-1, 1.01228536290376D-1,
100	*	3.30239355001260D-1, 3.12347077040003D-1,
101	*	2.60610696402935D-1,1.80648160694857D-1,
102	*	0.81274388361574D-1,2.95524224714753D-1,
103	*	2.69266719309996D-1,2.19086362515982D-1,
104	*	1.49451349150581D-1, 0.66671344308688D-1/
105	DATA	JUMPG/2/
106	END	

```
SUBROUTINE SHAPE(LL1,LL2,VGA,OUTS)
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
         COMMON/SH/ IPRF, REGO, IINT, DVPR, PDLR, PLNZ, VDLR, VLNZ, TAV,
3
                     PAV, ALOR(10), AKO(10), XS(10), KSHP, IVDY,
4
        *
                     LMOD(7), RMOD(7)
\mathbf{5}
        *
         COMMON/HA/ POSA(3000), STRA(3000), ENRA(3000), ALFA(3000),
6
        *ALFT(3000),CPLG(3000),STRT(3000),ISIA(3000),IQSW(3000)
\overline{7}
         COMMON/FA/ MOLL(7), AMASS(10), IFAR, OFWGS, IVI(7)
8
         OUTS = ODO
9
10
         DO 2O N = LL1, LL2
11
         М
              = ISIA(N)
         ALR = ALOR(M) * ALFA(N)
12
         POS = POSA(N)
13
         DIST=POS-VGA
14
         IF(IINT .EQ.
                          0) GOTO 25
15
16
         IF(DIST.LT.-DVPR.OR.DIST.LT.-RMOD(M)) GOTO 20
         IF(DIST.GT. DVPR.OR.DIST.GT. RMOD(M)) GOTO 21
17
      25 DIST=DABS(DIST)
18
         IF(DIST.GT.REGO.AND.IQSW(N).LT.0) GOTO 20
19
         IF(KSHP.EQ. 0) GOTO 500
20
21
         IF(KSHP.GT. 0) GOTO(194,195,196,196) ,KSHP
         IF(KSHP.EQ.-1) GOTO(500,194,195,196) ,LMOD(M)+1
22
     196 FLOR = ALR/3.1415926535897932D0/(ALR*ALR+DIST*DIST)
23
         IF(KSHP.EQ.4) THEN
24
         CALL WING(POS, VGA, TAV, LMOD(M), ALR, FLOR, OUTW)
25
         IF(OUTW.LT.ODO) GOTO 20
26
         OUTS = OUTS + STRT(N) * AMASS(M) * FLOR * OUTW
27
         GOTO 340
28
         END IF
29
         OUTS = OUTS + STRT(N) * AMASS(M) * FLOR
30
         GOTO 340
31
     195 X
              = XS(M) * DIST
32
         OUTS = OUTS + STRT(N) *
33
                                     AKO(M) * DEXP(-X*X)
34
         GOTO 340
    500 IF(DIST.GT.VLNZ.OR .PAV.GT.PLNZ) GOTO 196
35
         IF(DIST.LT.VDLR.AND.PAV.LT.PDLR) GOTO 195
36
     194 X
              = XS(M) * DIST
37
         Y
              = XS(M) * ALR
38
39
         IF(IVDY.EQ.0)OUTS=OUTS+ VOIGTD(X,Y) * AKO(M) * STRT(N)
         IF(IVDY.EQ.1)OUTS=OUTS+ VOIGTY(X,Y) * AKO(M) * STRT(N)
40
     340 IF(IPRF.EQ.1)WRITE(6, '(1X,3I4,3D13.8,2F11.6,4D11.4)')
41
        *N,M,KSHP,VGA,OUTS,STRT(N),POS,DIST,AMASS(M),AKO(M),ALR
42
      20 CONTINUE
43
      21 RETURN
44
         END
45
```

Appendix D

```
FUNCTION VOIGTY(X,Y)
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
         DIMENSION RA(32), CA(32), RB(32), CB(32), B(44), AK(5),
3
        *AM(5),DY(4),A(42),WWH(10),XXH(10)
\mathbf{4}
         X2=X*X
5
         Y2=Y*Y
6
         IF(X-1D1)200,201,201
\overline{7}
     200 IF(Y-1D0)202,202,203
8
     203 RA(1)=0D0
9
10
         CA(1)=ODO
11
         RB(1)=1D0
         CB(1)=0D0
12
         RA(2)=X
13
         CA(2)=Y
14
         RB(2) = 5D - 1 - X2 + Y2
15
16
         CB(2) = -2D0 * X * Y
         CB1=CB(2)
17
         UV1=0D0
18
         DO 250 J=2,31
19
         JMINUS=J-1
20
21
         JPLUS=J+1
         FLOATJ=DFLOAT(JMINUS)
22
         RB1=2D0*FLOATJ+RB(2)
23
         RA1=-FLOATJ*(2DO*FLOATJ-1DO)/2DO
24
         RA(JPLUS)=RB1*RA(J)-CB1*CA(J)+RA1*RA(JMINUS)
25
         CA(JPLUS)=RB1*CA(J)+CB1*RA(J)+RA1*CA(JMINUS)
26
         RB(JPLUS)=RB1*RB(J)-CB1*CB(J)+RA1*RB(JMINUS)
27
         CB(JPLUS)=RB1*CB(J)+CB1*RB(J)+RA1*CB(JMINUS)
28
         UV=(CA(JPLUS)*RB(JPLUS)-RA(JPLUS)*CB(JPLUS))/
29
        *
             (RB(JPLUS)*RB(JPLUS)+CB(JPLUS)*CB(JPLUS))
30
         IF(DABS(UV-UV1).LT.1D-6) GOTO 251
31
         UV1=UV
32
33
     250 CONTINUE
     251 VOIGTY=UV/1.77245385090552D0
34
         RETURN
35
     202 IF(X-2D0)301,301,302
36
     301 AINT=1D0
37
         MAX=12D0+5D0*X2
38
39
         KMAX=MAX-1
         DO 303 K=0,KMAX
40
         AJ=MAX-K
41
     303 AINT=AINT*(-2D0*X2)/(2D0*AJ+1D0)+1D0
42
         U=-2DO*X*AINT
43
         GOTO 304
44
     302 IF(X-4.5D0)305,306,306
45
```

```
305 B(43)=0D0
46
         B(44) = 0D0
47
         J=42
48
         DO 307 K=1,42
49
         B(J)=4D-1*X*B(J+1)-B(J+2)+A(J)
50
     307 J=J-1
51
         U=B(3)-B(1)
52
         GOTO 304
53
     306 AINT=1D0
54
         MAX=2D0+4D1/X
55
56
         AMAX=MAX
         DO 308 K=1,MAX
57
         AINT=AINT*(2D0*AMAX-1D0)/(2D0*X2)+1D0
58
     308 AMAX=AMAX-1D0
59
         U=-AINT/X
60
     304 V=1.7724538509055D0*DEXP(-X2)
61
         H=2D-2
62
         JM=Y/H
63
         IF(JM)310,311,310
64
     311 H=Y
65
66
     310 Z=0D0
         L=0
67
         DY(1)=0D0
68
     312 DY(2)=H/2D0
69
         DY(3)=DY(2)
70
71
         DY(4) = H
     318 AK(1)=0D0
72
         AM(1) = ODO
73
         DO 313 J=1,4
74
         YY=Z+DY(J)
75
         UU=U+5D-1*AK(J)
76
         VV=V+5D-1*AM(J)
77
         AK(J+1)=2DO*(YY*UU+X*VV)*H
78
         AM(J+1) = -2DO*(1DO+X*UU-YY*VV)*H
79
         IF(J-3)313,314,313
80
     314 \text{ AK}(4) = 2D0 * \text{AK}(4)
81
         AM(4)=2DO*AM(4)
82
     313 CONTINUE
83
         Z=Z+H
84
         L=L+1
85
         U=U+0.1666666666667DO*(AK(2)+2DO*AK(3)+AK(4)+AK(5))
86
         V=V+0.166666666666667D0*(AM(2)+2D0*AM(3)+AM(4)+AM(5))
87
         IF(JM)315,320,315
88
89
     315 IF(L-JM)318,317,320
     317 AJM=JM
90
```

Appendix D

```
H=Y-AJM*H
91
         GOTO 312
92
93
     320 VOIGTY=V/1.7724538509055D0
         RETURN
94
     201 F1=0D0
95
         DO 330 J=1,10
96
     330 F1=F1+WWH(J)/(Y2+(X-XXH(J))*(X-XXH(J)))+
97
        *WWH(J)/(Y2+(X+XXH(J))*(X+XXH(J)))
98
         VOIGTY=Y*F1/3.1415926535897D0
99
100
         RETURN
101
         DATA WWH/
        *4.622436696006D-1,2.866755053628D-1,1.090172060200D-1,
102
        *2.481052088746D-2,3.243773342238D-3,2.283386360163D-4,
103
        *7.802556478532D-6,1.086069370769D-7,4.399340992273D-10,
104
        *2.229393645534D-13/
105
106
         DATA XXH/
        *0.2453407083009D0,0.7374737285454D0,1.2340762153953D0,
107
        *1.7385377121166D0,2.2549740020893D0,2.7888060584281D0,
108
        *3.3478545673832D0,3.9447640401156D0,4.6036824495507D0,
109
        *5.3874808900112D0/
110
111
         DATA A/
        *0.0D 0,0.19999999D 0,0.0D 0,-0.18400000D 0,
112
        *0.0D 0,0.15583999D 0,0.0D 0,-0.12166400D 0,
113
        *0.0D 0,0.87708159D-1,0.0D 0,-0.58514124D-1,
114
        *0.0D 0,0.36215730D-1,0.0D 0,-0.20849765D-1,
115
        *0.0D 0,0.11196011D-1,0.0D 0,-0.56231896D-2,
116
        *0.0D 0,0.26487634D-2,0.0D 0,-0.11732670D-2,
117
        *0.0D 0,0.48995199D-3,0.0D 0,-0.19336308D-3,
118
        *0.0D 0,0.72287745D-4,0.0D 0,-0.25655512D-4,
119
        *0.0D 0,0.86620736D-5,0.0D 0,-0.27876379D-5,
120
        *0.0D 0,0.85668736D-6,0.0D 0,-0.25184337D-6,
121
        *0.0D 0,0.70936022D-7/
122
         END
123
```

Appendix D

```
FUNCTION VOIGTD(X,Y)
1
         DIMENSION B(22), RI(15), XN(15), YN(15), D0(25), D1(25),
\mathbf{2}
3
        *D2(25),D3(25),D4(25),HN(25),XX(3),HH(3),NBY2(19),C(21)
         IF(JUMP.GT.0) GOTO 104
\mathbf{4}
         JUMP=1
5
         DO 101 I=1,15
6
     101 RI(I) = -I/2.
\overline{7}
         DO 103 I=1,25
8
         HN(I) = H*(I-.5)
9
10
         CO=4.*HN(I)*HN(I)/25.-2.
11
         DO 102 J=2,21
     102 B(J+1)=C0*B(J)-B(J-1)+C(J)
12
         DO(I)=HN(I)*(B(22)-B(21))/5.
13
         D1(I)=1.-2.*HN(I)*D0(I)
14
         D2(I) = (HN(I) * D1(I) + D0(I))/RI(2)
15
16
         D3(I) = (HN(I) * D2(I) + D1(I)) / RI(3)
     103 D4(I) = (HN(I) * D3(I) + D2(I))/RI(4)
17
     104 IF (X-5.) 105,112,112
18
     105 IF (Y-1.) 110,110,106
19
     106 IF (X.GT.1.85*(3.6-Y)) GOTO 112
20
21
         IF (Y.LT.1.45)
                                   GOTO 107
         I=Y+Y
22
         GOTO 108
23
     107 I=11.*Y
24
     108 J=X+X+1.85
25
26
         MAX=XN(J)*YN(I)+.46
         MIN=JMINO(16,21-2*MAX)
27
         UU=Y
28
         VV=X
29
         DO 109 J=MIN,19
30
         U=NBY2(J)/(UU*UU+VV*VV)
31
32
         UU=Y+U*UU
33
     109 VV=X-U*VV
         VOIGTD=UU/(UU*UU+VV*VV)/1.772454
34
         RETURN
35
     110 Y2=Y*Y
36
         IF (X+Y.GT. 5.) GOTO 113
37
         N=X/H
38
39
         DX=X-HN(N+1)
         U = (((D4(N+1)*DX+D3(N+1))*DX+D2(N+1))*DX+D1(N+1))*
40
        *DX+DO(N+1)
41
         V=1.-2.*X*U
42
         VV=EXP(Y2-X*X)*COS(2.*X*Y)/1.128379-Y*V
43
         UU=-Y
44
         MAX=5.+(12.5-X)*.8*Y
45
```

```
DO 111 I=2,MAX,2
46
         U=(X*V+U)/RI(I)
47
         V = (X * U + V) / RI(I + 1)
48
         UU = -UU * Y2
49
     111 VV=VV+V*UU
50
         VOIGTD=1.128379*VV
51
         RETURN
52
     112 Y2=Y*Y
53
         IF (Y.LT.11.-.6875*X) GOTO 113
54
         U=X-XX(3)
55
56
         V=X+XX(3)
         VOIGTD=Y*(HH(3)/(Y2+U*U)+HH(3)/(Y2+V*V))
57
         RETURN
58
     113 U=X-XX(1)
59
         V = X + XX(1)
60
         UU=X-XX(2)
61
         VV = X + XX(2)
62
         VOIGTD=Y*(HH(1)/(Y2+U*U)+HH(1)/(Y2+V*V)+
63
        *HH(2)/(Y2+UU*UU)+HH(2)/(Y2+VV*VV))
64
         RETURN
65
66
         DATA JUMP/-1/
         DATA B(1), B(2)/0., .7093602E-7/
67
         DATA XN/10.,9.,2*8.,7.,6.,5.,4.,7*3./
68
         DATA YN/3*.6,.5,2*.4,4*.3,1.,.9,.8,2*.7/
69
         DATA H/.201/
70
         DATA XX/.5246476,1.65068,.7071068/
71
         DATA HH/.2562121,.02588268,.2820948/
72
         DATA NBY2/
73
        *9.5,9.,8.5,8.,7.5,7.,6.5,6.,5.5,5.,
74
        *4.5,4.,3.5,3.,2.5,2.,1.5,1.,.5/
75
         DATA C/
76
        * .7093602E-7, -.2518434E-6, .8566874E-6,
77
        *-.2787638E-5,.866074E-5,-.2565551E-4,.7228775E-4,
78
        *-.1933631E-3,.4899520E-3,-.1173267E-2,.2648762E-2,
79
        *-.5623190E-2,.1119601E-1,-.2084976E-1,.3621573E-1,
80
        *-.5851412E-1,.8770816E-1,-.121664,.15584,-.184,.2/
81
         END
82
```

Appendix D

1		SUBROUTINE WING(VA,VB,TA,IC,ALR,FLOR,OUTW)
2		IMPLICIT REAL*8(A-H,O-Z)
3		DV=DABS(VA-VB)
4		GOTO(10,20,30,40,50,60,70),IC
5	10	IF(DV.GT.3.5D0) GOTO 11
6		OUTW=1DO
7		RETURN
8	11	OUTW=DEXP(-1.4D0*(DV-3.5D0)**0.25D0)
9		RETURN
10	20	IF(DV.GE.5D-1) GOTO 21
11		OUTW=1DO
12		RETURN
13	21	IF(DV.GE.23D0) GOTO 22
14		OUTW=1.069*DEXP(-0.133*DV)
15		RETURN
16	22	IF(DV.GE.50D0) GOTO 23
17		OUTW=5D-2
18		RETURN
19	23	IF(DV.GE.25D1) GOTO 24
20		OUTW=0.133D0*DEXP(-0.0196*DV)
21		RETURN
22	24	OUTW=-1DO
23		RETURN
24	30	IF(DV.GE.11D0) GOTO 31
25		OUTW=(1D0+2D0*DV/11D0)*DEXP(-2D0*DV/11D0)
26		RETURN
27	31	OUTW=-1DO
28		RETURN
29	40	DW2=(VA+VB)*(VA+VB)
30		DEA=1DO-DEXP(-C2*VA/TA)
31		DEB=1D0-DEXP(-C2*VB/TA)
32		OUTW=VA*DEA*(1D0+ALR/(DW2+ALR*ALR)/PI/FLOR)/VB/DEB
33		RETURN
34	50	DW2=(VA+VB)*(VA+VB)
35		OUTW=VA*VA*(1DO+ALR/(DW2+ALR*ALR)/PI/FLOR)/VB/VB
36		RETURN
37	60	DW2=(VA+VB)*(VA+VB)
38		OUTW=VA*(1D0+ALR/(DW2+ALR*ALR)/PI/FLOR)/VB
39		RETURN
40	70	OUTW=2D0*VA/(1D0+DEXP(-C2*DV/TA))/VB
41		RETURN
42		DATA PI,C2/3.14159265358973,1.43879/
43		END

APPENDIX E

Listing of the Third Group of Programmes

SMTH COMP CHNL

Appendix E

```
PROGRAM SMTH
1
         IMPLICIT REAL*8(A-H,O-Z)
\mathbf{2}
         DIMENSION SM(25000), FR(25000), TRAB(200)
3
         OPEN(UNIT=4, TYPE='OLD', FILE='SMTH.INP')
\mathbf{4}
         OPEN(UNIT=8, TYPE='NEW', FILE='SMTH.DAT')
5
         READ(4,*)IRAD, TBOUND
6
         READ(4,*)WNUA,WNUB,DL,DD,WNU1,WNU2,DR,LE1,LE2,IT,IPD,IO
\overline{7}
         IF(IRAD.EQ.0) OPEN(UNIT=2,TYPE='OLD',FILE='TRAO.DAT')
8
         IF(IRAD.EQ.1) OPEN(UNIT=3,TYPE='OLD',FILE= 'RAD.DAT')
9
10
         IDAT=INT(WNU2-WNU1+1)
11
         IIR=INT(1D0/DR+DR)
         JF=0
12
         DO 100 L =1,IDAT
13
         DO 100 M=1,LE1
14
         IF(IRAD.EQ.1)THEN
15
16
                        READ(3,'(1X,F11.3)') WNUAV
                        READ(3, '(10(1X,E11.6))')(TRAB(I),I=1,IIR)
17
                        GOTO 97
18
                        END IF
19
         IF(IRAD.EQ.O)THEN
20
                        READ(2,*)LL, (TRAB(I), I=1, IIR), TRABS, WNUAV
21
                        END IF
22
      97 IF(M.NE.LE2) GOTO 100
23
         DO 98 LL=1,IIR
24
25
         KL=(L-1)*IIR+LL
         F=WNU1+(KL-1)*DR+DR/2D0-5D-1
26
         IF(F.LT.WNUA-DD) GOTO 98
27
         IF(F.GT.WNUB+DD) GOTO 96
28
         IF(IPD.EQ.1)WRITE(6, '(1X, 15, F10.3, F11.4)')KL, F, TRAB(LL)
29
         JF=JF+1
30
         FR(JF) = F
31
         SM(JF)=TRAB(LL)
32
33
      98 CONTINUE
     100 CONTINUE
34
      96 WRITE(6,*)'
                             JF = ', JF
35
         IF(IO.EQ.1) THEN
36
                      DO 101 I=1,JF
37
                      IF(FR(I).LT.WNUA) GOTO 101
38
39
                      IF(FR(I).GT.WNUB) GOTO 104
                      WRITE(8,*)FR(I),SM(I)
40
     101
                      CONTINUE
41
     104
                      WRITE(8,*)99.99, 99.99
42
                      IF(IT.EQ.0) GOTO 11
43
                      END IF
44
     103 IF(TBOUND.NE.ODO)THEN
45
```

```
DO 102 F=WNUA-DD,WNUB+DD,0.1
46
                        PL=C1*F*F*F/(DEXP(C2*F/TBOUND)-1)
47
    102
                        WRITE(8,*)F,PL
48
    105
                        WRITE(8,*)99.99, 99.99
49
                        END IF
50
        WRITE(6, *)
51
        IDD
             = INT(2D0*DD/DR+DR)
52
        IDL =INT(DL/DR+DR)
53
        WRITE(6,*)' KL = ',KL,'IDD=',IDD,'IDL=',IDL
54
        WRITE(6,*)
55
        WRITE(6,*)'I IDAT JDAT WNUAV TAVW IFIRST ILAST'
56
        WRITE(6,*)
57
        IF1=1
58
        DO 10 WNUAV=WNUA, WNUB, DL
59
        JDAT = 0
60
61
        TAVW
              = 0D0
        FWS=0
62
        DO 20 J=IF1,JF
63
        WNU = FR(J)
64
        IF(WNU.LT.WNUAV-DD) GOTO 19
65
66
        IF(WNU.GT.WNUAV+DD) GOTO 21
        JDAT = JDAT+1
67
        IF(IT.EQ.2) FW = 1DO-DABS(WNU-WNUAV)/DD
68
        IF(IT.EQ.1) FW = 1D0
69
        FWS = FWS+FW
70
        TAVW = TAVW + SM(J) * FW
71
       GOTO 20
72
     19 IF2=J
73
     20 CONTINUE
74
     21 IF1=IF2
75
       TAVW = TAVW/FWS
76
        WRITE(6, '(1X,315,5X,F10.2,F11.4,5X,215)')I,IDAT,JDAT,
77
78
       *WNUAV, TAVW, IF1, J-1
        WRITE(8,*)WNUAV,TAVW
79
     10 CONTINUE
80
        WRITE(8,*)99.99,99.99
81
     11 CONTINUE
82
        DATA C1, C2/ 1.1909596D-5,1.43879D0/
83
84
        END
85 C-----
86 C SMTH.INP
87 C O O
          IRAD TBOUND
88 C WNUA WNUB DL DD WNU1 WNU2 DR LE1 LE2 IT IPD IO
89 C 2135 2250 0.5 .05 1950 2250 0.01 1 1
                                                 0 0
                                                        1
90 C-----
```

Appendix E

```
PROGRAM COMP
1
         IMPLICIT REAL*8(A-H,O-Z)
\mathbf{2}
        DIMENSION SM(25000), FR(25000), TRAB(200),
3
                   FH(2050),H(2050),T(2050),R(2050),SL(3,2),
        *
4
                   PR(20), PT(20), QR(20), QT(20), RR(20), RT(20)
        *
5
         OPEN(UNIT=4,TYPE='OLD',FILE='COMP.INP')
6
         OPEN(UNIT=8, TYPE='NEW', FILE='COMP.DAT')
\overline{7}
         IPL=0
8
         READ(4,*)IPLOTS
9
10
   2000 IPL=IPL+1
11
         INPT=0
         READ(4,*)INPUTS, IGRAF, IRAD, IEQW, OF
12
   1000 \text{ INPT} = \text{INPT+1}
13
         INPTT = INPT
14
         READ(4,*)ITB, TBU, TBL, TBB1, TBB2, SCALE, DREF, DIV
15
16
         READ(4,*)WNUA,WNUB,DL,DD,WNU1,WNU2,DR,LE1,LE2,IT,IPD,IO
         READ(4,*)ICOM, IDEL, IDAY, IBAND
17
      1 FORMAT(1X, I3, 8F6.1)
18
      2 FORMAT(1X,2F7.2,2F7.4,2F7.2,F7.4,5I2)
19
      3 FORMAT(1X,415)
20
      4 FORMAT(/,/,10X,5HCASE:,12,/,/,10X,6HMEAN-H,2X,6HMEAN-F,
21
       *2X,6H MAX-H,2X,6H MAX-F,2X,6H STD-H,2X,6H STD-F,2X,
22
       *5H DATA,3X,11HWNUI [CM-1],/)
23
24 C-----
        IF(IRAD.NE.O.AND.IDAY.EQ.1)
25
                 OPEN(UNIT=3,TYPE='OLD',FILE= 'RAD.DAT;1')
26
         IF(IRAD.NE.O.AND.IDAY.EQ.2)
27
                 OPEN(UNIT=3,TYPE='OLD',FILE= 'RAD.DAT;2')
28
        *
         IF(IRAD.EQ.O.AND.IDAY.LE.1)
29
                 OPEN(UNIT=2,TYPE='OLD',FILE='TRAO.DAT;1')
30
         IF(IRAD.EQ.O.AND.IDAY.EQ.2)
31
                 OPEN(UNIT=2,TYPE='OLD',FILE='TRAO.DAT;2')
32
         IF(ICOM.NE.O)
33
                 OPEN(UNIT=9,TYPE='OLD',FILE= 'HCOM.DAT')
34
         IF(IDEL.NE.O.AND.INPT.EQ.1)
35
                 OPEN(UNIT=7,TYPE='NEW',FILE= 'SCOM.DAT')
36
         TTMAX=0D0
37
         TTMIN=1D10
38
39 C-----
40 C
             PLOT UPPER AND LOWER BOUNDARY TEMP. OR RAD.
       _____
41 C-
    103 IF(TBU.NE.ODO)THEN
42
                       DO 102 F=WNUA, WNUB
43
                       IF(ITB.EQ.0)PL=C1*F*F*F/(DEXP(C2*F/TBU)-1)
44
                       IF(ITB.EQ.1)PL=TBU
45
```

```
IF(TTMIN.GT.PL) TTMIN=PL
46
                       IF(TTMAX.LT.PL) TTMAX=PL
47
                       WRITE(8,*)F,PL
48
    102
                       CONTINUE
49
                       WRITE(8,*)99.99, 99.99
50
                       WRITE(6,*)' TTMIN:',TTMIN,' TTMAX:',TTMAX
51
                       END IF
52
        IF(TBL.NE.ODO)THEN
53
                       DO 105 F=WNUA,WNUB
54
                       IF(ITB.EQ.0)PL=C1*F*F*F/(DEXP(C2*F/TBL)-1)
55
                       IF(ITB.EQ.1)PL=TBL
56
                       IF(TTMIN.GT.PL) TTMIN=PL
57
                       IF(TTMAX.LT.PL) TTMAX=PL
58
                       WRITE(8,*)F,PL
59
    105
                       CONTINUE
60
61
                       WRITE(8,*)99.99, 99.99
                       WRITE(6,*)' TTMIN:',TTMIN,' TTMAX:',TTMAX
62
                       END IF
63
        IF(IO.EQ.O.AND.IT.EQ.O.AND.ICOM.LT.O) GOTO 50
64
             _____
65 C-----
66 C
                START TO RED TRANS. OR RAD. DATA
67 C-----
                      _____
        EQWS=ODO
68
        IDAT=INT(WNU2-WNU1+1)
69
        IIR=INT(1D0/DR+DR)
70
        WRITE(6,*)IDAT,IIR
71
        WRITE(6,*)
72
        JF=0
73
        DO 100 L =1,IDAT
74
        DO 100 M=1,LE1
75
        IF(IRAD.NE.O) THEN
76
                       READ(3,'(1X,F11.3)') WNUAV
77
                       READ(3, '(10(1X,E11.6))')(TRAB(I),I=1,IIR)
78
                       GOTO 97
79
                       END IF
80
        IF(IRAD.EQ.0)READ(2,*) LL,(TRAB(I),I=1,IIR),TRABS,WNUAV
81
     97 IF(M.NE.LE2) GOTO 100
82
        DO 98 LL=1,IIR
83
84
        KL=(L-1)*IIR+LL
        F=WNU1+(KL-1)*DR+DR/2D0-5D-1
85
        IF(F.LT.WNUA-DD) GOTO 98
86
        IF(F.GT.WNUB+DD) GOTO 96
87
        IF(IPD.EQ.1)WRITE(6, '(1X, 15, F10.4, F11.4)')KL, F, TRAB(LL)
88
        JF=JF+1
89
        FR(JF) = F
90
```

```
Appendix E
```

```
EQW=(1DO-TRAB(LL))*DR
91
         EQWS=EQWS+EQW
92
93
         IF(IEQW.EQ. 0) SM(JF) = TRAB(LL)
         IF(IEQW.EQ. 1) SM(JF) = 1DO-TRAB(LL)
94
         IF(IEQW.EQ.-1) SM(JF) = EQWS + OF
95
      98 CONTINUE
96
     100 CONTINUE
97
         WRITE(6,*)
98
      96 WRITE(6,*) 'POINTS BETWEEN WNUA-DD AND WNUB+DD :', JF
99
100
         WRITE(6,*)'EQUIVALENT WIDTH:',EQWS
101
         WRITE(6,*)
102 C-----
         IF(IO.EQ.1)THEN
103
                    DO 101 I=1,JF
104
                    IF(FR(I).LT.WNUA) GOTO 101
105
106
                    IF(FR(I).GT.WNUB) GOTO 104
         IF(ITB.EQ.1)SMI=C2*WNUAV/DLOG(C1*WNUAV**3/SM(I)+1)
107
         IF(ITB.EQ.O)SMI=SM(I)
108
                    IF(TTMIN.GT.SMI) TTMIN=SMI
109
                    IF(TTMAX.LT.SMI) TTMAX=SMI
110
                    WRITE(8,*)FR(I),SMI
111
112
     101
                    CONTINUE
                    WRITE(6,*)' TTMIN:',TTMIN,' TTMAX:',TTMAX
     104
113
                    END IF
114
         IF(IT.EQ.0) GOTO 111
115
         IF(IO.EQ.1) WRITE(8,*)99.99, 99.99
116
117 C----
         WRITE(6,*)
118
         IDD = INT(2D0*DD/DR+DR)
119
         IDL = INT(DL/DR+DR)
120
         WRITE(6, '(1X, 5HKL = ,16, 5X, 6HIDD = ,16, 5X, 6HIDL = ,
121
        *I6,/)') KL,IDD,IDL
122
         IF1=1
123
         IF2=1
124
         IF(ICOM.GT.0) GOTO 50
125
126 C-----
127 C
                         NORMAL SMOOTHING
128 C-----
129
         IF(IPD.EQ.2) THEN
                      WRITE(6,*)' I IDAT JDAT
                                                           WNUAV
130
                      TAVW
                                 IFIRST
                                           ILAST'
131
        *
                      WRITE(6, *)
132
                      END IF
133
134
         DO 10 WNUAV=WNUA, WNUB, DL
         JDAT = 0
135
```

```
TAVW = ODO
136
         FWS = ODO
137
         IF(IT.LT.3) DDD=DD
138
         IF(IT.EQ.3) DDD=1.2D0+(WNUAV-500D0)*8D-3
139
140
         IF(IT.EQ.4) THEN
           IF(WNUAV.LT.637D0) ADH=( 0.01074D0*WNUAV-3.28D0)/2D0
141
           IF(WNUAV.GE.637D0) ADH=(0.008041D0*WNUAV-2.69D0)/2D0
142
           IF(DD.NE.ODO)
                               ADH=DD/2D0
143
           DDD=3D0*ADH
144
           END IF
145
146
         IF(IT.EQ.5) DDD=DD*3.14159265D0*2D0
         IDD=INT(2D0*DDD/DR+DR)
147
         DO 20 J=IF1,JF
148
         WNU = FR(J)
149
         IF(WNU.LT.WNUAV-DDD) GOTO 19
150
151
         IF(WNU.GT.WNUAV+DDD) GOTO 21
         JDAT = JDAT+1
152
         IF(IT.EQ.1) FW = 1D0
153
         IF(IT.EQ.2.OR.IT.EQ.3) FW = 1D0 - DABS(WNU-WNUAV)/DDD
154
         IF(IT.EQ.4) FW = CC1*DEXP(-((WNU-WNUAV)*CC2/ADH)**2)/ADH
155
         IF(IT.EQ.5) THEN
156
               IF(WNU.EQ.WNUAV) FW=1D0
157
               IF (WNU.NE.WNUAV) FW=DSIN (WNU-WNUAV)/(WNU-WNUAV)
158
               END IF
159
         TAVW = TAVW + SM(J)*FW
160
         FWS = FWS + FW
161
         GOTO 20
162
      19 IF2=J
163
      20 CONTINUE
164
      21 IF1=IF2
165
         TAVW = TAVW/FWS
166
         IF(IPD.EQ.2)WRITE(6,'(1X,3I5,5X,F10.2,F11.4,5X,2I5)')
167
168
        *I, IDAT, JDAT, WNUAV, TAVW, IF1, J-1
         IF (ITB.EQ.1) TAVW=C2*WNUAV/DLOG (C1*WNUAV**3/TAVW+1)
169
         IF(TTMIN.GT.TAVW) TTMIN=TAVW
170
         IF(TTMAX.LT.TAVW) TTMAX=TAVW
171
         WRITE(8,*)WNUAV, TAVW
172
      10 CONTINUE
173
174
         WRITE(6,*)' TTMIN:',TTMIN,' TTMAX:',TTMAX
         IF(ICOM.EQ.O) GOTO 111
175
         WRITE(8,*)99.99,99.99
176
177 C-----
178 C
                      READ HIS DATA FOR COMPARISONS
179 C-----
                 _____
180
      50 IHIS=2049
```

```
Appendix E
```

```
READ(9,*)((SL(J,I),I=1,2),J=1,3)
181
          DO 22 J=1,2
182
183
          DO 22 I=1,2049
          READ(9,'(3(F8.2,2E10.5))')F1,H1,T1,F2,H2,T2,F3,H3,T3
184
          IF(J.NE.IDAY) GOTO 22
185
          IF(1.EQ.IBAND) THEN
186
                          H(I) = H1
187
                          T(I) = T1
188
                          FH(I) = F1
189
190
                          END IF
191
          IF(2.EQ.IBAND) THEN
                          H(I) = H2
192
                          T(I) = T2
193
                          FH(I) = F2
194
                          END IF
195
196
          IF(3.EQ.IBAND) THEN
                          H(I) = H3
197
                          T(I) = T3
198
                          FH(I) = F3
199
                          END IF
200
201
       22 CONTINUE
202
          IF(ITB.EQ.1) THEN
                        DO 33 I=1,IHIS
203
                        IF(T(I).EQ.ODO.OR.H(I).EQ.ODO) GOTO 33
204
                        H(I)=C2*FH(I)/DLOG(C1*FH(I)**3/H(I)+1)
205
206
                        T(I)=C2*FH(I)/DLOG(C1*FH(I)**3/T(I)+1)
       33
                        CONTINUE
207
                        END IF
208
       52 CONTINUE
209
210
          JHIS=0
          IF(IPD.EQ.2) WRITE(6, '(4X,1HI,2X,4HIDAT,2X,4HJDAT,
211
         *8X,5HWNUAV,2X,4HTAVW,6X,6HIFIRST,2X,5HILAST,/)'
212
213
          WNUAC=WNUA
214
          WNUBC=WNUB
          IF(WNUA.LT.SL(IBAND,1))WNUAC=SL(IBAND,1)
215
          IF(WNUB.GT.SL(IBAND,2))WNUBC=SL(IBAND,2)
216
          DO 110 I=1,IHIS
217
          WNUAV=FH(I)
218
219
          IF(WNUAV.LT.WNUAC) GOTO 110
          IF(WNUAV.GT.WNUBC) GOTO 112
220
          IF(JHIS.EQ.1) JHIS1=I-1
221
                  = 0
222
          JDAT
          TAVW
                  = 0D0
223
224
          FWS=0
          JHIS=JHIS+1
225
```

```
IF(ICOM.LT.0) GOTO 110
226
         IF(IT.LT.3) DDD=DD
227
228
         IF(IT.EQ.3) DDD=1.2D0+(WNUAV-500D0)*8D-3
         IF(IT.EQ.4) THEN
229
           IF(WNUAV.LT.637D0) ADH=( 0.01074D0*WNUAV-3.28D0)/2D0
230
           IF(WNUAV.GE.637D0) ADH=(0.008041D0*WNUAV-2.69D0)/2D0
231
           IF(DD.NE.ODO)
                               ADH=DD/2D0
232
           DDD=3D0*ADH
233
           END IF
234
         IF(IT.EQ.5) DDD=DD*3.14159265D0*2D0
235
236
         IDD=INT(2D0*DDD/DR+DR)
         DO 120 J=IF1,JF
237
         WNU = FR(J)
238
         IF(WNU.LT.WNUAV-DD) GOTO 119
239
         IF(WNU.GT.WNUAV+DD) GOTO 121
240
241
         JDAT = JDAT+1
         IF(IT.EQ.1) FW = 1D0
242
         IF(IT.EQ.2.OR.IT.EQ.3) FW = 1D0 - DABS(WNU-WNUAV)/DDD
243
         IF(IT.EQ.4) FW = CC1*DEXP(-((WNU-WNUAV)*CC2/ADH)**2)/ADH
244
         IF(IT.EQ.5) THEN
245
           IF(WNU.EQ.WNUAV) FW=1D0
246
           IF(WNU.NE.WNUAV) FW=DSIN(WNU-WNUAV)/(WNU-WNUAV)
247
           END IF
248
         TAVW = TAVW + SM(J)*FW
249
         FWS = FWS + FW
250
         GOTO 120
251
     119 IF2=J
252
     120 CONTINUE
253
     121 IF1=IF2
254
         TAVW = TAVW/FWS
255
         IF(IPD.EQ.2)WRITE(6, '(1X,3I5,5X,F10.2,F11.4,5X,2I5)')
256
        *I, IDAT, JDAT, WNUAV, TAVW, IF1, J-1
257
         IF(ITB.EQ.1)TAVW=C2*WNUAV/DLOG(C1*WNUAV**3/TAVW+1)
258
259
         R(I) = TAVW
     110 CONTINUE
260
     112 JHIS2=I-1
261
         KHIS=JHIS2-JHIS1+1
262
         WRITE(6, '(/,1X,8HJHIS1 = ,15,5X,8HJHIS2 = ,15,5X,
263
264
        *7HKHIS = ,I5,/)') JHIS1,JHIS2,KHIS
265 C-----
                                              _____
266 C
                            PLOT RESULRS
267 C-----
                    ______
         DO 987 I=JHIS1,JHIS2
268
269
         IF(TTMIN.GT.H(I)) TTMIN=H(I)
         IF(TTMIN.GT.R(I)) TTMIN=R(I)
270
```

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```

271		IF(TTMIN.GT.T(I).AND.IDEL.LT.O) TTMIN=T(I)
272		IF(TTMAX.LT.H(I)) TTMAX=H(I)
273		IF(TTMAX.LT.R(I)) TTMAX=R(I)
274		IF(TTMAX.LT.T(I).AND.IDEL.LT.O) TTMAX=T(I)
275	987	CONTINUE	
276		WRITE(6,*)' TT	MIN:',TTMIN,' TTMAX:',TTMAX
277		IF(ICOM.EQ1)	THEN
278			DO 1004 I=JHIS1,JHIS2
279	1004		WRITE(8,*)FH(I),H(I)
280			END IF
281		IF(ICOM.EQ2)	THEN
282			DO 1005 I=JHIS1,JHIS2
283	1005		WRITE(8,*)FH(I),T(I)
284			END IF
285		IF(ICOM.EQ3)	THEN
286			DO 1006 I=JHIS1,JHIS2
287	1006		WRITE(8,*)FH(I),H(I)
288			WRITE(8,*)99.99,99.99
289			DO 1007 I=JHIS1,JHIS2
290	1007		WRITE(8,*)FH(I),T(I)
291			END IF
292		IF(ICOM.EQ. 1)	THEN
293			DO 1113 I=JHIS1,JHIS2
294	1113		WRITE(8,*)FH(I),R(I)
295			END IF
296		IF(ICOM.EQ. 2)	THEN
297			DO 1114 I=JHIS1,JHIS2
298	1114		WRITE(8,*)FH(I),R(I)
299			WRITE(8,*)99.99,99.99
300			DO 1115 I=JHIS1,JHIS2
301	1115		WRITE(8,*)FH(I),H(I)
302			END IF
303		IF(ICOM.EQ. 3)	THEN
304			DO 1116 I=JHIS1,JHIS2
305	1116		WRITE(8,*)FH(I),R(I)
306			WRITE(8,*)99.99,99.99
307			DO 1117 I=JHIS1,JHIS2
308	1117		WRITE(8,*)FH(I),T(I)
309			END IF
310		IF(ICOM.EQ. 4)	THEN
311			DU 1118 I=JHIS1, JHIS2
312	1118		WRITE(8,*)FH(I),R(I)
313			WRITE(8,*)99.99,99.99
314			DU 1119 I=JHIS1, JHIS2
315	1119		WRITE(8,*)FH(I),H(I)

316		WRITE(8,*)99.99,99.99
317		DO 1120 I=JHIS1,JHIS2
318	1120	WRITE(8,*)FH(I),T(I)
319		END IF
320	C	
321	С	STAT BEGINS
322	C	
323		IF(IDEL.EQ.0) GOTO 111
324		WRITE(8,*)99.99,99.99
325		TB3=(TBB2-TBB1)/4D1+TBB1
326		TB1=TB3+(TBB2-TBB1)/4D1
327		TB2=TTMIN-(TBB2-TBB1)/2D1
328		SCALE=(TB2-TB1)/SCALE
329		DREF=SCALE*DREF
330		WTICK=(WNUB-WNUA)/1D1
331		TTICK=(WNUB-WNUA)/1D2
332		VTICK=(TB2 - TB1)/5D1
333		SHIFT=2D0*TTICK
334		TREF=(TB1+TB2)/2D0+DREF
335		WNUAA=WNUA+SHIFT
336		WNUBB=WNUB-SHIFT
337		IDV=(WNUB-WNUA)/IABS(IDEL)
338		WRITE(7,4) IDAY
339		WNUX=WNUA
340		MHIS=0
341		ARAV=ODO
342		ATAV=ODO
343		RRMA=ODO
344		TTMA=ODO
345		SDR =0D0
346		SDT =0D0
347		JDEL=IABS(IDEL)
348		DO 500 II=1,JDEL
349		LHIS=0
350		RMA=ODO
351		TMA=ODO
352		SDD1=0D0
353		SDD3=0D0
354		S2D1=0D0
355		S2D3=0D0
356		DO 1131 I=JHIS1,JHIS2
357		DINT1=WNUA+(WNUB-WNUA)/DFLOAT(JDEL)*(II-1)
358		DINT2=WNUA+(WNUB-WNUA)/DFLOAT(JDEL)*II
359		C=FH(I)
360		IF(C.LE.DINT1) GOTO 1131

```
Appendix E
```

```
IF(C.GT.DINT2) GOTO 499
361
362
          LHIS=LHIS+1
363
          A=C*C*C
          B=C/TREF
364
365
          IF(ITB.EQ.0)PL=C1*A/(DEXP(C2*B)-1)
          IF(ITB.EQ.1)PL=TREF
366
          D1=(H(I)-R(I))*SCALE+PL
367
          D2=(R(I)-T(I))*SCALE+PL
368
          D3=(H(I)-T(I))*SCALE+PL
369
370
          IF(C.LT.WNUA+SHIFT) GOTO 1132
371
          IF(C.GT.WNUB-SHIFT) GOTO 1132
          IF(D1.LT.TB1) D1=TB1
372
          IF(D1.GT.TB2) D1=TB2
373
          IF(D2.LT.TB1) D2=TB1
374
          IF(D2.GT.TB2) D2=TB2
375
376
          IF(D3.LT.TB1) D3=TB1
          IF(D3.GT.TB2) D3=TB2
377
   C----
378
          IF(ICOM.EQ.1.OR.ICOM.EQ.2.OR.ICOM.EQ.4) WRITE(8,*) C,D1
379
          IF(ICOM.EQ.3) WRITE(8,*) C,D2
380
          IF(ICOM.LT.0) WRITE(8,*) C,D3
381
   C----
382
    1132 CONTINUE
383
          DD1=H(I)-R(I)
384
          DD3=H(I)-T(I)
385
          IF(DABS(RMA).LT.DABS(DD1)) RMA=DD1
386
          IF(DABS(TMA).LT.DABS(DD3)) TMA=DD3
387
388
          SDD1=SDD1+DD1
          SDD3=SDD3+DD3
389
          S2D1=S2D1+DD1*DD1
390
          S2D3=S2D3+DD3*DD3
391
    1131 CONTINUE
392
          WRITE(8,*)99.99,99.99
393
394
      499 FK=DFLOAT(LHIS)
          RAV=SDD1/FK
395
          TAV=SDD3/FK
396
          RSD=DSQRT((FK*S2D1-SDD1*SDD1)/FK/(FK-1D0))
397
          TSD=DSQRT((FK*S2D3-SDD3*SDD3)/FK/(FK-1D0))
398
399
          WNUY=WNUX+IDV
          WRITE(6,'(8X,6F8.3,16,4X,F5.0,1H-,F5.0)')
400
         *RAV, TAV, RMA, TMA, RSD, TSD, LHIS, WNUX, WNUY
401
          WRITE(7,'(8X,6F8.3,16,4X,F5.0,1H-,F5.0)')
402
         *RAV, TAV, RMA, TMA, RSD, TSD, LHIS, WNUX, WNUY
403
          WNUX=WNUY
404
          PR(II)=DABS(RAV)
405
```

	PT(II)=DABS(TAV)
	QR(II)=DABS(RMA)
	QT(II)=DABS(TMA)
	RR(II)=RSD
	RT(II)=TSD
	ARAV=ARAV+RAV
	ATAV=ATAV+TAV
	SDR =SDR +RSD
	SDT =SDT +TSD
	IF(DABS(RRMA).LT.DABS(RMA)) RRMA=RMA
	IF(DABS(TTMA).LT.DABS(TMA)) TTMA=TMA
	MHIS=MHIS+LHIS
500	CONTINUE
	IF(ICOM.GT.O.AND.IDEL.LT.O) THEN
	DO 510 I=JHIS1,JHIS2
	DHT=(H(I)-T(I))*SCALE+TREF
	C=FH(I)
	IF(C.LT.WNUA+SHIFT) GOTO 510
	IF(C.GT.WNUB-SHIFT) GOTO 510
	IF(DHT.LT.TB1) DHT=TB1
	IF(DHT.GT.TB2) DHT=TB2
	WRITE(8,*)C,DHT
510	CONTINUE
	WRITE(8,*)99.99,99.99
	END IF
	DO 501 II=1,JDEL
	DINT1=WNUA+(WNUB-WNUA)/DFLOAT(JDEL)*(II-1)
	DINT2=WNUA+(WNUB-WNUA)/DFLOAT(JDEL)*II
	IF(PR(II).LE.PT(II)) THEN
	WRITE(8,*)DINT1,TB3-VTICK
	WRITE(8,*)DINT1,TB3+VTICK
	WRITE(8,*)DINT1,TB3
	WRITE(8,*)DINT2,TB3
	WRITE(8,*)DINT2,TB3-VTICK
	WRITE(8,*)DINT2,TB3+VTICK
	WRITE(8,*)DINT2,TB3
	WRITE(8,*)99.99,99.99
	END IF
501	CONTINUE
	FIDEL = DFLOAT(JDEL)
	ARAV=ARAV/FIDEL
	ATAV=ATAV/FIDEL
	SDR=SDR/FIDEL
	SDT=SDT/FIDEL
	WRITE(6,'(/,8X,6F8.3,I6,4X,F5.0,1H-,F5.0,1H*)')
	500

```
Appendix E
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451	:	*ARAV,ATAV,RRMA,TTMA,SDR,SDT,MHIS,WNUA,WNUB
452		WRITE(7,'(/,8X,6F8.3,I6,4X,F5.0,1H-,F5.0,2H *)')
453	:	*ARAV,ATAV,RRMA,TTMA,SDR,SDT,MHIS,WNUA,WNUB
454	C	
455	C	PLOT WINDOW
456	C	
457		WEILE(O,*)WNUAA, IKEF
458		DU 2101 F=WNUA+WIICK,WNUB-WIICK,WIICK
459		WRIIE(0,*)F, IREF
400		WRITE(0,*)F, TREF-VIICK
461		WRITE(0,*)F, IREF TO IION WRITE(8 *)F TREF
402	2101	CONTINIF
403	2101	WRITE(8 *)WNURB TREE
465		WRITE $(8 *)$ 99 99 99 99
466	C	-
467	C C	WRITE(8.*)WNUAA.TB2
468		DO 2102 F=WNUA+WTICK.WNUB-WTICK.WTICK
469		WRITE(8,*)F,TB2
470		WRITE(8,*)F,TB2-VTICK
471		WRITE(8,*)F,TB2
472	2102	CONTINUE
473		WRITE(8,*)WNUBB,TB2
474		WRITE(8,*)99.99,99.99
475	C	-
476		WRITE(8,*)WNUAA,TB1
477		DO 2103 F=WNUA+WTICK,WNUB-WTICK,WTICK
478		WRITE(8,*)F,TB1
479		WRITE(8,*)F,TB1+VTICK
480		WRITE(8,*)F,TB1
481	2103	CONTINUE
482		WRITE(8,*)WNUBB,TB1
483	~	WRITE(8,*)99.99,99.99
484	C	
485		DU 2104 ISUB=IREF, IB2, SCALE*DIV
486		WRIIE(8,*)WNUAA,ISUB
487		WRITE(8,*)WNUAA+IIICK,ISUB
488	0104	WRIIE(8,*)WNUAA,ISUB
489	2104	WRITE(8 *)WNIIAA TRO
490 701		WRITE $(3, *)$ whome, include when the second seco
491	C	-
493	0	DO 2105 TSUB=TREF.TB1SCALE*DIV
494		WRITE(8.*)WNUAA.TSUB
495		WRITE(8,*)WNUAA+TTICK,TSUB
		- · · · ·

```
WRITE(8,*)WNUAA,TSUB
496
    2105 CONTINUE
497
          WRITE(8,*)WNUAA,TB1
498
          WRITE(8,*)99.99,99.99
499
500 C-----
          DO 2106 TSUB=TREF, TB2, SCALE*DIV
501
          WRITE(8,*)WNUBB,TSUB
502
          WRITE(8,*)WNUBB-TTICK,TSUB
503
          WRITE(8,*)WNUBB,TSUB
504
    2106 CONTINUE
505
506
          WRITE(8,*)WNUBB,TB2
          WRITE(8,*)99.99,99.99
507
   C----
508
          DO 2107 TSUB=TREF, TB1, -SCALE*DIV
509
          WRITE(8,*)WNUBB,TSUB
510
511
          WRITE(8,*)WNUBB-TTICK,TSUB
          WRITE(8,*)WNUBB,TSUB
512
    2107 CONTINUE
513
          WRITE(8,*)WNUBB,TB1
514
515 C----
     111 CONTINUE
516
          IF(INPT.EQ.IGRAF) WRITE(8,*) -99.99,-99.99
517
          IF(INPT.NE.IGRAF.AND.IGRAF.NE.O.AND.INPT.NE.INPUTS)
518
                               WRITE(8,*) 99.99,99.99
519
         *
          IF (INPT.NE.IGRAF.AND.IGRAF.EQ.O.AND.INPT.NE.INPUTS)
520
         *
                               WRITE(8,*)-99.99,-99.99
521
      192 CONTINUE
522
          IF(ICOM.NE.O) THEN
523
524
                         REWIND 9
                         CLOSE UNIT=9
525
                         END IF
526
          IF(IRAD.NE.O) THEN
527
                         REWIND 3
528
                         CLOSE UNIT=3
529
                         END IF
530
          IF(IRAD.EQ.0) THEN
531
                         REWIND 2
532
                         CLOSE UNIT=2
533
534
                         END IF
          IF(INPT.LT.INPUTS) GOTO 1000
535
          WRITE(8,*) -99.99,-99.99
536
          IF(IPL .LT.IPLOTS) GOTO 2000
537
          DATA C1,C2,CC1,CC2/
538
         *0.119096D-4,1.43879D0,.46972D0,.83255D0/
539
          END
540
```

541 C-----542 C COMP.INP 543 C IPLOTS 544 C INPUTS IGRAF IRAD IEQW OF 545 C ITB TBU TBL TBB1 TBB2 SCALE DREF DIV 546 C WNUA WNU1 WNU2 DR LE1 LE2 IT IPD IO WNUB DL DD 547 C ICOM IDEL IDAY IBAND 548 C-----549 C 1 IPLOTS 550 C 1,0,1,0,0 INPUTS IGRAF IRAD IEQW OF 551 C 1,0,209.8,80,280,14,-1,1 552 C 610,630,0.5,0.56,610,630,0.005,1,1,2,0,0 553 C 2,-2,2,3 554 C-----555 C (FIG. III-3) 556 C 1 IPLOTS 557 C 5,3,0,0,0 INPUTS IGRAF IRAD IEQW OF 558 C 0,0,0,0,0,0,0,0 559 C 585,775,.1,0,580,780,.1,10, 6,4,0,0 560 C 0,0,0,0 ITRA I 6 561 C 0,0,0,0,0,0,0,0 562 C 585,775,.1,0,580,780,.1,10, 7,4,0,0 563 C 0,0,0,0 ITRA I 7 564 C 0,0,0,0,0,0,0,0 565 C 585,775,.1,0,580,780,.1,10, 8,4,0,0 566 C 0,0,0,0 ITRA I 8 567 C 0,0,0,0,0,0,0,0 568 C 585,775,.1,0,580,780,.1,10, 9,4,0,0 569 C 0,0,0,0 ITRA I 9 570 C 0,0,0,0,0,0,0,0 571 C 585,775,.1,0,580,780,.1,10,10,4,0,0 572 C 0,0,0,0 ITRA I 10 573 C-----

```
PROGRAM CHNL
1
\mathbf{2}
         IMPLICIT REAL*8(A-H,O-Z)
         COMMON/G/ XXG(60), WWG(60), XG(25), WG(29), WNUUU, WNUE,
3
                    DZ, IPRG, IGNU, EPS, IG, IGSC, PLY(50), TLY(50),
        *
\mathbf{4}
                    TRN(50), LAYER, TLA(50), TLB(50), TLC(50), TRA(50),
\mathbf{5}
        *
                    IRAD
6
        *
         DIMENSION
\overline{7}
        *SM(5000,50),TRAB(200,50),WN(5000),TAVW(50),WW(50),
8
        *PLYT(50), PLYW(50), PW(50), WNUC(25), DDC(25), ATMR(25,10)
9
10
        *,ALLR(25,10),ATMT(25,10),ALLT(25,10)
11
         OPEN(UNIT=4, TYPE='OLD', FILE= 'CHNL.INP')
         OPEN(UNIT=2,TYPE='OLD',FILE= 'TRAO.DAT')
12
         INPTS = 0
13
         INTS = 0
14
         READ (4,*)
                      INPUTS, IOPEN
15
16
    1000 READ (4,*)
                       IRAD, DR, IATM, IPR, NWNUAV, IPRG, IGNU, EPS
         READ (4,*) LW, LEVEL1, LEVEL2, IDIR, TSKIN, ITP
17
         READ (4,*)
                      ICH, IT, INORM
18
                       (WNUC(I),DDC(I),I=1,ICH)
         READ (4,*)
19
         IGSC=1
20
         IF(INPTS.EQ.0)THEN
21
22
         IF(IOPEN.EQ.1.OR.IOPEN.EQ.3)
        *
                        OPEN (UNIT=8, TYPE='NEW', FILE='TWCHN.DAT')
23
         IF(IOPEN.EQ.2.OR.IOPEN.EQ.3)
24
                        OPEN (UNIT=9, TYPE='NEW', FILE= 'RCHN.DAT')
25
        *
         IF(IATM.NE.O)OPEN(UNIT=3,TYPE='OLD',FILE='MODATM.DAT')
26
         IF(IATM.EQ.0)OPEN(UNIT=7,TYPE='OLD',FILE='PROFIL.DAT')
27
28
         IAM=IATM
         IF(IATM.EQ.O) IAR=7
29
         IF(IATM.NE.O) IAR=3
30
         IF(IATM.EQ.O) IAM=1
31
         READ (IAR,*)
32
33
        *((DUM,PLY(I),TLY(I),DUM,(DUM,J=1,7),I=1,LW),K=1,IAM)
         LEVEL=LEVEL2-LEVEL1+1
34
         LAYER=LEVEL-1
35
         IF(LEVEL.EQ.LW) GOTO 35
36
                           DO 36 I=1,LEVEL
37
                           PLY(I)=PLY(LEVEL1+I-1)
38
39
      36
                           TLY(I) = TLY(LEVEL1 + I - 1)
      35 IF(IDIR.EQ. 1)
                           GOTO 34
40
                           DO 37 I=1,LEVEL/2
41
                           CHEP=PLY(I)
42
                           CHET=TLY(I)
43
                           PLY(I)=PLY(LEVEL-I+1)
44
                           TLY(I)=TLY(LEVEL-I+1)
45
```

```
Appendix E
```

```
PLY(LEVEL-I+1)=CHEP
46
      37
                          TLY(LEVEL-I+1)=CHET
47
      34
                          DO 50 J=1,LAYER
48
                          PLYT(J)=PLY(J+1)
49
                          PLYW(J) = (PLY(J+1) + PLY(J))/2D0
50
                          PW(J) =DLOG(PLY(J+1))-DLOG(PLY(J))
51
      50
                          WRITE(6, '(1X, I5, 5D11.4)')
52
                           J,PLY(J),PLY(J+1),PLYT(J),PLYW(J),PW(J)
        *
53
         END IF
54
55 C----
56
         DO 101 I=1, LAYER
         IF(ITP.EQ.1) GOTO 60
57
         I2=I
58
         IF(I2 .EQ. 1) I2=I2+1
59
         I1=I2-1
60
61
         I3=I2+1
         V1=PLY(I1)
62
         V2=PLY(I2)
63
         V3=PLY(I3)
64
         C1=TLY(I1)
65
66
         C2=TLY(I2)
         C3=TLY(I3)
67
         A=C3/(V3-V2)/(V3-V1)+C2/(V2-V1)/(V2-V3)+
68
        * C1/(V1-V2)/(V1-V3)
69
         B=(C2-C3)/(V2-V3)-A*(V2+V3)
70
         C=C2-(A*V2+B)*V2
71
         PP=(PLY(I)+PLY(I+1))/2D0
72
         TT=(A*PP+B)*PP+C
73
         IF(TLY(I).LE.TT.AND.TT.LE.TLY(I+1)) GOTO 102
74
         IF(TLY(I).GE.TT.AND.TT.GE.TLY(I+1)) GOTO 102
75
      60 A=0D0
76
         B=(TLY(I)-TLY(I+1))/(PLY(I)-PLY(I+1))
77
         C=TLY(I)-B*PLY(I)
78
     102 WRITE(6, '(1X, I3, 5D13.4)') I, TLY(I), TLY(I+1), A, B, C
79
         TLA(I) = A
80
         TLB(I)=B
81
         TLC(I)=C
82
     101 CONTINUE
83
84 C-----
         IIRAD=0
85
         IF(IRAD.NE.O) INTS=INTS+1
86
         DO 500 ICN=1,ICH
87
         WNU=WNUC(ICN)
88
         DD = DDC(ICN)
89
         IIR=INT(1D0/DR+DR)
90
```

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```
JF=0
91
          NWNU=0
92
93
     100 IF(NWNU.EQ.NWNUAV) GOTO 200
          NWNU=NWNU+1
94
95 C----
          READ(2,*)
96
         *(LL, (TRAB(I, J), I=1, IIR), TRABS, WNUAV, J=1, LAYER)
97
98 C-----
99
          IF(IPR.EQ.1)WRITE(6,*) WNUAV
100
          WA= WNUAV-5D-1+DR/2D0
101
          WB= WNUAV+5D-1-DR/2D0
          W1= WNU-DD
102
          W2= WNU+DD
103
          IF(W1.GT.WB) GOTO 100
104
          IF(W2.LT.WA) GOTO 200
105
          DO 110 I=1,IIR
106
          WNUU=WNUAV-5D-1+DR/2DO+(I-1)*DR
107
          IF(WNUU.LT.W1) GOTO 110
108
          IF(WNUU.GT.W2) GOTO 200
109
          JF=JF+1
110
          WN(JF)=WNUU
111
          IF(IPR.EQ.1)WRITE(6,*)JF,WN(JF)
112
          IF(IRAD.EQ.0) GOTO 701
113
          TRN(1)=1D0
114
          DO 700 L=1,LAYER
115
          TRN(L+1)=TRAB(I,L)
116
          IF(TRN(L+1).LT.DZ) THEN
117
                               TRA(L)=ODO
118
                               GOTO 699
119
                               END IF
120
          TRA(L) = DLOG(TRN(L)/TRN(L+1))/(PLY(L+1)-PLY(L))
121
          IF(IDIR.EQ.-1) TRA(L) = -TRA(L)
122
     699 IF(IPRG.EQ.1) WRITE(6, '(1X, I3, 5D13.4)')
123
         *L,PLY(L),PLY(L+1),TRN(L),TRN(L+1),TRA(L)
124
     700 CONTINUE
125
          RAD=0D0
126
     701 DO 120 L=1,LAYER
127
          IF(IRAD.EQ.0)
                                GOTO 702
128
129
          RADD = ODO
          RADDA = ODO
130
          RADDB = ODO
131
          AA=TRN(L+1)
132
          BB=TRN(L)
133
          IF(TRA(L).LT.DZ) GOTO 119
134
          WNUUU=WNUU*WNUU*WNUU*CP1
135
```

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136	WNUE =W	NUU*CP2	
137	PA=WNUUU/(DEXP(WNUE/TLY(L+1))-1)		
138	PB=WNUU	U/(DEXP(WNUE/TLY(L))-1)	
139	IF(IRAD	.EQ1)THEN	
140		IF(AA/BB.LE.9D-1)	
141	*	RADDA=BB*PB-AA*PA+(PA-PB)*(AA-BB)/DLOG(AA/BB)	
142		IF(AA/BB.GT.9D-1)	
143	*	RADDB=(PA+PB)*(BB-AA)/2D0	
144		RADD=RADDA+RADDB	
145		RAD=RAD+RADD	
146		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,6E12.6)')	
147	*	L, BB, AA, RADDA, RADDB, RADD, RAD	
148		GOTO 119	
149		END IF	
150	IF(IRAD	.EQ2)THEN	
151		IF(L.EQ.1) RADD= BB*PB	
152		IF(L.EQ.LAYER) RADD=-AA*PA	
153		RADD=RADD-(BB+AA)*(PB-PA)/2D0	
154		RAD=RAD+RADD	
155		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,6E12.6)')	
156	*	L,BB,AA,PB,PA,RADD,RAD	
157		GOTO 119	
158		END IF	
159	IF(IRAD	.EQ3)THEN	
160		TAV = (TLY(L) + TLY(L+1))/2D0	
161		PL = WNUUU/(DEXP(WNUE/TAV)-1)	
162		RADD = PL*(BB-AA)	
163		RAD = RAD + RADD	
164		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,6E12.6)')	
165	*	L,BB,BB-AA,TAV,PL,RADD,RAD	
166		GOTO 119	
167		END IF	
168	IF(IRAD	.EQ4)THEN	
169		RADD=(PA+PB)*(BB-AA)/2D0	
170		RAD=RAD+RADD	
171		END IF	
172	IF(IRAD	.EQ.2) THEN	
173		PAV = (PLY(L+1)+PLY(L))/2D0	
174		TAV=TLC(L)+PAV*(TLB(L)+PAV*TLA(L))	
175		CC=BB*DEXP(-(PAV-PLY(L))*TRA(L))	
176		PC=WNUUU/(DEXP(WNUE/TAV)-1)	
177		RADD = (AA*PA+BB*PB+CC*PC)*(BB-AA)/(BB+AA+CC)	
178		RAD=RAD+RADD	
179		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,6E12.6)')	
180	*	L,BB,CC,AA,PB,PC,PA	

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181		GOTO 119
182		END IF
183	IF(IRAD	.EQ.3) THEN
184		RADD=(AA*PA+BB*PB)*(BB-AA)/(BB+AA)
185		RAD=RAD+RADD
186		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,4E12.6)')
187	*	L,BB,AA,PB,PA
188		GOTO 119
189		END IF
190	IF(IRAD	.EQ.4) THEN
191		PA=PLY(L+1)
192		PB=PLY(L)
193		TA=TLY(L+1)
194		TB=TLY(L)
195		HM=1D0/TRA(L)
196		B1M=DEXP(WNUE*(PA/TB-PB/TA)/(PA-PB))
197		B2M=WNUE*(1D0/TA-1D0/TB)/(PA-PB)
198		OG1=AA*DEXP(-B2M*PA)-BB*DEXP(-B2M*PB)
199		OG2=AA*DEXP(-2D0*B2M*PA)-BB*DEXP(-2D0*B2M*PB)
200		OG3=AA*DEXP(-3D0*B2M*PA)-BB*DEXP(-3D0*B2M*PB)
201		OG1=OG1/B1M/(B2M*HM+1D0)
202		OG2=OG2/B1M/B1M/(2D0*B2M*HM+1D0)
203		OG3=OG3/B1M/B1M/B1M/(3D0*B2M*HM+1D0)
204		RADD=-WNUUU*(OG1+OG2+OG3)
205		RAD=RAD+RADD
206		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,6E12.6)')
207	*	L,B1M,B2M,HM,OG1,OG2,OG3
208		GOTO 119
209		END IF
210	IF(IRAD	.EQ.5) THEN
211		PA=PLY(L+1)
212		PB=PLY(L)
213		TA=TLY(L+1)
214		TB=TLY(L)
215		HM=1D0/TRA(L)
216		B1M=DEXP(WNUE*(PA/TB-PB/TA)/(PA-PB))
217		B2M=WNUE*(1D0/TA-1D0/TB)/(PA-PB)
218		OG1=AA*DEXP(-B2M*PA)-BB*DEXP(-B2M*PB)
219		OG2=AA*DEXP(-2D0*B2M*PA)-BB*DEXP(-2D0*B2M*PB)
220		OG1=OG1/B1M/(B2M*HM+1D0)
221		OG2=OG2/B1M/B1M/(2D0*B2M*HM+1D0)
222		RADD=-WNUUU*(OG1+OG2)
223		RAD=RAD+RADD
224		IF(IPRG.EQ.1) WRITE(6,'(1X,I3,2X,5E12.6)')
225	*	L,B1M,B2M,HM,OG1,OG2

```
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```

```
GOTO 119
226
                   END IF
227
228
          IF(IRAD.EQ.1) THEN
                   AA=PLY(L)
229
                   BB=PLY(L+1)
230
                   IG=L
231
                   CALL GSC(AA, BB, WNUU, RADD)
232
                   RAD=RAD+RADD
233
                   GOTO 119
234
235
                   END IF
236
      119 SM(JF,L)=RAD
          IF(IPRG.EQ.1) WRITE(6, '(1X, I3, 2X, 2E12.6)') L, RADD, RAD
237
          GOTO 120
238
      702 SM(JF,L)=TRAB(I,L)
239
      120 CONTINUE
240
241
          IF(IRAD.NE.O) THEN
                   IF(TSKIN.NE.ODO)
242
                   RADD=TRN(LEVEL)*WNUUU/(DEXP(WNUE/TSKIN)-1)
243
         *
                    IF(TSKIN.EQ.ODO)
244
                   RADD=TRN(LEVEL)*WNUUU/(DEXP(WNUE/TLY(LEVEL))-1)
245
         *
                   RAD=RAD+RADD
246
                   SM(JF,LEVEL)=RAD
247
                   END IF
248
      110 CONTINUE
249
          GOTO 100
250
      200 WRITE(6,*)
251
          IF(IRAD.EQ.0) WRITE(6,*) ' JF=',JF
252
253
          WCVW = 1DO
          IF(IRAD.NE.O) WCVW=ODO
254
          WMW = ODO
255
          IF(IRAD.NE.O) IIRAD=1
256
          DO 400 L=1,LAYER+IIRAD
257
          TAVW(L)=ODO
258
259
          FWS=0D0
          DO 300 J=1,JF
260
          IF(IT.EQ.1) FW
                              = 1D0
261
          IF(IT.EQ.2) FW
                              = (DD-DABS(WN(J)-WNU))/DD/DD
262
          FWS = FWS + FW
263
      300 \text{ TAVW}(L) = \text{TAVW}(L) + \text{SM}(J,L) * FW
264
          TAVW(L) = TAVW(L)/FWS
265
          IF(IRAD.EQ.0)
                               WW(L) = (WCVW-TAVW(L))/PW(L)
266
                               WW(L) = TAVW(L) - WCVW
          IF(IRAD.NE.O)
267
          IF(WMW.LT.WW(L))
                               THEN
268
                               LMAXL=L
269
                               WMW=WW(L)
270
```

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271		END IF
272		WCVW = TAVW(L)
273	399	IF(IPR.EQ.2)WRITE(6,'(1X,I5,2F13.7,I5,F13.7)')
274	k	L,TAVW(L),WW(L),LMAXL,WMW
275	400	CONTINUE
276		IF(IOPEN.EQ.O) GOTO 601
277		DO 600 L=1,LAYER
278		WWM=WW(L)
279		IF(INORM.EQ.1)WWM=WWM/WMW
280		IF(IOPEN.EQ.1.OR.IOPEN.EQ.3) THEN
281		IF(IRAD.EQ.0) WRITE(8,'(1X,4F13.7)')
282	k	<pre>TAVW(L),PLYT(L),WWM,PLYW(L)</pre>
283		IF(IRAD.EQ.O.AND.L.EQ.LAYER)
284	k	<pre>wRITE(8,*) 99.99,99.99,99.99,99.99</pre>
285		END IF
286		IF(IOPEN.EQ.2.OR.IOPEN.EQ.3) THEN
287		IF(IRAD.NE.0) WRITE(9,'(1X,4F13.7)')
288	k	<pre>TAVW(L),PLYT(L),WWM,PLYW(L)</pre>
289		IF(IRAD.NE.O.AND.L.EQ.LAYER)
290	k	<pre>WRITE(9,*) 99.99,99.99,99.99,99.99</pre>
291		END IF
292	600	CONTINUE
293	601	IF(IRAD.NE.O) THEN
294		WNUUU=WNU*WNU*WNU*CP1
295		WNUE =WNU*CP2
296		WRITE(6,*)' JF, ICN, INTS :', JF,ICN,INTS
297		ATMR(ICN, INTS)=TAVW(LAYER)
298		ATMT(ICN, INTS)=WNUE/DLOG(WNUUU/TAVW(LAYER)+1)
299		ALLR(ICN, INTS)=TAVW(LEVEL)
300		ALLT(ICN, INTS)=WNUE/DLOG(WNUUU/TAVW(LEVEL)+1)
301		END IF
302	500	REWIND 2
303		INPTS=INPTS+1
304		IF(INPTS.LT.INPUTS) GOTO 1000
305		IF(IRAD.NE.O) THEN
306		WRITE(6,*)
307		DO 502 J = 1, INTS
308		DO 501 I = 1, ICH
309		WRITE(6, '(1X,14,F10.2,4F10.4)')
310	k	<pre></pre>
311	k	<pre>ALLR(I,J),ALLT(I,J)</pre>
312		IF(J.EQ.1)GOTO 501
313		ATMR(I,J) = -ATMR(I,J) + ATMR(I,1)
314		ATMT(I,J) = -ATMT(I,J) + ATMT(I,1)
315		ALLR(I,J) = -ALLR(I,J) + ALLR(I,1)

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316	3	ALLT(I,J)=-ALLT(I,J)+ALLT(I,1)
317	501	CONTINUE
318	502	WRITE(6,*)
319)	WRITE(6,*)'INPUTS,INTS :',INPUTS,INTS
320)	WRITE(6,*)
321	L	DO 503 I = 1,ICH
322	2 503	WRITE(6,'(1X,F6.1,1X,9F8.4)')
323	} *	WNUC(I),(ATMR(I,J),J=1,INTS)
324	1	WRITE(6,*)
325	5	DO 504 I = 1,ICH
326	504	WRITE(6,'(1X,F6.1,1X,9F8.4)')
327	7 *	WNUC(I),(ATMT(I,J),J=1,INTS)
328	3	WRITE(6,*)
329)	DO 505 I = 1,ICH
330	505	WRITE(6,'(1X,F6.1,1X,9F8.4)')
331	*	WNUC(I),(ALLR(I,J),J=1,INTS)
332	2	WRITE(6,*)
333	3	DO 506 I = 1,ICH
334	£ 506	WRITE(6,'(1X,F6.1,1X,9F8.4)')
335	5 *	WNUC(I),(ALLT(I,J),J=1,INTS)
336	3	WRITE(6,*)
337	7	END IF
338	B DATA	CP1,CP2,DZ/1.1909596D-5,1.43879D0,1D-10/
339	END	
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```
340 C-----
341 C CHNL.INP
342 C 3,0
343 C 1,0.1,6,2,120,0,10,0
344 C 50,1,50,1,0.,2
345 C 7,2,0
346 C 668, 3, 679, 10, 691, 12, 704, 16, 716, 16, 732, 16, 748, 16
347 C 2,0.1,6,0,120,0,2,0
348 C 50,1,50,1,0.,2
349 C 7,2,0
350 C 668,3,679,10,691,12,704,16,716,16,732,16,748,16
351 C 5,0.1,6,0,120,0,0,0
352 C 50,1,50,1,0.,2
353 C 7,2,0
354 C 668,3,679,10,691,12,704,16,716,16,732,16,748,16
355 C-----
356 C THIS SEQUENCE IS FOR THE HARTCOD REPORT SEE TABLE III-3.
357 C-----
```

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```
SUBROUTINE GSC(AA, BB, WNU, RADD)
1
\mathbf{2}
          IMPLICIT REAL*8(A-H,O-Z)
          COMMON/G/ XXG(60), WWG(60), XG(25), WG(29), WNUUU, WNUE,
3
                     DZ, IPRG, IGNU, EPS, IG, IGSC, PLY(50), TLY(50),
4
        *
                     TRN(50), LAYER, TLA(50), TLB(50), TLC(50), TRA(50),
5
        *
                     IRAD
\mathbf{6}
        *
         GOTO(20,5), IGSC
\overline{7}
       5 \text{ ER} = 0 \text{DO}
8
         FR = ODO
9
         F = ODO
10
11
       2 C = (BB - AA)/2D0
          IF(IGNU.NE.O) N=IGNU-1
12
          IF(IGNU.EQ.O)
                              N=0
13
       6 N1=N+1
14
          IF(N.GT.9) GOTO 8
15
16
       7 F=0D0
          IINXG=N*N1/2
17
         DO 4 I=1,N1
18
          INX=IINXG+I
19
          IF(IRAD.EQ.1) THEN
20
                   PLYGA =C*XXG(INX)+(BB+AA)/2D0
21
                   WEGA = TRA(IG)*TRN(IG)*DEXP(-TRA(IG)*(PLYGA-AA))
22
                   TPGA=TLC(IG)+PLYGA*(TLB(IG)+PLYGA*TLA(IG))
23
                   OUTP=WNUUU/(DEXP(WNUE/TPGA)-1)
24
                   F=F+WWG(INX)*OUTP*WEGA
25
                   IF(IPRG.EQ.2) WRITE(6, '(1X, I3, 5D12.4)')
26
                   IG, PLYGA, TPGA, WEGA, C, OUTP
27
        *
                   END IF
28
       4 CONTINUE
29
          F=F*C
30
          IF(IGNU.NE.O) GOTO 8
31
          ER=DABS(F-FR)/F
32
          IF(IPRG.EQ.3)WRITE(6,*)N1,F,ER
33
       3 IF(ER-EPS)8,8,9
34
       9 FR=F
35
         N=N+1
36
         GOTO 6
37
       8 CONTINUE
38
39
      11 RADD=F
      10 RETURN
40
      20 XXG(1)=0D0
41
          WWG(1) = 2D0
42
         KKX=0
43
          KKW=0
44
         DO 24 I=1,9
45
```

46		INXG=I*(I+1)/2
47		J=(I+1)/2
48		IF(I-(I/2)*2.EQ.0) GOTO 21
49		GOTO 22
50	21	KKW=KKW+1
51		XXG(INXG+J+1)=0D0
52		WWG(INXG+J+1)=WG(KKW)
53	22	DO 23 K=1,J
54		KK=I-K+2
55		KX=KKX+J-K+1
56		KW=KKW+J-K+1
57		XXG(INXG+KK) = XG(KX)
58		XXG(INXG+ K) = -XG(KX)
59		WWG(INXG+KK) = WG(KW)
60		WWG(INXG+ K) = WG(KW)
61	23	CONTINUE
62		KKX=KKX+J
63		KKW=KKW+J
64	24	CONTINUE
65		IGSC=2
66		RETURN

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67	DATA XG/ 5.	77350269189626D-1,
68	*7.74596669241483D-1,3.	39981043584856D-1,
69	*8.61136311594053D-1,5.	38469310105683D-1,
70	*9.06179845938664D-1,2.	38619186083197D-1,
71	*6.61209386466265D-1,9.	32469514203152D-1,
72	*4.05845151377397D-1,7.	41531185599394D-1,
73	*9.49107912342759D-1,1.	83434642495650D-1,
74	*5.25532409916329D-1,7.	96666477413627D-1,
75	*9.60289856497536D-1,3.	24253423403809D-1,
76	*6.13371432700590D-1,8.	36031107326636D-1,
77	*9.68160239507626D-1,1.	48874338981631D-1,
78	*4.33395394129247D-1,6.	79409568299024D-1,
79	*8.65063366688985D-1,9.	73906528517172D-1/
80	DATA WG/ 1.	0000000000000 0,
81	*8.88888888888889D-1,5.	55555555555556D-1,
82	*6.52145154862546D-1,3.	47854845137454D-1,
83	*5.6888888888889D-1,4.	78628670499366D-1,
84	*2.36926885056189D-1,4.	67913934572691D-1,
85	*3.60761573048139D-1,1.	71324492379170D-1,
86	*4.17959183673469D-1,3.	81830050505119D-1,
87	*2.79705391489277D-1,1.	29484966168870D-1,
88	*3.62683783378362D-1,3.	13706645877887D-1,
89	*2.22381034453374D-1,1.	01228536290376D-1,
90	*3.30239355001260D-1,3.	12347077040003D-1,
91	*2.60610696402935D-1,1.	80648160694857D-1,
92	*0.81274388361574D-1,2.	95524224714753D-1,
93	*2.69266719309996D-1,2.	19086362515982D-1,
94	*1.49451349150581D-1,0.	66671344308688D-1/
95	END	