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FURN3D: A Computer Code for Radiative Heat Transfer in Pulverized Coal Furnaces

by R. K. Ahluwalia and K. H. Im

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August 1992

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ABSTRACT

A computer code FURN3D has been developed for assessing the impact of burning different coals on heat absorption pattern in pulverized coal furnaces. The code is unique in its ability to conduct detailed spectral calculations of radiation transport in furnaces fully accounting for the size distributions of char, soot and ash particles, ash content, and ash composition. The code uses a hybrid technique of solving the three-dimensional radiation transport equation for absorbing, emitting and anisotropically scattering media. The technique achieves an optimal mix of computational speed and accuracy by combining the discrete ordinate method (S_4), modified differential approximation (MDA) and P_1 approximation in different range of optical thicknesses. The code uses spectroscopic data for estimating the absorption coefficients of participating gases CO_2, H_2O and CO. It invokes Mie theory for determining the extinction and scattering coefficients of combustion particulates. The optical constants of char, soot and ash are obtained from dispersion relations derived from reflectivity, transmissivity and extinction measurements. A control-volume formulation is adopted for determining the temperature field inside the furnace. A simple char burnout model is employed for estimating heat release and evolution of particle size distribution. The code is written in Fortran 77, has modular form, and is machine-independent. The computer memory required by the code depends upon the number of grid points specified and whether the transport calculations are performed on spectral or gray basis.

1. INTRODUCTION

Thermal radiation is the principal mode of heat transfer in pulverized coal (PC) furnaces. The radiative transfer is due to both band emission from gaseous molecules (CO_2, H_2O, CO, SO_2) and continuous emission from the various types of particles which occur in coal flames. Continuous or luminous radiation is a function of the type of particles, size distribution and concentration. Thus, different coals and coal preparations with different ash content, ash composition, coal grind, volatile matter and moisture/water content can exhibit different heat transfer characteristics. The purpose of this report is to document a computer model FURN3D that is sensitive to combustion particulate characteristics and thus capable of resolving the effect of coal preparation and substitution on furnace heat absorption.

A principal attribute of FURN3D is the ability to conduct radiation calculations on a detailed spectral basis. This is a computationally intensive process which necessitates development of an expedient technique for solving the radiation transport equation (RTE) without sacrifice of accuracy. Some of the various techniques of solving RTE in the order of computational requirement are the Monte Carlo method, zone method, discrete-ordinate method (S_N), modified differential approximation (MDA) and the differential approximation (P_1). The first two techniques are somewhat incompatible with finite-difference formulations and impractical for repetitive spectral calculations inside an iterative loop for unknown gas temperature field. The technique advocated in FURN3D is a hybrid of S_N, MDA and P_1. For a particular frequency and spectral extinction coefficient, the code selects one of the three techniques on the basis of computational speed and solution accuracy. In a given run, the code may use all three techniques at different frequencies. Depending upon the spectrum of extinction coefficients, the S_N technique may be invoked for more number of wave bands in one simulation than in another. Similarly, the code may select the P_1 approximation for more frequencies in some simulations than in others. The net outcome is that the computational time in FURN3D is problem dependent besides being grid dependent.

FURN3D employs Mie theory for determining the macroscopic absorption and scattering cross-section of combustion particles. Size distributions are

represented in form of histograms. For each frequency considered in the code, efficiency factors corresponding to particle size grids are calculated for char, soot, and ash; integrated over respective size spectra; summed; and combined with gas absorption coefficients to obtain the spectral extinction coefficients and scattering albedos of the gas-particle mixture.

For use in Mie theory, the work incorporates a comprehensive procedure for estimating the complex refractive indices of char, soot and ash particles. Dispersion relations for char are derived from experimental data on spectral efficiency factors, and those for soot are approximated by dispersion constants for soot from hydrocarbon fuels. The algorithm for refractive indices of ash follows recommendations based on experimental data for synthetic slags. The algorithm accounts for the SiO_2, $A\ell_2O_3$, FeO/Fe_2O_3, CaO, MgO and TiO_2 components of ash.

A control volume approach is adopted in FURN3D for the purpose of constructing heat balance and determining the temperature field. This approach avoids undue complications associated with solution of the fluid flow equations and targets the effort to an accurate determination of the radiation field. It also allows use of a non-linear equation solver leading to a rapid convergence for the temperature field. A simple char burnout model is incorporated to determine the heat release pattern inside the furnace.

This report serves the function of a computer code manual. It describes the underlying theory and its implementation, code structure, subroutines, input data and sample outputs. It does not discuss specific applications or results obtained from exercising the code. Three separate reports/papers are available for consultations regarding the aspects of code not discussed here. A technical report [Im and Ahluwalia, 1990] has been prepared on the radiation properties of coal flames. It assesses the existing experimental data and the theoretical bases for determining the absorption and scattering coefficients of products of coal combustion. It describes the results from a parametric study conducted to elucidate the role of char, soot and ash particulates in determining the radiation properties of coal flames. A technical paper [Park, Ahluwalia and Im, 1992] has been prepared on the numerical techniques for solving the radiation transport equation in three-dimensional absorbing, emitting and scattering media.

It evaluates S_4, MDA and P_1 approximation in terms of the computer memory requirement, CPU time and numerical accuracy. A technical report [Ahluwalia and Im, 1992] is being prepared to present results of a sensitivity study on furnace heat absorption for coals of different ash compositions, ash content (coal cleaning), grind (micronization), and moisture levels (slurries).

2. THEORY

The furnace model emphasizes detailed spectral calculations of three-dimensional radiation heat transfer from coal flames. A significant amount of effort is expended in determining the radiation properties of products of coal combustion. Luminous radiation from combustion particles is determined by applying Mie theory to a cloud containing char, soot and ash particles. Histogram representations are used to account for particle size distributions. Optical constants of char and soot are determined from dispersion relations and those of ash from empirical information. A separate report is available on the effects of coal preparation, ash content and ash composition on radiation properties of coal flames.

A hybrid technique is used to solve the three-dimensional radiation transport equation in absorbing, emitting and anisotropically scattering media. The technique selects P_1 approximation, modified differential approximation and the discrete ordinate method for solving RTE in different range of optical thicknesses. The selection process considers method applicability, accuracy and computational efficiency. The basis of the method is discussed elsewhere [Ahluwalia and Im, 1992].

A control volume formulation is used to construct heat balance and calculate temperature field. Solution of RTE has also been coupled to an elaborate three-dimensional fluid flow code in a separate effort and is not described here.

2.1 RADIATION PROPERTIES OF COAL FLAMES

In coal furnaces, radiative heat transfer is due to both band emission from CO_2 and H_2O and continuous emission from the various types of particles (coal, char, soot and flyash) that occur in the flame. The parameters determining continuous radiation are particle mass fraction and distribution in the flow field, particle size distribution, and the complex refractive index generally represented as n + ik where n is the refractive index and k the absorption index. For given n and k, Mie theory for homogeneous spherical particles is used for calculating the efficiency factors for extinction (Q_e) and scattering (Q_s) as a

function of $2\pi r/\lambda$. A histogram representation is adopted for particle size distribution (psd). The efficiency factors are calculated for each size, weighted over cross-sectional area and integrated over psd to obtain macroscopic absorption and scattering cross-sections. On combining with gas absorption coefficient, one obtains the spectral extinction coefficient and the scattering albedo as

$$\beta = \kappa + \int Q_e \pi r^2 n dr \tag{2.1}$$

$$\omega = \int Q_s \pi r^2 n dr / \beta \tag{2.2}$$

2.2 GAS ABSORPTION COEFFICIENTS

In coal combustion, CO_2, H_2O, and trace amounts of CO and SO_2 are produced which participate in radiant heat transfer by the virtue of interaction of infrared radiation with vibrational and rotational modes of energy absorption by the gaseous molecules. The line structure of the vibration-rotation bands may be described by postulating a random spectrum of Lorentz lines of equal widths (Goody model). This postulate leads to the following definition of absorptivity of a homogeneous gas path of length L for ith species and jth band.

$$\alpha_{ij} = 1 - \exp\{-(s/d)_{ij}\rho_i L[1 + 2(s/d)_{ij}\rho_i L/(2\pi\gamma/d)_{ij}]^{-1/2}\} \tag{2.3}$$

where s is mean intensity, d is line spacing, γ is mean line width, ρ is the density of absorber and L is the mean beam length. In radiation transport calculations, one needs to determine the absorption coefficient. It is possible to define an 'apparent' absorption coefficient of gas as

$$\kappa = \sum_i \sum_j \frac{(s/d)_{ij}\rho_i}{[1 + 2(s/d)_{ij}\rho_i L/(2\pi\gamma/d)_{ij}]^{1/2}} \tag{2.4}$$

In a narrow band model, an extensive data base is developed on the mean intensity to line spacing ratio s/d and the line density 1/d over the entire infrared spectrum for every vibration and rotation band of a gaseous species. An empirical correlation is constructed to determine the line width as a function of broadening pressures and gas temperatures. A comprehensive set of tabulations has been produced for the 1.14, 1.38, 1.87, 2.7 and 6.3 μm banks of H_2O, 2.0,

2.7, 4.3, 9.4, 10.4 and 15 μm bands of CO_2, 2.35 and 4.7 μm bands of CO, and 4.0, 4.3, 7.4, 8.7 and 19.3 μm bands of SO_2. Wide band models are constructed by prescribing a variation of s/d and γ/d versus υ within a band. In an exponential wide band model, such as due to Edwards [1976] used in this work, s/d is assigned an exponential shape.

2.3 CHAR OPTICAL CONSTANTS

Optical constants of char have been derived from the extinction efficiency data of Brewster and Kunitomo [1984], and represented by a dispersion relation as a combination of three bound-electron oscillators and a free-electron oscillator.

$$n^2 - k^2 = n_\infty^2 + \sum_j \frac{\omega_{pj}^2(\omega_j^2 - \omega^2)}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\,\omega^2} - \frac{\omega_f^2}{\omega^2 + \gamma_f^2} \tag{2.5}$$

$$2nk = \sum_j \frac{\omega_{pj}^2\gamma_j\omega}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\omega^2} + \frac{\omega_f^2\gamma_f}{\omega(\omega^2 + \gamma_f^2)} \tag{2.6}$$

Mie theory was employed to determine theoretical extinction efficiency factors corresponding to n and k calculated from the dispersion relation. A non-linear optimizer was used to determine dispersion constants that yielded best least-square fit of the efficiency factor data. Table 2.1 lists the oscillator parameters determined in this manner.

Table 2.1 Oscillator Parameters for Char

	Saraji Char	West Char	Sufco Char
n_∞	2.046×10^{-2}	1.896×10^{-2}	3.012×10^{-2}
ω_f, cm^{-1}	1.371×10^4	1.286×10^4	9.157×10^3
γ_f, cm^{-1}	4.522	1.548×10^{-1}	5.187×10^1
ω_{p1}, cm^{-1}	3.550×10^4	3.542×10^4	2.252×10^4
ω_1, cm^{-1}	1.357×10^4	1.357×10^4	1.357×10^4
γ_1, cm^{-1}	6.259×10^3	3.418×10^3	9.868×10^3
ω_{p2}, cm^{-1}	4.5×10^3	4.499×10^3	4.506×10^3
ω_2, cm^{-1}	3.597×10^4	3.597×10^4	3.597×10^5
γ_2, cm^{-1}	7.622×10^5	7.622×10^5	7.622×10^5
ω_{p3}, cm^{-1}	3.435×10^4	3.450×10^5	3.950×10^4
ω_3, cm^{-1}	7.593×10^3	7.593×10^3	7.593×10^3
γ_3, cm^{-1}	2.166×10^4	1.964×10^4	3.896×10^4

2.4 SOOT OPTICAL CONSTANTS

There are no extant data on optical properties of coal soot, although voluminous data may be found on soot produced from other hydrocarbon fuel. Lee and Tien [1981] analyzed the optical constants of soot using dispersion theory applied to two bound and one free electron oscillators. They determined some dispersion parameters rigorously and deduced the remaining unknowns from in-situ flame transmission data. Their results indicate that the infrared optical properties of soot are relatively independent of the fuel hydrogen to carbon ratio and the molecular structure of soot. Thus their dispersion constants can be regarded as some mean values applicable to many fuels including coal. Table 2.2 lists the dispersion constants ($n_\infty = 1$) at reference temperatures of 1450 and 300 K. At other temperatures, damping frequencies γ_f and γ_j at 1450 K may be corrected by multiplication with the factor $(T/1450)^{1/2}$.

Table 2.2. Soot Dispersion Constants

	1450 K	300 K
n_∞	1	1
ω_f, cm^{-1}	5.049×10^4	5.049×10^4
γ_f, cm^{-1}	4.0×10^4	1.819×10^4
ω_{p1}, cm^{-1}	1.201×10^5	1.201×10^5
ω_{01}, cm^{-1}	4.167×10^4	4.167×10^4
γ_1, cm^{-1}	1.967×10^5	8.947×10^4
ω_{p2}, cm^{-1}	3.979×10^5	3.979×10^5
ω_2, cm^{-1}	2.417×10^5	2.417×10^5
γ_2, cm^{-1}	1.867×10^5	8.492×10^4

2.5 ASH OPTICAL CONSTANTS

Goodwin [1986] has performed systematic measurements of transmittance through, and, near-normal reflectance on, thin polished wafers cut from coal slags, from which the ash optical constants were determined. The wafers were cut from synthetic slags, prepared from oxide powder mixtures, and natural slags, prepared by remelting flyash or gasifier slag. The transmittance spectra were measured at room temperature from 0.19 to 8 μm and the reflectance spectra from

1 to 13 μm. The optical constants were determined from the transmittance and reflectance data at wavelengths where both sets of data were available. At wavelengths longer than 8 μm the wafers were opaque, and a Kramers-Kronig analysis of the spectral reflectance data was made to compute the optical constants.

A mixture rule was developed to predict the real part of the refractive index from 1 to 8 μm in terms of the mass fraction (Y) of the mineral constituents SiO_2, $A\ell_2O_3$, CaO, MgO and Fe_2O_3.

$$n(\lambda) = \left[\frac{1 + 2\rho\Sigma Y_i F_i(\lambda)}{1 - \rho\Sigma Y_i F_i(\lambda)}\right]^{1/2} \tag{2.7}$$

$$\rho = 2.54 + 0.00978\ Y_{Fe_2O_3} \tag{2.8}$$

$$F_i(\lambda) = (a_i\lambda^2 - b_i)/(c_i\lambda^2 - d_i) \tag{2.9}$$

The parameters a,b,c and d are 0.9389, 53, 5.001 and 420 for SiO_2; 1.914, 174, 10.36 and 1633.8 for $A\ell_2O_3$; 4.25, 827.7, 16.63 and 6102.3 for CaO; 1.647, 0, 11.36 and 0 for Fe_2O_3; 2.72, 260, 15.8 and 1954.4 for TiO_2; and 1.278, 136.9, 7.433 and 1200.9 for MgO.

According to Goodwin's data, the imaginary part of the refractive index depends primarily on the iron, silica and OH contents of the slag. Iron is the primary absorber for $\lambda < 4$ μm. A correlation was developed for the effect of Fe in this wavelength region, accounting for both Fe^{2+} ligand-band absorption and Fe^{2+} - Fe^{3+} intervalence charge transfer absorption. The correlation is given in terms of the molar concentrations of Fe^{2+} and Fe^{3+}.

$$k(\lambda) = A_1 e^{1.75/\lambda} + A_2 g(\lambda) \tag{2.10}$$

$$A_1 = 2.30 \times 10^{-5}[Fe^{2+}]\ [Fe^{3+}] \tag{2.11}$$

$$A_2 = 7.685 \times 10^{-5}[Fe^{2+}] + 7.037 \times 10^{-6}[Fe^{2+}]^2 \tag{2.12}$$

$$[Fe] = \frac{2\rho}{MW_{Fe_2O_3}}\ Y_{Fe_2O_3} \tag{2.13}$$

$$g(\lambda) = a_1(\lambda - \lambda_u) + b_1 \quad \lambda_\ell < \lambda < \lambda_u \tag{2.14}$$

Table 2.3 provides the parameters comprising the $g(\lambda)$ expression.

Table 2.3. Parameters Defining $g(\lambda)$

λ_ℓ	λ_u	a_1	b_1
0.0	1.1	5.5	2.5
1.1	1.54	-1.3529	2.18
1.54	1.9	0.7778	2.46
1.9	2.3	-0.9150	2.094
2.3	2.6	-0.6533	1.898
2.6	4	0.1877	2.153

In the intermediate wavelength region, $4 < \lambda < 8$ μm, the absorption index is dominated by vibrational absorption due to Si-O-Si and Si-O^-.

$$k(\lambda) = \frac{\rho}{\rho_0} Y_{SiO_2} k_0(\lambda) \tag{2.15}$$

where ρ_0, the specific gravity of fused silica, is 2.19. Table 2.4 lists the spectral variation in $k_0(\lambda)$ at T_0 = 300 K. In the intermediate wavelength region, the following temperature correction may be applied to the absorption index.

$$k(T) = k(T_0)[1 + \frac{2}{\exp(7194/\lambda T) - 1}] \tag{2.16}$$

Table 2.4. Silica Absorption Index, $k_0(\lambda)$

λ, μm	k_0, m^{-1}	λ, μm	k_0, m^{-1}	λ, μm	k_0, m^{-1}
4.00	5.79×10^{-5}	5.00	3.98×10^{-3}	6.667	7.16×10^{-3}
4.082	7.99×10^{-5}	5.063	5.12×10^{-3}	6.897	8.51×10^{-3}
4.167	1.07×10^{-4}	5.128	5.18×10^{-3}	7.143	1.06×10^{-2}
4.255	1.32×10^{-4}	5.263	5.49×10^{-3}	7.407	1.48×10^{-2}
4.348	2.13×10^{-4}	5.333	5.69×10^{-3}	7.692	3.72×10^{-2}
4.396	2.65×10^{-4}	5.405	5.72×10^{-3}	7.752	4.74×10^{-2}
4.444	2.84×10^{-4}	5.556	5.63×10^{-3}	7.813	7.68×10^{-2}
4.494	2.84×10^{-4}	5.882	5.94×10^{-3}	7.874	0.132
4.545	2.56×10^{-4}	6.061	6.32×10^{-3}	7.937	0.216
4.651	2.62×10^{-4}	6.154	6.46×10^{-3}	8.00	0.323
4.762	4.85×10^{-4}	6.250	6.52×10^{-3}		
4.878	1.82×10^{-3}	6.452	6.57×10^{-3}		

The optical constants in the wavelength range 8 to 13 μm were observed to be dominated by three absorption bands. The first absorption peak at 9.4 μm was attributed to Si-O vibration associated with bridging oxygen (i.e., Si-O-Si). The second peak at 10.4 μm was observed to increase in strength with Fe_2O_3 content. This peak is associated with $Si\text{-}O^-$ vibration (non-bridging oxygen). The third peak at approximately 13 μm was similar to the peak seen in the fused silica spectrum, and may be due to the occurrence of ring groups. The experimental data were curve-fitted by a three-oscillator model of Eqs. (2.5)-(2.6) with $n_\infty = 1.47$ and $\omega_f = 0$. The resonant frequencies and the damping constants of the bound-electron oscillators in pairs are 1062.8 and 164.7, 955.8 and 79.1, and 702.8 and 27.5 cm^{-1}. The plasma frequencies were expressed as a function of silica and iron mass fractions in ash.

$$(\omega_{p1}/\omega_1)^2 = (0.425 - 0.60\, Y_{Fe_2O_3})(Y_{SiO_2}/0.52) \tag{2.17}$$

$$(\omega_{p2}/\omega_2)^2 = (0.175 + 0.75\, Y_{Fe_2O_3})(Y_{SiO_2}/0.52) \tag{2.18}$$

$$(\omega_{p3}/\omega_3)^2 = 0.053(Y_{SiO_2}/0.52) \tag{2.19}$$

Table 2.5. Oscillator Constants for $A\ell_2O_3$ and MgO Restrahlen Bands

Oscillator	1	2	3	4
a) $A\ell_2O_3$, $n_\infty^2 = 3.01$				
ω_{pj}, cm^{-1}	210.9	726.3	639.1	347.8
ω_j, cm^{-1}	383	442	369	635
γ_j, cm^{-1}	0.015	0.01	0.02	0.02
b) MgO, $n_\infty^2 = 3.01$				
ω_{pj}, cm^{-1}	1030.2	135.8		
ω_j, cm^{-1}	401	640		
γ_j, cm^{-1}	7.62	102.6		

No experimental data are reported for the long wavelength region $\lambda > 13$ μm. At the suggestion of Goodwin, the optical constants in this range are assumed to be dominated by the Restrahlen bands of $A\ell_2O_3$ and MgO. A four-oscillator fit is

used to describe the $A\ell_2O_3$ spectrum and a two-oscillator fit for MgO Restrahlen band. Table 2.5 summarizes the oscillator parameters for $A\ell_2O_3$ and MgO bands. In lieu of any better information, we adopt a simple mixture rule in which n and k for $A\ell_2O_3$ and MgO bands are mass-fraction averaged to obtain the optical constants for ash in the long wavelength region.

2.6 RADIATION HEAT TRANSFER

For a three-dimensional absorbing, emitting and scattering rectangular enclosure, the radiation transport equation (RTE) is

$$\nabla\cdot(\hat{s}I) + \beta I = (1 - \omega)\beta I_b + \frac{\omega\beta}{4\pi}\int_{4\pi} I(\vec{r},\hat{s}')\phi(\hat{s},\hat{s}')d\Omega' \tag{2.20}$$

where I is the spectral radiation intensity in the beam direction $\hat{s}$, β and ω are respectively the spectral extinction coefficient and scattering albedo, I_b is the Planck function, ϕ is the scattering phase function and Ω denotes the solid angle. The boundary conditions for diffusely reflecting walls are:

$$I(\vec{r},\hat{s}) = \epsilon I_b + \frac{(1 - \epsilon)}{\pi}\int_{\hat{n}\cdot\hat{s}<0}|\hat{n}.\hat{s}|I(\vec{r},\hat{s}')d\Omega' . \tag{2.21}$$

Three of the many methods of solving RTE are the differential approximation (P_1), modified differential approximation (MDA), and the discrete ordinate method (S_4). Each method has its own advantages and disadvantages. Of the three methods, P_1 approximation is computationally the fastest but accurate only in the optically thick limit. MDA is accurate for all β but has shown slow convergence in the optically thin limit. S_4 is also accurate for all β but is computationally slow particularly for large β. We have developed a hybrid scheme with optimal mix of computational speed and accuracy. In this scheme, P_1 approximation is used for $\beta > \beta_{max}$, MDA for $\beta_{min} < \beta < \beta_{max}$, and S_4 for $\beta < \beta_{min}$. Typically, β_{min} and β_{max} are respectively of the order of 0.01 m^{-1} and 2.0 m^{-1}. Although not specifically required, the scattering phase function is assumed to be linearly anisotropic of the form,

$$\phi(\hat{s},\hat{s}') = 1 + a_1(\hat{s}.\hat{s}') \tag{2.22}$$

2.7 P_1 APPROXIMATION

Governing equations for P_1 approximation may be derived by expanding the radiation intensity in terms of a truncated series of spherical harmonic functions or by employing the lowest-order moment method. For a linearly anisotropic phase function and diffusely reflecting walls, the method reduces to determining the incident radiation from

$$\nabla\cdot\left(\frac{1}{\beta_1}\nabla G\right) - 3(1-\omega)\beta G = -12\pi(1-\omega)\beta I_b \tag{2.23}$$

subject to wall boundary conditions

$$-\frac{\gamma}{3\beta_1}\hat{n}.\nabla G + G = 4\pi I_{bw} \tag{2.24}$$

where

$$\beta_1 = \beta(1 - \omega_1) \tag{2.25}$$

$$\omega_1 = a_1\omega/3, \text{ and} \tag{2.26}$$

$$\gamma = 2/3(2/\epsilon - 1) . \tag{2.27}$$

Equation (2.23) is solved numerically by using a cell-centered finite difference technique.

2.8 MODIFIED DIFFERENTIAL APPROXIMATION

Following Modest [1989], the radiation intensity I is decomposed into two parts: one I_s, that may be traced to emission from the enclosure walls, and the second, I_m, that may be traced to emission from the medium. The two components of intensity are governed by the following equations.

$$\nabla.[\hat{s}I_s(\vec{r},\hat{s})] + \beta I_s(\vec{r},\hat{s}) = 0 \tag{2.28}$$

$$\nabla.[\hat{s}I_m(\vec{r},\hat{s})] + \beta I_m(\vec{r},\hat{s}) = (1 - \omega)\beta I_b + \frac{\omega\beta}{4\pi}\int_{4\pi} I(\vec{r},\hat{s}')\phi(\hat{s},\hat{s}')d\Omega' \tag{2.29}$$

I_s field, given by Eq. (2.28), accounts for radiation emitted by the furnace

walls after attenuation by medium absorption and scattering by wall reflection. It is solved by the discrete ordinate method (S_4) subject to the following wall boundary condition.

$$I_s(\vec{r},\hat{s}) = \epsilon I_b(\vec{r}) + \frac{(1-\epsilon)}{\pi}\int_{\hat{n}.\hat{s}<0} |\hat{n}.\hat{s}| I_s(\vec{r},\hat{s}')d\Omega' \tag{2.30}$$

Following Modest [1989] whereas I_s with its origin from the radiation emitted by the wall has highly irregular angular distribution, I_m with its origin linked to medium emission is expected to be near isotropic. Thus, Eq. (2.29) describing I_m can be simplified by applying the P_1 approximation. For a linear anisotropic phase function, the following equation for the incident radiation G_m may be derived.

$$\nabla.\frac{1}{\beta_1}\nabla G_m - 3(1-\omega)\beta G_m = -12\pi(1-\omega)\beta I_b - 3\omega\beta[1 + \frac{a_1}{3(1-\omega_1)}]G_s \tag{2.31}$$

For a diffusely reflecting surface, G_m admits Marshak's boundary condition for a cold surface

$$-\frac{\gamma}{3\beta_1}\hat{n}.\nabla G_m + G_m = -\frac{\gamma\omega_1}{1-\omega_1}\vec{q}_s.\hat{n} \tag{2.32}$$

Equation (2.31) is solved numerically for G_m by using a cell-centered finite difference technique. As pointed out by Modest, MDA reduces to the correct limits for optically-thin as well as optically-thick mediums. In the thin limit, the medium emission related contribution to heat transfer becomes vanishingly small. In the thick limit, the MDA solution converges to the P_1 approximation.

2.9 DISCRETE ORDINATE METHOD

In the S_4 method, RTE is solved for twenty-four ordinate directions and the integrals are replaced by a quadrature summed over the ordinate directions. For a discrete direction Ω_ℓ defined by directional cosines μ_ℓ, ξ_ℓ and η_ℓ, RTE is written as

$$\mu_\ell\frac{\partial I^\ell}{\partial x} + \xi_\ell\frac{\partial I^\ell}{\partial y} + \eta_\ell\frac{\partial I^\ell}{\partial z} + \beta I^\ell = (1-\omega)\beta I_b + \frac{\omega\beta}{4\pi}S_\ell \tag{2.33}$$

where S_ℓ is the source term for in-scattered radiation.

$$S_\ell = \sum_{\ell=1}^{N_\ell'} w_{\ell'} \phi_{\ell\ell'} I^{\ell'} \tag{2.34}$$

$$w_{\ell'} = \pi/4 \tag{2.35}$$

The finite-difference form of S_4 solution is developed by integrating RTE over a control volume. For positive directional cosines,

$$I_p^\ell = \frac{\mu_\ell A I_i^\ell + \xi_\ell B I_j^\ell + \eta_\ell C I_k^\ell + \alpha[(1-\omega)\beta I_b + S_\ell]V_p}{\mu_\ell A + \xi_\ell B + \eta_\ell C + \alpha\beta V_p} \tag{2.36}$$

where

$$A = \Delta x \Delta y \tag{2.37}$$

$$B = \Delta x \Delta z \tag{2.38}$$

$$C = \Delta x \Delta y \tag{2.39}$$

$$V_p = \Delta x \Delta y \Delta z \tag{2.40}$$

$$I_p^\ell = \alpha I_i^\ell + (1-\alpha) I_{i+1}^\ell = \alpha I_j^\ell + (1-\alpha) I_{j+1}^\ell = \alpha I_k^\ell + (1-\alpha) I_{k+1}^\ell \tag{2.41}$$

The interpolation parameter α varies between 0.5 and 1. The overall solution is developed by visiting the finite-difference grid in the direction of the beam. More details of the solution procedure are given in Carlson and Lathrop [1968].

2.10 HEAT BALANCE

For heat balance purposes, the furnace is divided into three types of zones: a hopper zone designated as zone 1, a burner belt zone designated as zone 2, and heat absorption zones. Recirculated flue gas is directed into the hopper zone. Fuel and oxidizer enter the furnace in the burner belt zone. A recirculation pattern exchanges flow between zones 1 and 2. With this flow representation, the following heat balance equations may be written.

$$\dot{m}_r(h_r - h_1) + \dot{m}_R(h_2 - h_1) = \iint_{V_1} \nabla.\vec{q}\,dVd\nu \tag{2.42}$$

$$\dot{m}_f(h_f - h_2) + \dot{m}_a(h_a - h_2) + (\dot{m}_r + \dot{m}_R)(h_1 - h_2) + F_2\dot{m}_f Q_{hv} = \iint_{V_2} \nabla.\vec{q}\,dVd\nu \tag{2.43}$$

$$(\dot{m}_r + \dot{m}_f + \dot{m}_a)(h_i - h_{i+1}) + F_i\dot{m}_f Q_{hv} = \iint_{V_i} \nabla.\vec{q}\,dVd\nu,\ i > 2 \tag{2.44}$$

In the foregoing equations, F is fractional heat release, h is the enthalpy, $\dot{m}$ is the flow rate and Q_{hv} denotes the heating value. The subscripts a, f, r and R designate air, fuel, recirculated flue gas and recirculated combustion gas, respectively. The divergence of heat flux may be determined from the following equation.

$$\nabla.\vec{q} = 4\pi(1 - \omega)\beta(I_b - \frac{G_m + G_s}{4\pi}) \tag{2.45}$$

The energy equations are coupled and nonlinear in zone temperatures. A hybrid non-linear equations solver based on steepest descent method and Newton update algorithm is used to determine the gas temperature.

3. PROGRAM DESCRIPTION

The theory described in Chapter 2 has been encapsulated in a computer code FURN3D. The code is written in a modular form in Fortran 77 language. Each subroutine is self contained and can be modified and compiled separately. All common blocks are segragated in a file furn3d.h and positioned in subroutines by means of an include command. Sizes of arrays appearing in common blocks are specified through a parameter statement. Thus, the array sizes can be easily manipulated through integer variables specifying the dimensions in a single statement in furn3d.h.

3.1 LOGIC FLOW

The flow diagram of FURN3D is sketched in Figs. 3.1 through 3.3. The program starts with a call to the INPUT subroutine which reads the input data and prints an image form of the input data.

Within MAIN, Fortran function dtime is invoked to initialize variable tstart. This variable is utilized in subsequent steps to track expenditure of CPU resources in different portions of the computer code.

Structure of MAIN can be best explained in terms of four segments: setup, G_s, G_m and post-processing. The setup segment consists of subroutines INPUT, INIT, GRID, COMPSN, COMBDRV and OPTDRV. The purpose of these subroutines is respectively to define the problem; initialize the variables; initialize the finite-difference grid; determine the gas composition; calculate ash and soot particle size distributions; determine evolution of char psd and heat release; and calculate the spectral absorption coefficients and scattering albedos. COMBDRV is actually a driver subroutine which calls DIFFUS for diffusivity of gaseous species, CONDUC and VISCOS for gas conductivity and viscosity, and BURNOUT for char combustion and heat release. Similarly, OPTDRV is a driver subroutine which calls OPTPROP for radiation properties.

Figure 3.2 shows the interrelationship between the radiation property subroutines. Calculation of particle efficiency factors for extinction and scattering depends on the values of indices, incl(1), incl(2) and incl(3),

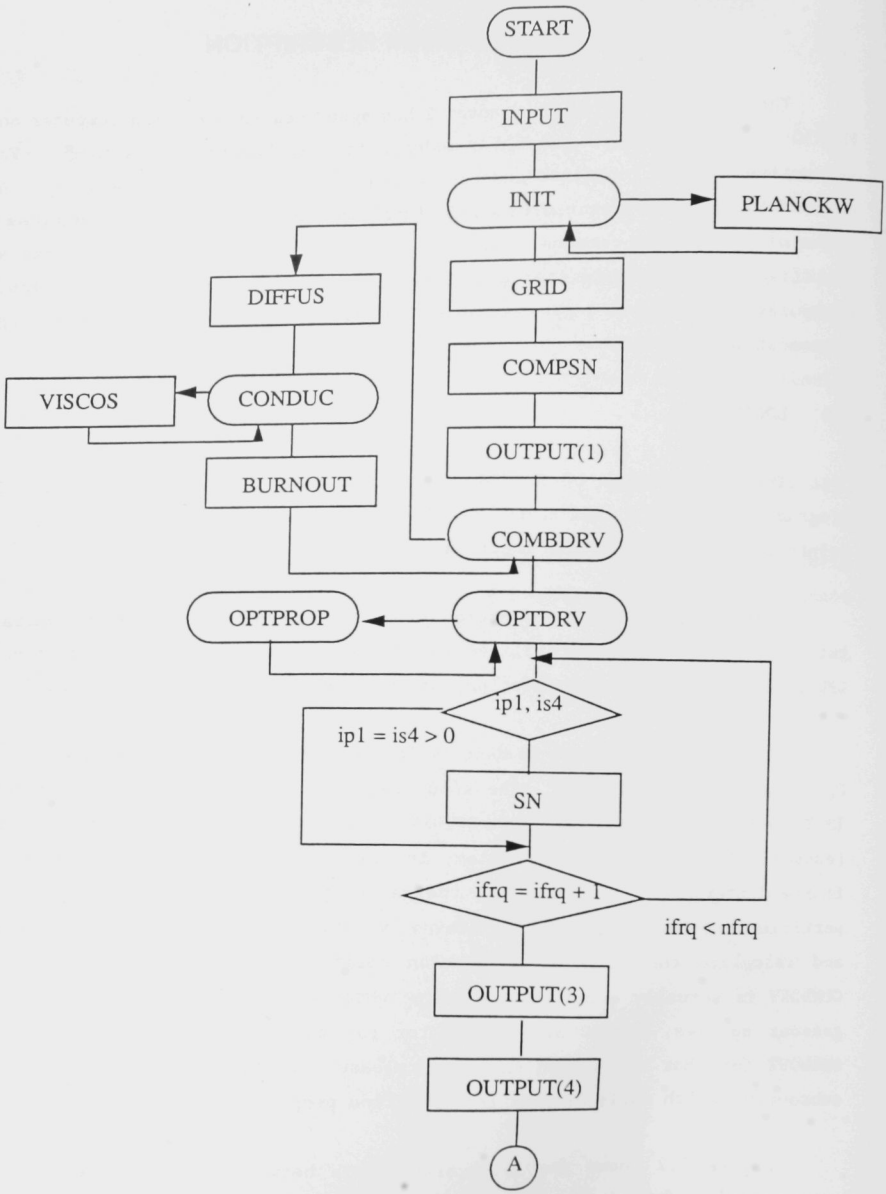

Fig. 3.1. Setup and G_s Segments of FURN3D.

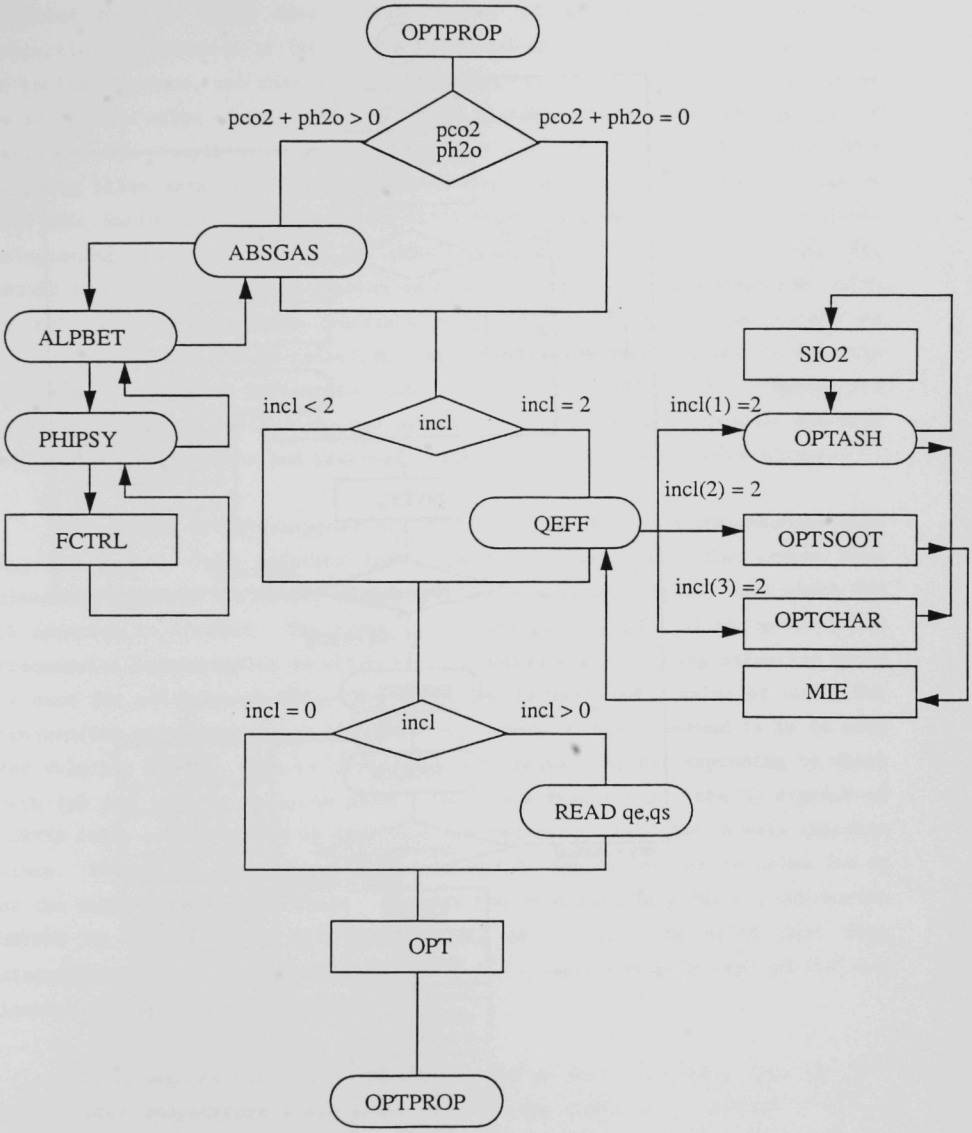

Fig. 3.2. Radiation Properties Subroutines.

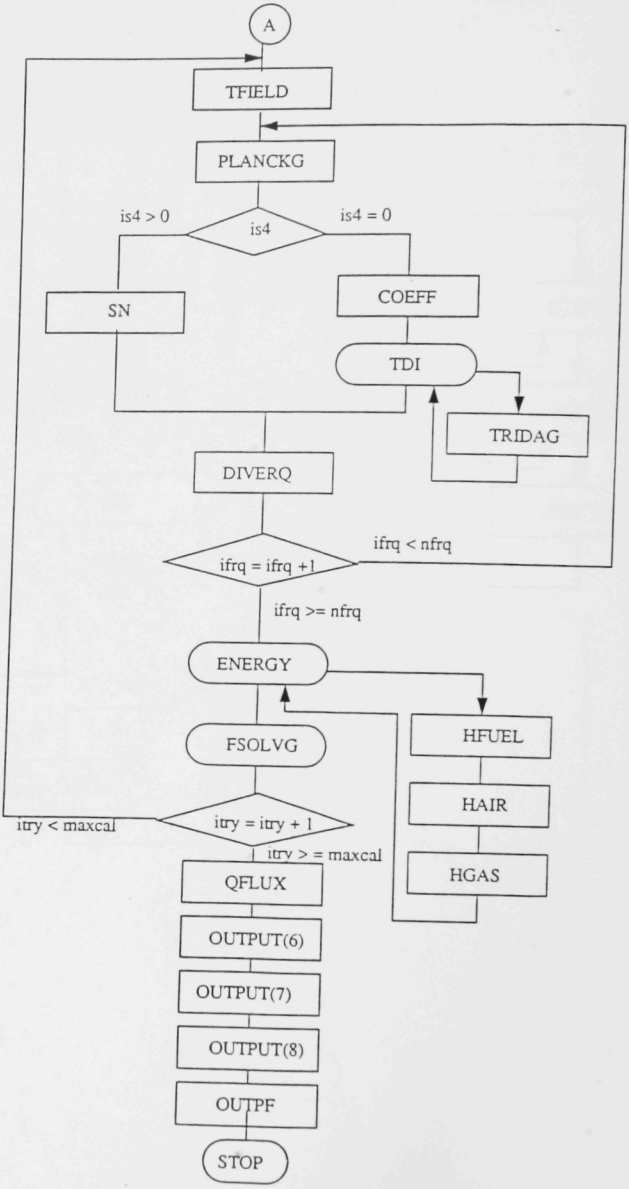

Fig. 3.3. G_m and Post-processing Segments of FURN3D.

supplied through input data. Contribution of ash particles to radiation properties is excluded if incl(1) is specified as zero, that of soot particles if incl(2) is zero, and that of char particles if incl(3) is zero. If the index is assigned a value of one, the efficiency factors of the corresponding kind of particles are simply read as a function of particle size and frequency from existing files qash, qsoot or qchar. Alternately, if the index has a value of two, the extinction and scattering efficiency factors are updated by first calculating optical constants followed with use of Mie theory. Within OPT, ABSGAS is called for gas absorption coefficients if the partial pressure of CO_2 or H_2O is non-zero. The particle efficiency factors are multiplied by geometrical area to obtain radiation cross sections and then integrated over size spectrum to obtain extinction and scattering coefficients. These are appropriately combined with the gas absorption coefficients to generate spectral extinction coefficients and scattering albedos of the gas-particle mixture.

Subroutine OPTDRV examines the field distribution of β and compares with β_{min} and β_{max} to load solution index arrays ipl and is4. The arrays have dimension equal to the number of frequencies or wavebands (nfrq) into which the IR spectrum is divided. The array ipl is assigned a value of unity for those frequencies corresponding to which $\beta > \beta_{max}$ everywhere and P_1 approximation is to be used for solution of RTE. The array is4 is assigned a value of unity for frequencies corresponding to which $\beta < \beta_{min}$ anywhere and S_4 method is to be used for solution of RTE. MDA is to be used for frequencies corresponding to which both ipl and is4 are equal to zero. For these frequencies, the G_s segment of FURN3D calls subroutine SN to determine the radiation field due to wall emission alone. Within SN, the index is4 is examined to decide whether to solve for G_s or the complete radiation field. Outside the frequency loop for G_s, subroutine OUTPUT is called twice with nout values of 3 and 4 to print heat flux distribution due to G_s and the G_s field if the corresponding indices iout(3) and iout(4) are specified to be unity.

The G_m segment (see Fig. 3.3) consists of an inner frequency loop imbedded in an outer temperature iteration loop. In the inner loop, subroutine SN is called for those frequencies with is4 equal to unity. SN solves the RTE for total incident radiation by the discrete ordinate method (S_4). Subroutine COEFF is called for frequencies with is4 equal to zero. COEFF assembles the finite-

difference coefficients of MDA equation for G_m if the index ipl has a zero value, or of P_1 equation for G is ipl carries a value of unity. The resulting finite difference equations are solved in subroutine TDI and TRIDAG. Knowing G_s, G_m and G, spectral and total divergence of heat flux is determined in DIVERQ.

The outer iteration loop proceeds with initialization or update of temperature field in TFIELD. PLANCKG is called to calculate spectral black body emissive power at specified gas temperatures. The inner frequency loop is executed to establish total divergence of radiation heat flux in the furnace control volumes. Subroutine ENERGY is called to perform heat balance and calculate residuals in the energy equations. The residuals are supplied to the non-linear equation solver FSOLVG which in turn returns a fresh gusss for the temperature field. The iteration loop is reexecuted until the magnitude of residuals becomes smaller than the specified accuracy (acc). The procedure is terminated with an appropriate message if the maximum number of iterations (maxcal) is exceeded or divergence is detected in FSOLVG.

In the post-processing segment of FURN3D, QFLUX is called to determine spectral and total heat flux to different walls of the furnace. Subroutine OUTPUT is called repeatedly with nout equal to 6, 7 and 8 to print spectral wall heat flux, divergence of heat flux and the gas temperature field if the corresponding indices iout(6), iout(7) or iout(8) are specified to be unity. Finally OUTPF is called to print partial pressures, particle size spectra, radiation properties, wall heat transfer, and a summary output of flow rates and heat balance.

3.2 DESCRIPTION OF SUBROUTINES

FURN3D subroutines have been assembled in three groups and arranged alphabetically in each group. Group A represents subroutines related to solution of radiation transport and heat balance equations. Group B contains subroutines dedicated to determining radiation properties of the products of coal combustion. Group C is a compilation of Input/Output (I/O) subroutines and BLOCK DATA. Table 3.1 lists and classifies each subroutine. Appendices A, B and C describe the purpose, arguments and main equations solved in each subroutine.

Table 3.1. Classification of Subroutines

A.1	BURNOUT	B.1	ABSGAS	C.1	BLOCK DATA DATA1
A.2	COEFF	B.2	ALPBET	C.2	BLOCK DATA DATA2
A.3	COMBDRV	B.3	FCTRL	C.3	INPUT
A.4	COMPSN	B.4	MIE	C.4	OUTPF
A.5	CONDUC	B.5	OPT	C.5	OUTPUT
A.6	DIFFUS	B.6	OPTASH		
A.7	DIVERQ	B.7	OPTCHAR		
A.8	ENERGY	B.8	OPTDRV		
A.9	FRAC	B.9	OPTPROP		
A.10	FSOLVG	B.10	OPTSOOT		
A.11	GRID	B.11	PHIPSY		
A.12	HAIR	B.12	QEFF		
A.13	HFUEL	B.13	SIO2		
A.14	HGAS				
A.15	INIT				
A.16	PLANCKG				
A.17	PLANCKW				
A.18	QFLUX				
A.19	SN				
A.20	TDI				
A.21	TFIELD				
A.22	TRIDAG				
A.23	VISCOS				

3.3 INPUT DATA

As mentioned earlier, the dimensions of adjustable arrays in the common blocks are specified in furn3d.h by means of the parameter command. Since the size of the common blocks must be declared in advance, the dimensions of the arrays are fixed during compilation. In problems requiring larger size arrays, the variables specifying the dimensions in the paprameter statement must be increased and the code recompiled. The following integer variables are available for modification.

imx	The maximum number of grid points in x-direction.
jmx	The maximum number of grid points in y-direction.
kmx	The maximum number of grid points in z-direction.
nf	The maximum number of frequencies into which the IR spectrum is divided. Admissible values are 1 for gray gas treatment or 37 for spectral calculations.
nv	The maximum number of control volumes for performing heat balance.

Problem specific data are specified as 28 items. A title card generally precedes a data item. It can be used to identify the data following it. It can be up to 80 characters long and must be enclosed in quotation marks. All numeric data are in free format. Individual data items are explained below in their order of appearances.

Item 1 'Title card for the problem'

Item 2 'Debug output indices'
iout(1) iout(2)-------- iout(16)

Explanation: Sixteen indices are provided for debugging or in-depth output. A particular output is suppressed if the

corresponding iout index is specified to zero. Since some of the outputs can be voluminous, it is recommended that all indices except iout(1) be initially set to zero. Following is the relationship between the indices and variable printed.

iout(1)	mass fraction of combustion products
iout(2)	not used
iout(3)	spectral heat flux due to G_s
iout(4)	G_4
iout(5)	G_m
iout(6)	spectral heat flux due to G_s and G_m
iout(7)	divergence of heat flux
iout(8)	gas temperature at interior nodes
iout(9)	convergence information on S_4 solution
iout(10)	convergence information on G_m solution
iout(11)-iout(13)	not used
iout(14)	detailed output from non-linear equations solver
iout(15)-iout(16)	not used

Item 3 'Number of frequencies used in spectral calculations'
nfrq

Explanation: Admissible values of nfrq are 1 for a gray gas and 37 for spectral calculations.

Item 4 'RTE solution criteria and S_4 relaxation parameter'
betamx betamn alpha

Explanation: Variables betamx and betamn are used to initialize arrays ipl(nfrq) and is4(nfrq) according to the following criteria.

ipl(i) = 1 if β > betamx everywhere
= 0 Otherwise

is4(i) = 1 if β < betamn everywhere

= 0 Otherwise

Variable α is a relaxation parameter used in solving S_4 equations.

Item 5 'Maximum/minimum number of iterations'

nitergm nitgmmn niterj maxcal

Explanation:

nitergm	maximum number of iterations in G_m solution
nitgmmn	minimum number of iterations in G_m solution
niterj	maximum number of iterations in S_4 solutions
maxcal	maximum number of iterations in heat balance equations

Item 6 'Non-linear equations solver: accuracy and temperature increment'

acc deltg

Explanation:

acc	accuracy to which heat balance equations are solved
deltg	temperature increment used in evaluating the differential of the heat balance equation

Item 7 'Grid and control volume information'

imax jmax kmax nvol kvol(1)-----kvol(nvol)

Explanation: In conducting heat balance, the first control volume is designated as the hopper zone. The second control volume is where volatile matter (VM) is released, soot is formed, and VM and soot complete burnout. Char combustion is determined from a burnout model.

imax	number of grids in x direction, imax < imx
jmax	number of grids in y direction, jmax < jmax
kmax	number of grids in z direction, kmax < kmx
nvol	number of control volumes for heat balance equations, nvol < nv

kvol(ivol) demarcation of control volumes, kvol(nvol) = kmax.

Item 8 'Convective heat transfer coefficients, $W/m^2.K$'
hcoef(1) hcoef(2)-------- hcoef(nvol)

Explanation: Number of data points should equal the number of control volumes, nvol.

Item 9 'Spectral surface emissivity'
ew(1) ew(2)------ ew(nfrq)

Explanation: The required number of data points are one for a gray medium and 37 for spectral calculations. Table 3.2 lists the band centers and the band width corresponding to which the surface emissivities must be specified.

Item 10 'Spectral anisotropic scattering factors'
al(1) al(2)----- al(nfrq)

Explanation: In solving the radiation transport equation, the scattering phase function is expressed as a linear function of the cosine of the scattering angle.

$$P(\cos\theta_0) = 1 + a_1\cos\theta_0$$

$$\cos\theta_0 = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi - \phi')$$

Item 11 'Over-relaxation parameter'
omega

Explanation: Variable omega is used as the starting over-relaxation parameter in solving the finite difference equations for G_m. During iterations, the relaxation parameter is gradually increased from omega to 2.

Table 3.2. Wavebands for Spectral Calculations

ifrq	υ_{min} cm^{-1}	υ_{max} cm^{-1}	υ_c cm^{-1}	$\Delta\upsilon$ cm^{-1}	ifrq	υ_{min} cm^{-1}	υ_{max} cm^{-1}	υ_c cm^{-1}	$\Delta\upsilon$ cm^{-1}
1	200	370	285	170	20	6350	6780	6565	430
2	370	640	505	270	21	6780	7000	6890	220
3	640	870	755	230	22	7000	7500	7250	500
4	870	1240	1055	370	23	7500	7800	7650	300
5	1240	1380	1310	140	24	7800	8150	7975	350
6	1380	1880	1630	500	25	8150	8500	8325	350
7	1880	2160	2020	280	26	8500	9000	8750	500
8	2160	2570	2365	410	27	9000	10000	9500	1000
9	2570	2950	2760	380	28	10000	11000	10500	1000
10	2950	3120	3035	170	29	11000	12000	11500	1000
11	3120	3480	3300	360	30	12000	13000	12500	1000
12	3480	3860	3670	380	31	13000	14000	13500	1000
13	3860	4100	3980	240	32	14000	15000	14500	1000
14	4100	4400	4250	300	33	15000	16000	15500	1000
15	4400	4800	4600	400	34	16000	17000	16500	1000
16	4800	5200	5000	400	35	17000	18000	17500	1000
17	5200	5630	5415	430	36	18000	19000	18500	1000
18	5495	5965	5730	470	37	19000	20000	19500	1000
19	6100	6350	6225	250					

Item 12 'Furnace dimensions, m'

xmax ymax zmax

Explanation: Furnace is modeled as a rectangular box of dimensions xmax × ymax × zmax

Item 13 'Furnace wall temperatures, K'

txm txp tym typ tzm tzp

Explanation: Wall temperatures are read in the following order: x-minus wall, x-plus wall, y-minus wall, y-plus wall, bottom wall, and top wall.

Item 14 'Ultimate analysis of coal'

fuel(1) fuel(2) fuel(3) fuel(4) fuel(5)

Explanation: The first five elements of fuel array contain mass fractions of carbon, hydrogen, sulfur, nitrogen and oxygen in that order. Together with the coal moisture content and ash mass fraction, read as fuel(6) and fuel(7) in item 15, they should equal one.

Item 15 'Proximate analysis of coal'

fuel(6) fuel(7) fuel(8) fuel(9) fuel(10)

Explanation: Variables fuel(6), fuel(7), fuel(8), and fuel(9) should add up to 1.

fuel(6) mass fraction of moisture in coal

fuel(7) ash mass fraction

fuel(8) mass fraction of volatile matter

fuel(9) fixed carbon content

fuel(10) fraction of volatile matter that forms soot

Item 16 'Air composition (O_2, N_2, H_2O) and excess air'

air(1) air(2) air(3) air(4)

Explanation: Variables air(1), air(2) and air(3) should add up to 1.

air(1) mass fraction of O_2 in air

air(2) mass fraction of N_2 in air

air(3) moisture content of air

air(4) excess air, i.e., combustion air/theoretical air - 1.

Item 17 'Fractional gas recirculation'

fracr(1) fracr(2)

Explanation: The first variable, fracr(1), represents the fraction of flue gas externally recirculated from furnace exit to the hopper zone. The second variable, fracr(2), refers to the fraction of fuel and air internally recirculated from the combustion zone to the bottom hopper zone.

Item 18 'Fractional heat loss'

aloss(1) aloss(2) aloss(3)

Explanation: Heat losses are specified as fractions of the high heating value. Variable aloss(1) refers to unburnt carbon loss, aloss(2) to unaccounted losses, and aloss(3) to radiation losses.

Item 19 'Fuel, air, recirculating gas temperatures, K'

temp(1) temp(2) temp(3)

Explanation:

temp(1) fuel temperature, K

temp(2) air temperature, K

temp(3) recirculating flue gas temperature, K

Item 20 'High heating valve (J/kg) and furnace rating'

hhv qfurn

Explanation:

hhv high heating value of coal, J/kg

qfurn furnace rating, W

Item 21 'Ash composition'

yash(1) yash(2) yash(3) yash(4) yash(5)

Explanation: Ash composition is used in the program to determine the optical constants. The five data points refer to the mass fractions of SiO_2, $A\ell_2O_3$, CaO, Fe_2O_3 and MgO.

Item 22 'Inclusion indices: ash, soot and char'

incl(1) incl(2) incl(3)

Explanation: Index array incl is a convenient way to dictate the manner in which the contributions of ash, soot and char particles to radiation properties is included. Particle contribution can be excluded by assigning zero value to a particular index. The efficiency factors are read from an existing file if the index is specified to be one. The efficiency factors are recomputed and stored in files qash, qsoot and/or qchar if the index equals two. Contributions of gaseous species H_2O, CO_2 and CO are always included.

Item 23 'Cumulative mass fraction of char particles'

ypt(1,1) ypt(1,2) ypt(1,3)... ypt(1,40)

Explanation: Within the program, particle number density is calculated by differentiating the cumulative mass fraction function. User must input ypt at discrete sizes listed in Table 3.3. The following is the relationship between number density and cumulative mass fraction.

$$ypt(i) = \sum_{j=1}^{i} r_j^3 N_j / \sum_{j=1}^{40} r_j^3 N_j$$

Item 24 'Cumulative mass fraction of soot particles'

ypt(2,1) ypt(2,2) ypt(2,3)... ypt (2,40)

Table 3.3. Particle Size Grid

	Radius, μm				Radius, μm		
Grid	Ash	Soot	Char	Grid	Ash	Soot	Char
1	0.10	0.01	0.10	21	12.0	0.21	12.0
2	0.25	0.02	0.25	22	14.0	0.22	14.0
3	0.50	0.03	0.50	23	16.0	0.23	16.0
4	0.75	0.04	0.75	24	18.0	0.24	18.0
5	1.00	0.05	1.00	25	20.0	0.25	20.0
6	1.25	0.06	1.25	26	22.0	0.26	22.0
7	1.50	0.07	1.50	27	24.0	0.27	24.0
8	1.75	0.08	1.75	28	26.0	0.28	26.0
9	2.00	0.09	2.0	29	28.0	0.29	28.0
10	2.5	0.10	2.5	30	30.0	0.30	30.0
11	3.0	0.11	3.0	31	32.0	0.32	32.0
12	3.5	0.12	3.5	32	34.0	0.34	34.0
13	4.0	0.13	4.0	33	36.0	0.36	36.0
14	4.5	0.14	4.5	34	38.0	0.38	38.0
15	5.0	0.15	5.0	35	40.0	0.40	40.0
16	6.0	0.16	6.0	36	42.0	0.42	42.0
17	7.0	0.17	7.0	37	44.0	0.44	44.0
18	8.0	0.18	8.0	38	46.0	0.46	46.0
19	9.0	0.19	9.0	39	48.0	0.48	48.0
20	10.0	0.20	10.0	40	50.0	0.50	50.0

Explanation: See item 23 and Table 3.2.

Item 25 'Cumulative mass fraction of char particles'

ypt(3,1) ypt(3,2) ypt(3,3)... ypt(3,40)

Explanation: See item 23 and Table 3.2.

Item 26 'Material densities of ash, soot and char, kg/m^3'

rhopt(1) rhopt(2) rhopt(3)

Explanation: Material densities contained in rhopt array are used in number density calculations.

Item 27 'Files for ash, soot and char efficiency factors'

qash qsoot qchar

Explanation: Files may be assigned any alphanumeric names up to fifteen characters long. The files must contain efficiency factors if the option incl(i) equal to 1 is used. The file contents are updated for incl(i) equal to 2 option.

Item 28 'Furnace pressure (atm) and reference temperatures (K)'

pgas trad(1) trad(2)..... trad(nvol)

Explanation: Control volume temperatures specified in trad constitute the reference temperatures for calculating radiation properties. These are also used as starting values in the temperature iteration loop. Section 5.2 may be consulted for recommended method of obtaining the reference temperatures.

4. SAMPLE PROBLEM

Consider a medium-size utility furnace 12.7 m x 12.7 m in cross-section and 47.6 m in height. The furnace is fired with high-volatile bituminous coal of 28.6 MJ/kg high heating value and carries a thermal rating of 915.1 MWt. Field tests indictate combustion losses amounting to 0.25% unburnt carbon, 0.19% radiation loss and 1.5% unaccounted losses. According to ultimate analysis, coal has 71.08% carbon content, 4.86% hydrogen, 2.91% sulfur, 1.41% nitrogen, and 8.04% oxygen by difference. Proximate analysis of coal indicates 38.7% fixed carbon, 43.8% volatile matter, 11.7% ash, and 5.8% moisture. Following is the composition of ash: 47.52% silica, 17.87% alumina, 5.75% calcium oxide, 20.13% iron oxide, and 1.02% magnesium oxide. The furnace uses 20% excess air for complete combustion. Air has 1.3% moisture content and is preheated to 573 K. Coal is dried by preheating to 373 K. The furnace system does not use flue gas recirculation. Flow tests point to the existence of an internal recirculation pattern by which up to 30% of combustion air is directed to the hopper region. The apparent temperature and emissively of furnace surfaces exposed to the combustion gas are estimated from radiometric measurements as 1080 K and 0.70 respectively. Height of the burner belt zone atop the 7.5 m hopper zone is 9.3 m. It is desired to calculate the furnace exit temperature and the heat absorption pattern.

Figure 4.1 shows the size distributions of char and flyash measured using Malvern sizer and optical probes. It is estimated that 10% of the volatile matter completes combustion via soot formation and oxidation. The best guess of soot size distribution is also shown in Fig. 4.1.

4.1 INPUT DATA

Table 4.1 lists the input data for the sample problem. Item 1 identifies the problem with a title. Item 2 selects the data to be printed. All indices except iout(1), iout(9) and iout(14) have been set to zero. Thus, only information pertaining to combustion gas composition and flow rates, convergence of S_4 solution, and progress of non-linear solver will be printed out.

Item 3 dictates that the radiation calculations are to be conducted on a

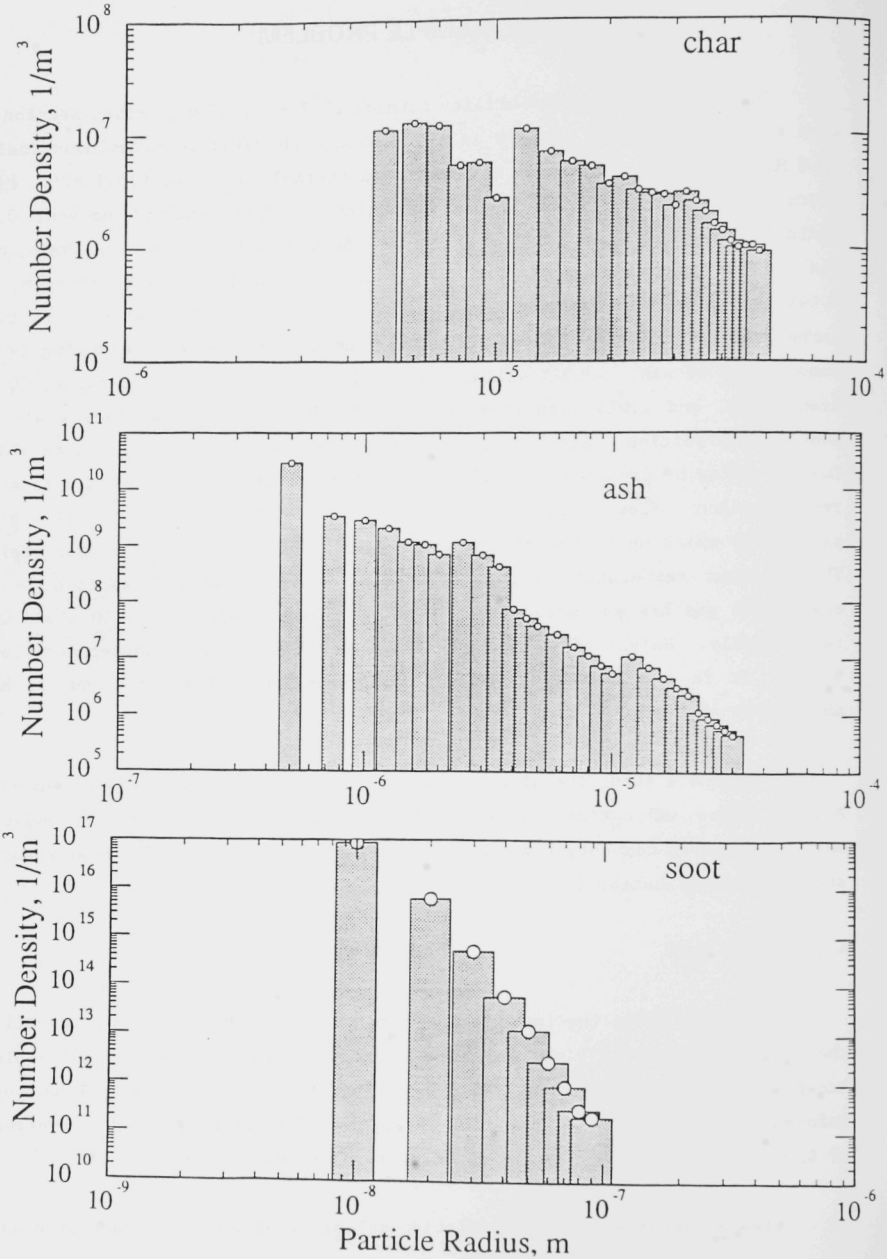

Fig. 4.1. Size Distributions of Char, Ash and Soot Particles.

Table 4.1 Sample Input Data

```
' Sample Problem '

' Yg J(i) qs Gs  Gm  qv  div.q  Tg  covergency <not active> conv <not active>'
  1   0  0  0   0   0     0     0    0   0     0   0   0    0     0    0

' input: 1 for gray medium or 37 for spectral medium'
   37

' betamx(P1 for beta>beatmx),betamn(S4 for beta<betamn) and alpha'
   1.5    0.05    0.8

'  nitergm  nitgmmn  niterj  maxcal / max iterations(do not change)'
   30        2       20       25

'   acc    deltg  / nonlinear solver parameters(do not change)'
  1.e2    0.1

'  imax jmax kmax  nvol    (kvol(n), n = 1 , nvol) / node structure'
   15   15   51    7      8 18 24 30 36 42 51

' convective heat transfer coefficients in W/m**2.K (h(n),n=1,nvol)'
   15.  15.  15.  15.  15.  15.  15.

' wall emissivity: fused surface at 1080K '
  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7
  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7
  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7  0.7
  0.7

' non-isotropicity factors '
  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
  1.0

' relaxation parameter(do not change)'
  1.2

'  xmax   ymax   zmax  /furnace size'
  12.7   12.7   47.6

'   txm   txp    tym     typ   tzm     tzp / wall temperature:'
  1080.  1080.  1080.  1080.  1080.   1080.

'   C        H2        S        N2        O2     /ultimate analysis '
 0.66413  0.04537  0.02722  0.01320   0.07507


'  H2O    ASH    VM      FC    (soot(%VM))/ proximate analysis '
 0.058  0.117  0.438  0.387    0.10

' oxygen  nitrogen  moisture  excess air /air data '
 0.2315   0.7685    0.013    0.20

' flue gas   combus gas  / gas recirculation '
  0.0        0.30

'unburnt carb  unacc loss    rad loss / combustion losses'
  0.0025       0.0150        0.0019

'  fuel    air     recirc  /gas temperatures'
 373.0   573.0    750.0
```

Table 5.1 Sample Input Data cont'd

```
'fuel HV(J/kg)   heat input (Watts)'
   27.86d+06          915.1e+06

' SiO2    Al2O3    CaO     Fe2O3    MgO   /ash composition'
 0.4752  0.1787   0.0575  0.2013   0.0102


'cumulative mass of ash particles'
 0.000  0.000  0.013  0.018  0.028  0.042  0.056  0.076  0.096
 0.160  0.226  0.291  0.308  0.325  0.342  0.363  0.383  0.404
 0.424  0.444  0.513  0.582  0.649  0.714  0.780  0.824  0.868
 0.912  0.956  1.000  1.000  1.000  1.000  1.000  1.000  1.000
 1.000  1.000  1.000  1.000


'cumulative mass of soot particles'
 0.555  0.868  0.957  0.982  0.992  0.996  0.998  0.999  1.000
 1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000
 1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000
 1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000
 1.000  1.000  1.000  1.000

'cumulative mass of char particles'
 0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
 0.000  0.000  0.000  0.000  0.000  0.001  0.003  0.006  0.008
 0.011  0.013  0.027  0.041  0.058  0.080  0.101  0.133  0.165
 0.203  0.249  0.294  0.366  0.438  0.507  0.571  0.636  0.697
 0.759  0.832  0.916  1.000


'  ash       soot       char  / material density'
  1500.0    1000.0    1000.0

'     qash          qsoot     qchar   / file names'
  'qash.samp'     'qsoot'   'qchar'

' ash  soot  char / include indices'
  1    1     1

' Pg(atm) (Tref(i),i=1,nvol)'
  1.000
  1.588E+03 1.832E+03 1.754E+03 1.681E+03  1.618E+03 1.563E+03 1.489E+03
```

spectral basis.

Item 4 stipulates that P_1 approximation be used to solve RTE for all frequencies with $\beta > 1.5\ m^{-1}$, S_4 for all frequencies with $\beta < 0.05\ m^{-1}$ and MDA for $0.05 < \beta < 1.5\ m^{-1}$. An interpolation factor of 0.8 is to be used in determining radiation intensity by S_4.

Item 5 specifies the maximum number of iterations (25) in solving for G_m/G by MDA/P_1, minimum iterations (2) for G_m/G by MDA/P_1, maximum iteration (20) for radiation intensity/G_s by MDA/S_4, and maximum iteration (25) for heat balance equations.

Item 6 directs the accuracy (100 W) to which the heat balance equations are to be solved and increment in temperature (0.1 K) for numerical evaluation of the derivative of the objective function.

Item 7 sets up a 15x15x51 grid for numerical solution of RTE. It also selects 7 control volumes for solving the heat balance equations. The control volumes extend from axial grid points 1-8, 9-18, 19-24, 25-30, 31-36, 37-42 and 43-51. The first control volumes refers to the hopper zone and the second to the burner belt zone.

Item 8 provides estimates of convective heat transfer coefficients (15 W/m^2 K) for each of the seven control volumes.

Item 9 specifies spectral wall emissivity (0.7) for each of the thirty-seven wavebands.

Item 10 initializes anisotropic scattering factor (1.0) for nfrq wavebands. A value of 0 implies isotropic scattering and 1 forward scattering.

Item 11 initializes the relaxation parameter as 1.2 for SOR solution of G_m/G by MDA/P_1.

Item 12 sizes the furnace as 12.7 m x 12.7 m x 47.6 m.

Item 13 inputs the temperatures of the x-minus, x-plus, y-minus, y-plus, bottom and top walls of the furnace as 1080 K.

Item 14 supplies the results from ultimate analysis of coal on a fractional basis as 0.7108 carbon, 0.0486 hydrogen, 0.0291 sulfur, 0.0141 fuel-bound nitrogen and 0.0804 oxygen.

Item 15 states the results from proximate analysis of coal on a fractional basis as 0.058 moisture, 0.117 ash, 0.438 volatile matter and 0.387 fixed carbon. It also specifies the fraction (0.1) of volatile matter that transforms into soot.

Item 16 provides the composition of dry air on a mass fraction basis as 0.2315 oxygen and 0.7685 nitrogen. It also specifies that on a fractional basis air contains 0.013 moisture and that 0.20 excess air is used for coal combustion.

Item 17 specifies that the furnace does not employ flue gas recirculation and a fraction 0.30 of combustion gas is directed from the burner belt zone to the hopper zone.

Item 18 specifies combustion losses as a fraction of coal high heating value: 0.0025 due to unburnt carbon, 0.015 unaccounted and 0.0019 due to radiation.

Item 19 prescribes fuel, air and recirculating flue gas temperatures as 373 K, 573 K and 750 K respectively.

Item 20 specifies coal high heating value as 28.6 MJ/kg and the furnace rating as 915.1 MWt.

Item 21 provides input data pertaining to elemental composition of ash on a fractional basis as 0.475 silica, 0.1787 alumina, 0.0575 calcia, 0.2013 magnetite and 0.0102 magnesia.

Items 22, 23 and 24 prescribe cumulative size distributions of ash, soot and char particles derived from data presented in Figs. 4.1.

Item 25 specifies material densities of ash (1500 kg/m^3), soot (1000 kg/m^3) and char (1000 kg/m^3).

Item 26 names files for storing efficiency data of ash (qash.Ill No6), soot (qsoot) and char (qchar.BYU).

Item 27 specifies that contributions of ash, soot and char to radiation cross-sections are to be included and that existing efficiency data in files named in item 26 are to be used for this purpose.

Item 28 inputs furnace pressure as 1 atm and supplies reference temperatures for each of the seven control volumes.

4.2 SAMPLE OUTPUT

Depending upon the specified values of indices array iout, an extensive amount of output may be generated. This type of output is primarily for debugging purposes and is not discussed here.

Subroutine OUTPF prints a five-part summary of results. Table 4.2 presents size distribution of ash, soot and char particles in the flame zone (control volume 2) of furnace. Similar output is also produced for bottom zone (control volume 1) and for a representative heat absorption zone (control volume 3). To help interpret the output, column headings are identified below.

inum	size bin
rash	radius of ash particles, m
rash	number density of ash particles, #/m^3
rsot	radius of soot particles, m
nsot	number density of soot particles, #/m^3
rchr	radius of char particles, m
nchr	number density of char particles, #/m^3

Printed at the bottom of table are average ash, soot and char loadings, and the partial pressures of CO_2, H_2O and CO.

Table 4.2 Particle Size Spectra and Gas Composition

ash/soot/char size spectrum in flame zone

inum	rash m	nash #/m3	rsot m	nsot #/m3	rchr m	nchr #/m3
1	1.000E-07	0.000E+00	1.000E-08	9.640E+16	1.000E-07	0.000E+00
2	2.500E-07	0.000E+00	2.000E-08	6.796E+15	2.500E-07	0.000E+00
3	5.000E-07	3.217E+10	3.000E-08	5.726E+14	5.000E-07	0.000E+00
4	7.500E-07	3.666E+09	4.000E-08	6.785E+13	7.500E-07	0.000E+00
5	1.000E-06	3.093E+09	5.000E-08	1.390E+13	1.000E-06	0.000E+00
6	1.250E-06	2.217E+09	6.000E-08	3.217E+12	1.250E-06	0.000E+00
7	1.500E-06	1.283E+09	7.000E-08	1.013E+12	1.500E-06	0.000E+00
8	1.750E-06	1.154E+09	8.000E-08	3.393E+11	1.750E-06	0.000E+00
9	2.000E-06	7.733E+08	9.000E-08	2.383E+11	2.000E-06	0.000E+00
10	2.500E-06	1.267E+09	1.000E-07	0.000E+00	2.500E-06	0.000E+00
11	3.000E-06	7.561E+08	1.100E-07	0.000E+00	3.000E-06	0.000E+00
12	3.500E-06	4.690E+08	1.200E-07	0.000E+00	3.500E-06	0.000E+00
13	4.000E-06	8.217E+07	1.300E-07	0.000E+00	4.000E-06	0.000E+00
14	4.500E-06	5.771E+07	1.400E-07	0.000E+00	4.500E-06	0.000E+00
15	5.000E-06	4.207E+07	1.500E-07	0.000E+00	5.000E-06	6.139E+06
16	6.000E-06	3.007E+07	1.600E-07	0.000E+00	6.000E-06	7.105E+06
17	7.000E-06	1.804E+07	1.700E-07	0.000E+00	7.000E-06	6.712E+06
18	8.000E-06	1.269E+07	1.800E-07	0.000E+00	8.000E-06	2.998E+06
19	9.000E-06	8.486E+06	1.900E-07	0.000E+00	9.000E-06	3.158E+06
20	1.000E-05	6.187E+06	2.000E-07	0.000E+00	1.000E-05	1.535E+06
21	1.200E-05	1.235E+07	2.100E-07	0.000E+00	1.200E-05	6.217E+06
22	1.400E-05	7.778E+06	2.200E-07	0.000E+00	1.400E-05	3.915E+06
23	1.600E-05	5.060E+06	2.300E-07	0.000E+00	1.600E-05	3.185E+06
24	1.800E-05	3.448E+06	2.400E-07	0.000E+00	1.800E-05	2.895E+06
25	2.000E-05	2.552E+06	2.500E-07	0.000E+00	2.000E-05	2.014E+06
26	2.200E-05	1.278E+06	2.600E-07	0.000E+00	2.200E-05	2.306E+06
27	2.400E-05	9.846E+05	2.700E-07	0.000E+00	2.400E-05	1.776E+06
28	2.600E-05	7.744E+05	2.800E-07	0.000E+00	2.600E-05	1.659E+06
29	2.800E-05	6.200E+05	2.900E-07	0.000E+00	2.800E-05	1.608E+06
30	3.000E-05	5.041E+05	3.000E-07	0.000E+00	3.000E-05	1.279E+06
31	3.200E-05	0.000E+00	3.200E-07	0.000E+00	3.200E-05	1.686E+06
32	3.400E-05	0.000E+00	3.400E-07	0.000E+00	3.400E-05	1.406E+06
33	3.600E-05	0.000E+00	3.600E-07	0.000E+00	3.600E-05	1.135E+06
34	3.800E-05	0.000E+00	3.800E-07	0.000E+00	3.800E-05	8.950E+05
35	4.000E-05	0.000E+00	4.000E-07	0.000E+00	4.000E-05	7.794E+05
36	4.200E-05	0.000E+00	4.200E-07	0.000E+00	4.200E-05	6.318E+05
37	4.400E-05	0.000E+00	4.400E-07	0.000E+00	4.400E-05	5.585E+05
38	4.600E-05	0.000E+00	4.600E-07	0.000E+00	4.600E-05	5.755E+05
39	4.800E-05	0.000E+00	4.800E-07	0.000E+00	4.800E-05	5.829E+05
40	5.000E-05	0.000E+00	5.000E-07	0.000E+00	5.000E-05	5.210E+05

average ash loading = 1.944E-03kg/m**3
average soot loading = 7.276E-04kg/m**3
average char loading = 3.217E-03kg/m**3

partial pressure of CO2 = 1.379E-01atm
partial pressure of H2O = 8.448E-02atm
partial pressure of CO = 0.000E+00atm

Table 4.3 presents the spectral optical properties of combustion gas corresponding to gas compositions and reference temperatures in control volumes, 1, 2 and 3. For each waveband identified by ifrq, the table lists extinction coefficients (bet1, bet2, bet3), scattering albedos (omg1, omg2, omg3), and RTE solution indices ipl and is4. As explained earlier, P_1 approximation is employed for waveband ifrq if ipl(ifrq) equals one, S_4 if is4(ifrq) is assigned a value of one, and MDA if both ipl(ifrq) and is4(ifrq) equal zero.

Table 4.4 presents the spectral heat transfer for each of the seven control volumes. Heat transfer surfaces for control volumes 2 through nvol-1 consist of four side walls, control volume 1 also contains the bottom wall, and control volume nvol also contains the top wall. Tabulated spectral heat transfer is in units of W rather than W/cm so that a linear addition over wavebands yields the total heat transfer.

Table 4.5 presents further information on heat transfer (Qrate, W), heat flux (Qflux, W/m^2) and rate of heat release from coal combustion (Qrel, W). The information is presented for each of the seven control volumes after excluding the bottom wall from control volume 1 and the top wall from control volume nvol. Total heat transfer is also listed in this table.

Table 4.6 provides a summary of calculations. Various columns in the table correspond to temperature (temp, K), flow rate (flow, kg/s), specific enthalpy (enth, J/kg), total enthalpy at entrance (hin, W), total enthalpy at exit (hout, W), and divergence of heat flux (divq, W). Various rows in the table designate fuel (fuel), combustion air (air), recirculating flue gas (recg), control volumes (vol1-vol7), and overall furnace (furn). The entry for row designated fuel and column hin corresponds to total heating value of coal, and that under column hout to total heat release after accounting for combustion and moisture losses. In the rows designated as vol1-vol7, the difference (hin - hout) represents heat exchange with other control volumes and furnace walls, whereas (hin - hout - divq) represents convective heat transfer to the adjacent walls of the furnace. The entry under column divq in row furn contains the total convective and radiative heat transfer to the furnace walls. Numerically, it equals the difference between the entries under the columns hin and hout along the row furn. Finally, a breakdown is given of CPU time expenditure in optical property

Table 4.3 Radiation Properties of Combustion Gas and Solution Indices

Optical Properties of Combustion Gas

ifrq	bet1 m-1	omg1	bet2 m-1	omg2	bet3 m-1	omg3	ip1	is4
1	1.308E+00	2.767E-02	1.546E+00	1.453E-01	1.299E+00	2.971E-02	0	0
2	4.269E+00	1.020E-01	4.353E+00	1.366E-01	4.372E+00	1.062E-01	1	0
3	1.976E+00	1.982E-01	2.308E+00	1.974E-01	1.970E+00	2.120E-01	1	0
4	6.014E-01	2.838E-01	9.663E-01	2.554E-01	6.175E-01	2.948E-01	0	0
5	2.868E-01	3.741E-01	7.385E-01	2.673E-01	2.979E-01	3.840E-01	0	0
6	5.055E-01	6.614E-01	1.055E+00	3.798E-01	5.279E-01	6.754E-01	0	0
7	5.621E-01	8.776E-01	1.262E+00	4.366E-01	5.932E-01	8.868E-01	0	0
8	2.498E+00	2.185E-01	3.603E+00	1.706E-01	2.432E+00	2.395E-01	1	0
9	5.720E-01	9.653E-01	1.637E+00	3.864E-01	6.092E-01	9.666E-01	0	0
10	5.650E-01	9.568E-01	1.773E+00	3.527E-01	6.017E-01	9.583E-01	0	0
11	6.052E-01	8.794E-01	1.954E+00	3.166E-01	6.392E-01	8.880E-01	0	0
12	1.141E+00	4.604E-01	2.715E+00	2.255E-01	1.155E+00	4.851E-01	0	0
13	6.736E-01	7.765E-01	2.353E+00	2.593E-01	7.059E-01	7.902E-01	0	0
14	5.831E-01	9.039E-01	2.374E+00	2.585E-01	6.187E-01	9.085E-01	0	0
15	5.707E-01	9.430E-01	2.499E+00	2.494E-01	6.080E-01	9.440E-01	0	0
16	5.803E-01	9.123E-01	2.652E+00	2.322E-01	6.170E-01	9.151E-01	0	0
17	6.219E-01	8.677E-01	2.821E+00	2.216E-01	6.588E-01	8.736E-01	0	0
18	5.751E-01	9.318E-01	2.887E+00	2.155E-01	6.129E-01	9.324E-01	0	0
19	5.706E-01	9.344E-01	2.961E+00	2.095E-01	6.085E-01	9.344E-01	0	0
20	5.712E-01	9.301E-01	3.025E+00	2.046E-01	6.090E-01	9.303E-01	0	0
21	5.812E-01	9.016E-01	3.092E+00	1.983E-01	6.177E-01	9.048E-01	0	0
22	6.763E-01	7.737E-01	3.246E+00	1.888E-01	7.100E-01	7.859E-01	0	0
23	5.803E-01	8.962E-01	3.194E+00	1.912E-01	6.171E-01	8.987E-01	0	0
24	5.702E-01	9.103E-01	3.220E+00	1.895E-01	6.080E-01	9.104E-01	0	0
25	5.758E-01	9.066E-01	3.263E+00	1.879E-01	6.141E-01	9.066E-01	0	0
26	5.831E-01	9.024E-01	3.315E+00	1.863E-01	6.219E-01	9.024E-01	0	0
27	5.819E-01	9.027E-01	3.394E+00	1.822E-01	6.206E-01	9.027E-01	0	0
28	5.838E-01	9.034E-01	3.509E+00	1.776E-01	6.226E-01	9.034E-01	0	0
29	5.789E-01	9.008E-01	3.636E+00	1.710E-01	6.174E-01	9.008E-01	0	0
30	5.726E-01	8.953E-01	3.785E+00	1.635E-01	6.107E-01	8.953E-01	0	0
31	5.793E-01	8.896E-01	3.973E+00	1.579E-01	6.178E-01	8.896E-01	0	0
32	5.602E-01	8.758E-01	4.171E+00	1.472E-01	5.975E-01	8.758E-01	0	0
33	5.450E-01	8.583E-01	4.407E+00	1.371E-01	5.813E-01	8.583E-01	0	0
34	5.368E-01	8.407E-01	4.688E+00	1.284E-01	5.725E-01	8.407E-01	0	0
35	5.324E-01	8.197E-01	5.015E+00	1.205E-01	5.678E-01	8.197E-01	0	0
36	5.115E-01	7.900E-01	5.374E+00	1.107E-01	5.455E-01	7.900E-01	0	0
37	5.019E-01	7.628E-01	5.794E+00	1.033E-01	5.353E-01	7.628E-01	0	0

Table 4.4 Spectral Heat Transfer to Sidewall in Control Volumes

Spectral Heat Transfer

ifrq	1	2	3	4	5	6	7
1	2.46E+02	3.74E+02	3.61E+02	3.12E+02	2.71E+02	2.36E+02	1.90E+02
2	7.64E+02	1.17E+03	1.06E+03	9.25E+02	8.14E+02	7.22E+02	5.97E+02
3	1.88E+03	2.79E+03	2.59E+03	2.29E+03	2.02E+03	1.79E+03	1.49E+03
4	6.12E+03	9.38E+03	8.89E+03	7.73E+03	6.82E+03	6.01E+03	4.88E+03
5	3.13E+03	5.20E+03	4.76E+03	4.00E+03	3.52E+03	3.10E+03	2.45E+03
6	1.42E+04	2.55E+04	2.20E+04	1.82E+04	1.59E+04	1.38E+04	1.08E+04
7	7.99E+03	1.89E+04	1.35E+04	9.99E+03	8.43E+03	7.20E+03	5.28E+03
8	1.93E+04	2.73E+04	2.71E+04	2.36E+04	2.06E+04	1.81E+04	1.47E+04
9	1.15E+04	3.59E+04	1.91E+04	1.02E+04	7.70E+03	6.35E+03	4.42E+03
10	5.91E+03	1.72E+04	9.55E+03	5.44E+03	4.19E+03	3.47E+03	2.43E+03
11	1.69E+04	3.79E+04	2.74E+04	2.00E+04	1.65E+04	1.38E+04	9.94E+03
12	2.51E+04	3.76E+04	3.92E+04	3.26E+04	2.73E+04	2.30E+04	1.77E+04
13	1.35E+04	2.55E+04	2.18E+04	1.70E+04	1.41E+04	1.17E+04	8.56E+03
14	1.34E+04	3.16E+04	2.16E+04	1.48E+04	1.19E+04	9.78E+03	6.86E+03
15	1.53E+04	4.05E+04	2.40E+04	1.45E+04	1.12E+04	9.07E+03	6.26E+03
16	1.56E+04	3.77E+04	2.51E+04	1.66E+04	1.31E+04	1.06E+04	7.29E+03
17	1.65E+04	3.69E+04	2.76E+04	1.96E+04	1.56E+04	1.24E+04	8.56E+03
18	1.45E+04	3.73E+04	2.30E+04	1.42E+04	1.08E+04	8.58E+03	5.78E+03
19	6.56E+03	1.73E+04	1.04E+04	6.28E+03	4.71E+03	3.68E+03	2.45E+03
20	1.01E+04	2.67E+04	1.63E+04	9.87E+03	7.35E+03	5.69E+03	3.75E+03
21	4.83E+03	1.22E+04	8.22E+03	5.30E+03	3.96E+03	3.03E+03	1.97E+03
22	1.08E+04	2.40E+04	2.03E+04	1.45E+04	1.09E+04	8.29E+03	5.46E+03
23	4.82E+03	1.25E+04	8.41E+03	5.34E+03	3.91E+03	2.93E+03	1.86E+03
24	4.78E+03	1.28E+04	8.16E+03	4.97E+03	3.59E+03	2.67E+03	1.69E+03
25	4.07E+03	1.11E+04	7.08E+03	4.30E+03	3.08E+03	2.27E+03	1.42E+03
26	4.76E+03	1.32E+04	8.44E+03	5.11E+03	3.62E+03	2.63E+03	1.62E+03
27	6.56E+03	1.87E+04	1.19E+04	7.00E+03	4.83E+03	3.43E+03	2.06E+03
28	3.83E+03	1.15E+04	7.13E+03	4.07E+03	2.71E+03	1.86E+03	1.07E+03
29	2.19E+03	6.81E+03	4.19E+03	2.32E+03	1.49E+03	9.89E+02	5.49E+02
30	1.22E+03	3.94E+03	2.42E+03	1.31E+03	8.13E+02	5.20E+02	2.78E+02
31	6.61E+02	2.23E+03	1.37E+03	7.26E+02	4.36E+02	2.70E+02	1.39E+02
32	3.55E+02	1.23E+03	7.70E+02	4.02E+02	2.34E+02	1.40E+02	6.91E+01
33	1.86E+02	6.71E+02	4.27E+02	2.21E+02	1.24E+02	7.18E+01	3.41E+01
34	9.56E+01	3.59E+02	2.33E+02	1.19E+02	6.48E+01	3.61E+01	1.65E+01
35	4.82E+01	1.89E+02	1.26E+02	6.33E+01	3.34E+01	1.80E+01	7.89E+00
36	2.40E+01	9.81E+01	6.74E+01	3.35E+01	1.71E+01	8.91E+00	3.75E+00
37	2.39E+01	1.07E+02	7.31E+01	3.46E+01	1.65E+01	8.06E+00	3.13E+00

Table 4.5 Furnace Heat Transfer

Wall Heat Flux and Heat Transfer Rate Distribution

	Qrate	Qflux	Qrel
vol1	5.364E+07	2.752E+05	0.000E+00
vol2	1.487E+08	6.159E+05	9.146E+08
vol3	6.472E+07	4.448E+05	0.000E+00
vol4	4.580E+07	3.130E+05	0.000E+00
vol5	3.681E+07	2.508E+05	0.000E+00
vol6	3.023E+07	2.054E+05	0.000E+00
vol7	3.296E+07	1.485E+05	0.000E+00
bott	2.463E+07	1.527E+05	
top	1.065E+07	6.601E+04	
totl	4.482E+08		

Table 4.6 Summary of Results and CPU breakdown

summary output

	temp K	flow kg/s	enth J/kg	hin W	hout W	divq W
fuel	3.730E+02	3.285E+01	0.000E+00	9.151E+08	8.927E+08	
air	5.730E+02	3.599E+02	2.858E+05	1.029E+08		
recg	7.500E+02	0.000E+00	4.914E+05	0.000E+00		
vol1	1.584E+03	1.178E+02	1.535E+06	2.219E+08	1.809E+08	3.815E+07
vol2	1.845E+03	3.927E+02	1.883E+06	1.176E+09	9.615E+08	2.090E+08
vol3	1.759E+03	3.927E+02	1.768E+06	7.396E+08	6.942E+08	4.251E+07
vol4	1.679E+03	3.927E+02	1.661E+06	6.942E+08	6.524E+08	3.928E+07
vol5	1.611E+03	3.927E+02	1.571E+06	6.524E+08	6.170E+08	3.314E+07
vol6	1.553E+03	3.927E+02	1.494E+06	6.170E+08	5.865E+08	2.842E+07
vol7	1.476E+03	3.927E+02	1.393E+06	5.865E+08	5.469E+08	3.711E+07
furn	1.476E+03	3.927E+02	1.393E+06	9.956E+08	5.469E+08	4.482E+08

1

time spent in optical props 6.396E+01 secs
time spent in Gs computation 1.145E+03 secs
time spent in Gm computation 4.426E+03 secs
time spent in Planck Function 9.228E+02 secs

calculations, determination of G_s field by MDA, determination of G_m/G field by MDA/P_1/S_4, evaluation of Planck function at gas temperatures, and non-linear equation solver.

5. RECOMMENDATIONS

FURN3D is a modular code written in Fortran 77. The code and input data are structured to permit a user to conduct many different types of calculations: spectral vs gray body, isotropic vs anisotropic scattering, with or without ash particles, with or without char particles, with or without soot particles, P_1 approximation vs MDA vs S_4 method, fine vs course grid, limited vs extensive printout, etc. Different choices of input data affect results in magnitude, accuracy, speed or printout. This flexibility in input is useful for conducting sensitivity analysis or gaining understanding of the results of calculations. Discussed below are our recommendations of input data choices which are not specific to a particular problem.

5.1 OUTPUT CONTROL

Optional printout is controlled by item 2 input data. Generally, output pertaining to wall heat flux due to G_s (Q_s), G_s field, G_m field, total heat flux (Q) and divergence of heat flux should be suppressed by assigning a value of zero to indices iout(3) - iout(7). Each of these quantities is four dimensional (three field variables and one spectral) and generates a lengthy output. Arrays G_s and Q_s are non-zero only for frequencies corresponding to which MDA is used to solve RTE. The boundary conditions used on constructing G_s solution are hot walls and cold gas. Thus, Q_s is always negative signifying that heat transfer is from the walls to the gas. On the other hand, total heat transfer Q in practical furnaces should be positive. A negative value for Q represents non-convergent solution by MDA.

Index iout(8) controls printout of the three-dimensional temperature field. We recommend setting iout(8) equal to zero since a more concise output of temperatures is available elsewhere.

5.2 SPECTRAL VS. GRAY CALCULATIONS

Meaningful and consistent results are obtained only if full spectral calculations are performed by setting nfrq equal to 37 in data item 3. The code does require estimates of reference temperatures as data in item 28. These

estimates are used in determining radiation properties of the products of combustion. The estimates can be obtained by making a quick run with nfrq set equal to one (gray body calculation). The code will print an error message and terminate if nfrq is assigned a value different than 1 or 37.

5.3 RTE SOLUTION

As explained earlier, FURN3D employs a hybrid technique in which S_4 is used to solve RTE for $\beta < \beta_{min}$, MDA for $\beta_{min} < \beta < \beta_{max}$ and P_1 for $\beta > \beta_{max}$. The recommended initial values of β_{max} and β_{min} to be specified in data item 3 are 1.5 and 0.05, respectively. Both computational speed and accuracy are affected by choice of β_{max} and β_{min}. Computational speed can be enhanced by choosing smaller β_{max} but at the expense of invoking P_1 approximation in the range where it is less accurate. Too high a value of β_{max} lends to use of MDA in the range where small inaccuracy in G_s solution is known to lead to non-physical results. Similarly, faster solutions can be obtained by increasing β_{min} and using MDA for frequencies for which S_4 would be used otherwise. However, the line-by-line method of inverting algebraic equations for G_m has shown slow convergence in the limit of small β.

Recommended value for the interpolation parameter α is 0.8. This is a reasonable compromise between 0.5, where S_4 solution has second-order accuracy, and 1, where upwind differening is used and negative intensities are not produced in intermediate steps.

5.4 ITERATIVE SOLUTION

Number of iterations required to solve the finite-difference equations for G_m/G by MDA/P_1 may depend upon the choice of β_{min} and β_{max}. In our experience, a choice of 30 as maximum number of iterations and 2 as minimum has generally proved adequate. A message is automatically printed if convergence is not achieved within the specified number of iterations. Subroutines related to solution of G_m/G by MDA/P_1 are called from inside a temperature iteration loop. In a well-behaved problem, fewer iterations are needed to solve for G_m/G as the temperature field approaches the converged value and increments in temperatures from one iteration to the next decrease in magnitude. Thus, it is possible to

have a situation in which convergence in G_m/G is not obtained initially but is attained subsequently as the temperature field is iterated upon.

Number of iterations needed for solving G_s/G by S_4 depends upon the magnitude of β_{min}. For $\beta_{min} < 0.05$, 20 iterations are generally sufficient. Convergence behavior of S_4 can be monitored by specifying iout(9) equal to one.

Number of iterations needed by the non-linear solver is proportional to the specified number of control volumes over which heat balance is conducted. Twenty-five iterations are generally sufficient for up to seven control volumes and prescribed accuracy of 100 W in heat rate. We recommend that a temperature increment of 0.1 K (deltg) be prescribed for numerically calculating the gradient of the objective function. Numerical differentiation becomes inaccurate if too large a value of deltg is used and convergence shows down. Round off errors degrade convergence if deltg is made too small.

The non-linear equations solver based on steepest descent and Newton update has proved robust in our experience. Past failures to solve heat balance equations have been associated with non-convergent or inconsistent solutions of RTE. These could always be resolved by proper selections of β_{min}, β_{max} and α. Progress of the non-linear solver can be followed by assigning a value of unity to iout(14).

The algebraic equations for G_m/G obtained from applying MDA/P_1 to RTE and finite differencing are solved by a line-by-line inversion technique in conjunction with successive overrelaxation (SOR). It has been found that convergence can be speeded by gradually decreasing the SOR parameter from one iteration to the next. Numerical experimentation has shown that a starting value of 1.2 for the relaxation parameter is near optimum under many conditions and is recommended.

5.5 NUMERICAL GRID

FURN3D has been extensively executed on SUN SPARC workstations. In simulations for typical industrial furnaces, grid fineness has been limited by availability of computer memory rather than being determined from numerical

accuracy. For a 15 x 15 x 51 grid as used in Table 3.1, FURN3D requires more than 16 Mb of storage if calculations are performed in double precision. Much of the storage requirement (11 Mb) is imposed by arrays for spectral quantities G_m and G_s and angular intensity I. Thus, for all practical purposes the largest grid than can be accommodated on a computer should be used. In certain cases, run cost may also be a determining factor.

In any run the number of grid points (imax, jmax, kmax) and control volumes (nvol) should be smaller than the maximum allowable (imx, jmx, kmx, nv). The code will terminate the run with an appropriate message if this condition is violated. The user can than either decrease the number of grid points or recompile FURN3D with larger dimensions specified in the parameter statement. We also recommend that user select imax, jmax and kmax to produce a near cubicle grid.

5.6 RADIATION PROPERTIES

Determination of efficiency factors for ash, soot and char can be a computer time intensive process since for each kind of particle Mie theory must be invoked 44,400 times (number of particle size bins x number of wave bands x number of subdivisions within a wave band). Mie solution is tedious to execute as it involves complex number algebra, complex trigonometric functions and infinite series summation. A file management and a particle size grid systems have been set up in FURN3D to minimize expenditure of computer resources on Mie solution. A file index array incl(3) has been provided through which the user can specify whether the efficiency factors are to be read from existing files, or calculated and stored in new or existing files. Efficiency factors for char and soot only need to be calculated once since the optical constants for these particles are independent of composition. Efficiency factors for ash need to be updated for different ash composition.

The foregoing method of file management works because the efficiency factors in Mie theory are function of $2\pi r/\lambda$ and optical constants, and we have fixed the particle size grid and the wavebands. The absorption and scattering cross-sections do depend on particle size distributions and these are calculated in every run. However, different size distributions can be accommodated with a

single database for efficiency factors.

5.7 HARDWARE REQUIREMENT

As mentioned earlier, requirement of computer memory depends on the grid parameters imx, jmx, kmx and nv, and the number of frequencies nf. Table 5.1 summarizes the total memory occupied by the major arrays in FURN3D and also provides a breakdown in terms of variables related to the Planck function (I_b), heat flux (q), divergence of heat flux ($\nabla.q$), S_4 subroutines, and G_m/G subroutines. Memory required by $\nabla.q$ and S_4 solution arrays is independent of nf. For the coarsest 5x5x15 grid tabulated, random access memory (RAM) is determined by S_4 arrays for gray-body calculations, and by I_b, q, S_4 and G_m/G arrays for spectral calculations. For spectral calculations on the finest 18x18x60 grid listed, more than half of 22 Mb RAM needed is occupied by arrays needed in G_m/G solution. In gray-body calculations on the finest grid listed, 67% of 7.6 Mb RAM needed is taken up by variables appearing in S_4 solution. The portion of heat flux (q) arrays dependent on nf is for output purposes only and can be trimmed with slight reprogramming for machines with limited RAM. The spectral arrays involved in G_m/G subroutines greatly expedite solution convergence. On machines with limited RAM, these can be substituted by ROM (read only memory) at the expense of greatly increased I/O time.

5.8 GETTING STARTED

The complete code package consists of seven source and data files and an optional output file. The fortran source code is contained in file furn3d.f. Common blocks are stored separately in file furn3d.h. During compilation, furn3d.f extracts the common-block information from furn3d.h through include statements. Many workstations require that furn3d.f and furn3d.h be stored in the same directory.

File cp.d contains curve-fit coefficients for calculating specific heats and enthalpies of CO_2, H_2O, SO_2, N_2, O_2, carbon, ash and coal. Contents of this file, read by furn3d during execution using formatted statements, should not be altered.

Table 5.1. Computer Memory Requirement

Grid Parameters					Memory Required, Mb					
imx	jmx	kmx	nv	nf	Total	I_b	q	$\nabla.q$	S_4	G_m/G
5	5	15	5	37	0.75	0.11	0.11	<0.01	0.17	0.25
5	5	15	5	1	0.31	<0.01	<0.01	<0.01	0.17	0.04
10	10	30	5	37	4.00	0.44	0.43	0.02	0.94	2.02
10	10	30	5	1	1.41	0.04	0.02	0.02	0.94	0.29
15	15	51	10	37	13.36	1.13	1.07	0.09	3.10	7.71
15	15	51	10	1	4.65	0.12	0.06	0.09	3.10	1.10
18	18	60	15	37	21.71	1.63	1.51	0.16	5.01	13.06
18	18	60	15	1	7.56	0.20	0.08	0.16	5.01	1.87
18	18	60	8	37	21.70	1.63	1.51	0.16	5.01	13.06
18	18	60	8	1	7.55	0.20	0.08	0.16	5.01	1.87

Remaining files have variable names. An input data file, say furn3d.d, should contain problem specific data as explained in Section 3.3. Included in data are names of files to be used for reading efficiency factors for scattering and extinction by char, soot and ash. Internally, furn3d.f assigns them names qchar, qsoot, and qash. These files may be new or existing, empty or full. Generally, contents of files referenced by qchar and qsort should not be changed from data documented in Appendices G and H. Contents of file referenced by qash should be updated for ashes of different compositions using procedures outlined in Sections 3.3 and 5.6. On workstations, it may be convenient to store all files in a single directory.

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APPENDIX A. FURNACE HEAT TRANSFER SUBROUTINES

A.1 SUBROUTINE BURNOUT

PURPOSE To calculate char particle temperature, fractional carbon burnout, remaining char concentration and oxygen partial pressure.

ARGUMENTS nsize, anumc, rc, akg, diff02, tg, tp, amcf, p02, rhochar, rhoc, dtm.

MAIN EQUATIONS

1. Char Oxidation Rate

$$q = A\exp(-E/RT_P)P_{O_2,s}^n$$

2. CO/CO_2 Product Ratio

$$f = A_c\exp(-E_c/RT_P)$$

3. Burning Mode

$$P/P_0 = (m/m_0)^\alpha$$

$$d/d_0 = (m/m_0)^{(1-\alpha)/3}$$

4. Swelling Factor

$$\omega = d_o/d_c$$

5. Heat Release

$$Q_c = q(\Delta H_{CO_2} + f\Delta H_{CO})/(1 + f)$$

6. Heat Transfer

$$Q = \frac{(k_g Nu)}{d}(T_p - T_g) + \epsilon\sigma(T_p^4 - T_W^4)$$

7. Oxygen Partial Pressure

$$q\frac{(1+f/2)}{(1+f)}\frac{MW_{O_2}}{MW_c} = \left(\frac{Nu_m D_{O_2}}{d}\right)\left(\frac{P}{RuT_g}\right)(P_{O_2} - P_{O_2,s})$$

SUBROUTINES CALLED None

DATA

$\Delta H_{CO} = 9.283 \times 10^6$ J/kg

$\Delta H_{CO_2} = 3.28 \times 10^7$ J/kg

$Nu = Nu_m = 2$

DESCRIPTION Equations for char oxidation kinetics, heat release, heat transfer and oxygen mass transfer are coupled and non-linear functions of particle temperature T_p and oxygen partial pressure $P_{O_2,S}$ These are rearranged in terms of a single unknown, T_p. Starting from initial bounds of T_p, a bisection method is used to successively halve the bound interval until convergence to 10^{-4}K is achieved. The procedure is repeated for each particle size in char histogram.

The burnout results are integrated over particle size to obtain char spray density and reduction in oxygen partial pressure.

REFERENCE Hurt, R. H. and Hardesty, D. R., 'Rates and Mechanisms of Pulverized Coal Char Combustion,' Seventh Annual Coal Preparation, Utilization, and Environmental Control Contractor Conference Proceedings, Pittsburgh, PA, July 1991.

A.2 SUBROUTINE COEFF

PURPOSE To assemble coefficients of finite difference equations for G_m.

ARGUMENTS ifrq

MAIN EQUATIONS

1. $A^E = \Delta y_j \Delta z_k / (\beta_{1i+1/2jk} \Delta x_{i+1/2})$

2. $A^W = \Delta y_i \Delta z_k / (\beta_{1i-1/2jk} \Delta x_{i-1/2})$

3. $A^N = \Delta x_i \Delta z_k / (\beta_{1ij+1/2k} \Delta y_{j+1/2})$

4. $A^S = \Delta x_i \Delta z_k / (\beta_{1ij-1/2k} \Delta y_{j-1/2})$

5. $A^H = \Delta x_i \Delta y_j / (\beta_{1ijk+1/2} \Delta z_{k+1/2})$

6. $A^L = \Delta x_i \Delta y_i / (\beta_{1ijk-1/2} \Delta z_{k-1/2})$

7. $$A^P = A^E + A^W + A^N + A^S + A^H + A^L + 3(1 - \omega_{ijk})\beta_{ijk} \Delta x_i \Delta y_j \Delta z_k$$

8. $$S_{ijk} = 12\pi(1-\omega_{ijk})\beta_{ijk} I_{bijk} \Delta x_i \Delta y_j \Delta z_k + 3\omega_{ijk}[1+a_{ijk}/3(1-\omega_{1ijk})] G_{sijk} \Delta x_i \Delta y_j \Delta z_k$$

SUBROUTINES CALLED None

DATA None

DESCRIPTION Subroutine COEFF is called from MAIN for frequencies for which P_1 approximation or MDA is used. The coefficients A^E, A^W, A^N, A^S, A^L, A^H and S_{ijk} are modified for grid points adjacent to walls to account for diffusely reflecting boundary conditions.

REFERENCE Park, H. M., Ahluwalia, R. K. and Im, K. H., 'Three-Dimensional Radiation in Absorbing-Emitting-Scattering Media Using the Modified Differential Approximation,' to appear in International Journal of Heat and Mass Transfer, 1992.

A.3 SUBROUTINE COMBDRV

PURPOSE To determine heat release from char and volatile matter combustion and evolution of char size distribution in different control volumes.

ARGUMENTS None

MAIN EQUATIONS None

SUBROUTINES CALLED

1. BURNOUT (nsize, anumc, rc, akg, diff02, tgas, tp, amcf, p02, rhochar, rhopt(3), dtm)
2. CONDUCT(nspe, x, t, visc, akg)

DATA None

DESCRIPTION COMBDRV is a driver module that coordinates calls to other subroutines for estimating the heat release source term appearing in the energy equation and the char size distribution required for radiation property calculations. All calculations are based on initial gas temperature estimates supplied as input data.

REFERENCE None

A.4 SUBROUTINE COMPSN

PURPOSE

To determine fuel and oxidizer flow rates, gas throughout, flue gas recirculation rate, combustion gas recirculation rate, gas composition, partial pressures of participating gases, flyash size distribution, soot size distribution and initial char size distribution.

ARGUMENTS

None

MAIN EQUATIONS

$$hv = hhv(1- \Sigma losses)-Fuel(6)\times 2.41722\times 10^6$$

$$\dot{m}_f = Q_F/hhv$$

$$C + O_2 = CO_2$$

$$H_2 + 1/2\ O_2 = H_2O$$

$$S + O_2 = SO_2$$

$$P_{CO_2} = X_{CO_2}P$$

$$P_{H_2O} = X_{H_2O}P$$

SUBROUTINES CALLED

None

DATA

None

DESCRIPTION

COMPSN utilizes input data on furnace rating, high heating value, ultimate analysis of coal, fuel and air moisture contents, combustion losses and fractional recirculation rate to calculate gas composition and various flow rates. Input data on cumulative size distributions are used to determine ash, soot and char (initial) number density in specified size bins and furnace control volumes.

REFERENCE

None

A.5 SUBROUTINE CONDUC

PURPOSE To calculate thermal conductivity of gaseous mixture.

ARGUMENTS nspe, x, t, visc, akg

MAIN EQUATIONS

1. Specific Heat of Species i

$$c_{pi} = ac_{pi} + bc_{pi}T + cc_{pi}T^2 + dc_{pi}T^3$$

2. Thermal Conductivity of Species i

$$c_{vi} = c_{pi} - R$$

$$\alpha = c_{vi}/R - 3/2$$

$$\beta = 0.762 - 0.7109\omega_i + 1.3168\omega_i^2$$

$$Z = 2 + 10.5(T/T_{ci})^2$$

$$\psi = 1 + \alpha([0.215 + 0.28288\alpha - 1.068\beta + 0.26665Z] / [0.6366 + \beta Z + 1.061\alpha\beta])$$

$$k_i = 3750\left(\frac{R\psi}{MW_i}\right)\mu_i$$

3. Thermal Conductivity of Gaseous Mixture

$$A_{ij} = \frac{[1 + (\mu_i/\mu_j)^{1/2} (MW_j/MW_i)^{1/4}]^2}{[8(1 + MW_i/MW_j)]^{1/2}}$$

$$k_g = \sum_{i=1}^{n} \frac{X_i k_i}{\sum_{j=1}^{n} X_j A_{ij}}$$

SUBROUTINES CALLED None

DATA Arrays ac_{pi}, bc_{pi}, cc_{pi}, dc_{pi}, ω_i and T_{ci} are initialized in a BLOCK DATA statement.

DESCRIPTION Prior to calling CONDUC, subroutine VISCOS must be called for calculating viscosity μ_i. The algorithm for estimating the thermal conductivity of a pure gas is due to Chung et al.

theory of gases. The interaction parameters and the collision integral are based on Lennard Jones 12-6 potential.

REFERENCES

Reid, R. C., Prausnitz, J. M., Polling, B. E., The Properties of Gases and Liquids, Fourth Edition, Chapter 11, McGraw-Hill Book Company, 1987.

A.7 SUBROUTINE DIVERQ

PURPOSE To calculate divergence of radiation heat flux.

ARGUMENTS ifrq

MAIN EQUATIONS Divergence of Heat Flux

$$\nabla . \vec{q} = \int 4\pi(1-\omega)\beta(I_b - \frac{G_m + G_s}{4\pi})d\nu$$

SUBROUTINES CALLED None

DATA None

DESCRIPTION DIVERQ is called from MAIN for each frequency band. It calculates the spectral quantity and integrates it for total divergence of heat flux.

REFERENCE None

A.8 SUBROUTINE ENERGY

PURPOSE

To calculate the residual functions which must be reduced to zero for proper convergence of the energy equations.

ARGUMENTS

itry

MAIN EQUATIONS

1. Radiative Heat Transfer

$$Q_{ri} = \int_{Vi} \nabla . \vec{q}_r dV$$

2. Convective Heat Transfer

$$Q_{ci} = \sum_{Walls} h_i A_i (T_{gi} - T_{wi})$$

3. Residual Enthalphy Function for Control Volume 1

$$F_1 = \dot{m}_r (h_r - h_1) + \dot{m}_R (h_2 - h_1) - Q_{c1} - Q_{r1}$$

4. Residual Enthalpy Function for Control Volume 2

$$F_2 = \dot{m}_f (h_f + f_2 hv - h_2) + \dot{m}_a (h_a - h_2)$$
$$+ (\dot{m}_r + \dot{m}_R)(h_1 - h_2) - Q_{c2} - Q_{r2}$$

5. Residual Enthalpy Function for Other Control Volumes

$$F_i = \dot{m}_f f_i hv + (\dot{m}_f + \dot{m}_a + \dot{m}_r)(h_{i-1} - h_i)$$
$$- Q_{ci} - Q_{ri}$$

SUBROUTINES CALLED

1. HFUEL(temp(1), cp)
2. HAIR(temp(2), air, cp)
3. HGAS(temp(3), gas, cp)
4. HGAS(tg(ivol), gas, cp)

DATA

None

DESCRIPTION

ENERGY is called inside a temperature iteration loop in MAIN. For specified temperature fields, the radiation field is updated prior to entering this subroutine.

REFERENCE None

A.9 FUNCTION FRAC

PURPOSE To calculate fractional emission in a waveband.

ARGUMENTS v1, v2

MAIN EQUATIONS

$$v = C_2 \upsilon / T$$

$$f(v_1, v_2) = f(0 \rightarrow v_1) - f(0 \rightarrow v_2)$$

$$f(0 \rightarrow v) = \frac{15}{\pi^4} \sum_{n=1}^{\infty} \frac{e^{-nv}}{n} \left(v^3 + \frac{3v^2}{n} + \frac{6v}{n^2} + \frac{6}{n^3} \right)$$

SUBROUTINES CALLED None

DATA None

DESCRIPTION FRAC is called from PLANCKG and PLANCKW to calculate fractional blackbody emission in a wave band bounded by v_2 and v_1. The summation process indicated in F(0-v) infinite series is performed until incremental contribution decreases to 10^{-4}.

REFERENCE Chang, S. L. and Rhee, K. T., "Blackbody Radiation Functions," International Communications Heat Mass Transfer, Vol. 11, 1984, pp. 451-455.

A.10 SUBROUTINE FSOLVG

PURPOSE To solve a set of nonlinear algebraic equations.

ARGUMENTS x, f ,bl, bu, acc, del, n, i, maxi, prt, a

MAIN EQUATIONS See references cited below.

SUBROUTINES CALLED

1. jacob(x, f, bl, bu, xs, fs, xsc, fsc, b, bi, ait, del, tl, n, it, print)
2. update(x, f, dx, df, xs, fs, wl, w2, b, bi, n)
3. steps(wl, w2, fs, b, bi, tl, t2, n)
4. newx(x, bl, bu, wl, w2, xs, dx, xsc, b, amu, n, it, print)
5. invt(a, n, m, del)

DATA None

DESCRIPTION FSOLVG, developed by H. Geyer, implements the algorithm of M. J. D. Powell for solving a set of nonlinear equations. The algorithm is based on Newton's update and steepest descent methods. The subroutine is structured in a reverse calling sequence which means that when called it returns with an update of the solution vector without calling any functional subroutines. Various arguments of the subroutine are identified below.

x(n)	independent variable vector
f(n)	residual vector
bl(n)	lower bound vector on x
bu(n)	upper bound vector on x
acc	accuracy criteria
del	x increment used to calculate gradient
n	number of equations to be solved
i	iteration counter
maxi	maximum number of iterations
prt	print switch: 0 for no printing, 1 or 2 for

		printing
	a	work array of dimension 2*n*n+8*n+6

REFERENCES

1. Geyer, H. K., Personal Communications, 1990.
2. Powell, M. J. D., "A Hybrid Method for Nonlinear Equations," Numerical Methods for Nonlinear Algebraic Equations, Gordon and Breach Science Publishers, New York, 1970.

A.11 SUBROUTINE GRID

PURPOSE	To generate finite-difference grid system and calculate diffusion distances and geometrical areas.
ARGUMENTS	None
MAIN EQUATIONS	None
SUBROUTINES CALLED	None
DATA	None
DESCRIPTION	The subroutine subdivides the furnace of dimensions XMAX, YMAX, and ZMAX into a uniform IMAXxJMAXxKMAX grid.
REFERENCE	None

A.12 FUNCTION HAIR

PURPOSE

To calculate enthalpy of air at air inlet temperature.

ARGUMENTS

t, air, cp

MAIN EQUATIONS

1. Enthalpy of Air Components (O_2, N_2, H_2O)

$$h_i = Cp_{1i} + (Cp_{2i}/2)T + (Cp_{3i}/3)T^2 + Cp_{4i}/4)T^3 + (Cp_{5i}/5)T^4 + Cp_{6i}/T$$

2. Mixture Enthalpy

$$\Delta h = \sum_i \frac{RuY_i}{MW_i}[h_i(T_i) - h_i(T_r)]$$

SUBROUTINES CALLED

None

DATA

T_r = 298K. Arrays Cp_1, Cp_2, Cp_3, Cp_4, Cp_5 and Cp_6 are read from file cp.d in subroutine INPUT.

DESCRIPTION

HAIR is called only once from MAIN. All enthalpics in the computer code are referenced to 298K.

REFERENCE

Gordon, S. and McBride, B. J., "Computer Program for Calculation of Complex Chemical Equilibrium Composition, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouquet Detonations," NASA SP-273, 1971.

A.13 FUNCTION HFUEL

PURPOSE To calculate sensible enthalpy of fuel at fuel inlet temperature.

ARGUMENTS t, cp

MAIN EQUATIONS

1. $$h = Cp_{18} + (Cp_{28}/2)T + (Cp_{38}/3)T^2 + (Cp_{48}/4)T^3 + (Cp_{58}/5)T^5 + Cp_{68}/T$$

2. $$\Delta h_f = \frac{Ru}{MW_8}[h(T) - h(T_r)]$$

SUBROUTINES CALLED None

DATA $T_r = 298$

DESCRIPTION HFUEL is called only once from MAIN. Numerical values of Cp_{18}, Cp_{28}, Cp_{38}, Cp_{48}, Cp_{58}, Cp_{68} and MW_8 correspond to carbon data.

REFERENCE Gordon, S. and McBride, B. J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouquet Detonations," NASA SP-273, 1971.

A.14 FUNCTION HGAS

PURPOSE To calculate enthalpy of combustion gas at control volume temperatures.

ARGUMENTS t, gas, cp

MAIN EQUATIONS

1. Component enthalpy (CO_2, H_2O, SO_2, CO, O_2, C)

$$h_i = Cp_{1i} + (Cp_{2i}/2)T + (Cp_{3i}/3)T^2 + (Cp_{4i}/4)T^3 + (Cp_{5i}/5)T^4 + Cp_{6i}/T.$$

2. Mixture Enthalphy

$$\Delta h = \sum \frac{RuY_i}{MW_i}[h_i(T) - h_i(T_r)]$$

SUBROUTINES CALLED None

DATA $T_r = 298$ K

DESCRIPTION HGAS is called from MAIN inside a temperature iteration loop.

REFERENCE Gordon, S. and McBride, B. J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouquet Detonations," NASA SP-273, 1971.

A.15 SUBROUTINE INIT

PURPOSE	To initialize variables.
ARGUMENTS	None
MAIN EQUATIONS	None
SUBROUTINES CALLED	PLANCKW
DATA	None
DESCRIPTION	INIT is called from MAIN after reading the input data. Arrays zeroed out are those corresponding to total heat flux, divergence of heat flux, spectral heat flux, incident radiation G_m, incident radiation G_s, radiation intensity, and direction cosine indices. Mean beam length is estimated for use in gas property calculations. A call is made to PLANCKW for determining spectral radiation intensity at wall temperatures. The lower and upper bounds for gas temperature arrays are set as 273 and 3500 K, respectively.
REFERENCE	None

A.16 SUBROUTINE PLANCKG

PURPOSE To calculate spectral Planck function at gas temperature.

ARGUMENTS ifrq

MAIN EQUATIONS

1. Gray Gas

   $I_b = \sigma T^4/\pi$

2. Spectral Band

   $\Delta\upsilon = \upsilon_1 - \upsilon_2$

   $I_b = f(C_2\upsilon_1/T, C_2\upsilon_2/T)\ (\sigma T^4/\pi)\ (1/\Delta\upsilon)$

SUBROUTINES CALLED FRAC (f1, f2)

DATA

$\sigma = 5.669 \times 10^{-8}\ W/m^2.K^4$

$C_2 = 1.43883$ cm.K

DESCRIPTION PLANCKG is called from MAIN inside a gas temperature iteration loop. It returns spectral Planck function, after averaging over the limits of the wave band.

REFERENCE Chang, S. L. and Rhee, K. T., "Blackbody Radiation Functions," International Communications Heat Mass Transfer, Vol. 11, 1984, pp. 451-455.

A.17 SUBROUTINE PLANCKW

PURPOSE	To calculate spectral Planck function at wall temperture.
ARGUMENTS	ifrq
MAIN EQUATIONS	Same as for PLANCKG
SUBROUTINES CALLED	None
DATA	$\sigma = 5.669 \times 10^{-8}$ $W/m^2.K^4$ $C_2 = 1.43883$ cm.K
DESCRIPTION	PLANCKW is called once from INIT. It returns spectral Planck function at wall temperatures after averaging over the limits of the wave band.
REFERENCE	Chang, S. L. and Rhee, K. T., "Blackbody Radiation Functions, International Communications Heat Mass Transfer, Vol. 11, 1984, pp. 451-455.

A.18 SUBROUTINE QFLUX

PURPOSE To calculate wall heat flux attributable to diffusion approximation.

ARGUMENTS None

MAIN EQUATIONS

1. Modified Differential Approximation

$$\vec{q}_m \cdot \hat{n} = - G_{mw}/[2(2/\epsilon_w - 1)]$$

2. Combined Heat Flux

$$\vec{q}_\nu = \vec{q}_m + \vec{q}_s$$

3. P_1 Approximation

$$\vec{q}_\nu \cdot \hat{n} = -(G_w - 4\pi I_{bw})/[2(2/\epsilon_w - 1)]$$

4. Total Heat Flux

$$\vec{q} = \int \vec{q}_\nu d\nu$$

SUBROUTINES CALLED None

DATA None

DESCRIPTION G_{mw} is determined by finite-differencing the Marshak's boundary conditions for G_m. The boundary conditions for MDA and P_1 are different by inclusion or exclusion of the wall emission term. In MDA, q_m is added to q_s to obtain net heat flux. Spectral integration is performed to obtain the total heat flux.

REFERENCE Park, H. M., Ahluwalia, R. K. and Im, K. H., "Three-Dimensional Radiation in Absorbing-Emitting-Scattering Media Using the Modified Differential Approximation," to appear in International Journal of Heat and Mass Transfer, 1992.

A.19 SUBROUTINE SN

PURPOSE

To solve the radiation transport equation by the discrete ordinate technique for G_s if modified differential approximation is used and G if S_4 is specified.

ARGUMENTS

ifrq

MAIN EQUATIONS

1. Radiation intensity by S_4

$$\mu_\ell \frac{\partial I^\ell}{\partial x} + \xi_\ell \frac{\partial I^\ell}{\partial y} + \eta_\ell \frac{\partial I^\ell}{\partial z} + \beta I^\ell = (1 - \omega)\beta I_b + \frac{\omega\beta}{4\pi} S_\ell$$

$$I_p^\ell = \frac{\mu_\ell A I_i^\ell + \xi_\ell B I_j^\ell + \eta_\ell C I_k^\ell + \alpha[(1 - \omega)\beta I_b + S_\ell] V_p}{\mu_\ell A + \xi_\ell B + \eta_\ell C + \alpha\beta V_p}$$

$$A = \Delta x \Delta y$$

$$B = \Delta x \Delta z$$

$$C = \Delta x \Delta y$$

$$V_p = \Delta x \Delta y \Delta z$$

2. G_s for modified differential approximation

$$\mu_\ell \frac{\partial I^\ell}{\partial x} + \xi_\ell \frac{\partial I^\ell}{\partial y} + \eta_\ell \frac{\partial I^\ell}{\partial z} + \beta I^\ell = 0$$

$$I_p^\ell = \frac{\mu_\ell A I_i^\ell + \xi_\ell B I_j^\ell + \eta_\ell C I_k^\ell}{\mu_\ell A + \xi_\ell B + \eta_\ell C + \alpha\beta V_p}$$

3. Incident radiation

$$G = \sum w_\ell I^\ell$$

4. Surface radiation flux

$$Q = \pi \epsilon_w I_{bw} - \epsilon_w \sum w_\ell \mu_\ell I^\ell$$

SUBROUTINES CALLED

None

DATA

Direction cosines, μ_ℓ, ξ_ℓ and η_ℓ, and weights w_ℓ are initialized in a BLOCK DATA STATEMENT.

DESCRIPTION

The finite difference analogs of the radiation transport equation are valid when the direction cosines are positive.

The equations are solved by a point-to-point successive substitution technique. The grid points in the computational domain are visited according to the direction of the radiation beam. The face intensities I_i^ℓ, I_j^ℓ and I_k^ℓ are related to the cell center intensities through linear interpolation.

REFERENCES

1. Carlson, B. G. and Lathrop, K. D., Transport Theory - The Method of Discrete Ordinates in Computing Methods in Reactor Physics, edited by Greenspan, Kelber, and Okrent, Gordon and Breach, New York, 1968.

2. Fiveland, W. A. and Jamaluddin, A. S., "Three-Dimensional Spectral Radiative Heat Transfer Solutions by the Discrete-Ordinate Method," J. Thermophysics, Vol. 5, No. 3, pp. 335-339, July-September 1991.

A.20 SUBROUTINE TDI

PURPOSE To solve the algebraic equations formed from finite-differencing the G_m transport equation.

ARGUMENTS ifrq

MAIN EQUATIONS

$$A^P G_{mijk} = A^E G_{mi+1jk} + A^W G_{mi-1jk} + A^N G_{mij+1k} + A^S G_{mij-1k} + A^H G_{mijk+1} + A^L G_{mijk-1} + S_{ijk}$$

SUBROUTINES CALLED TRIDAG

DATA None

DESCRIPTION Subroutine TDI is called from MAIN after assembling the coefficients A^P, A^E, A^W, A^N, A^S, A^H and A^L and the source term S in COEFF. It solves the finite-difference equations by an iterative line-by-line elimination procedure. In this procedure, the equations are solved alternately along lines of constant x, y and z. When a line of constant x is solved, the contributions from the adjacent constant x lines is added to the source term, thus reducing the equations to a tridiagonal form, which is easily solved by the Gauss elimination procedure in TRIDAG. A similar procedure is repeated when solving along lines of constant y and constant z. The grid is visited alternately along lines of contstant x, y and z until the change in G_m on consecutive iterations becomes smaller than the prescribed tolerance.

REFERENCES None

A.21 SUBROUTINE TFIELD

PURPOSE	To maintain consistent temperature fields in radiation transport and heat balance equations.
ARGUMENTS	None
MAIN EQUATIONS	None
SUBROUTINES CALLED	None
DATA	None
DESCRIPTION	TFIELD equates the three-dimensional temperature field used in the radiation transport equation to the one-dimensional temperature field employed in the heat balance equations.
REFERENCES	None

A.22 SUBROUTINE TRIDAG

PURPOSE To solve a tridiagonal set of algebraic equations.

ARGUMENTS a, b, c, r, u, n

MAIN EQUATIONS $b_i u_2 = a_i u_{i-1} + c_i u_{i+1} + r_i$

SUBROUTINES CALLED None

DATA None

DESCRIPTION TRIDAG, called from TDI, is an implementation of the Thomas algorithm for solving a tridiagonal set of algebraic equations. Depending upon the direction of sweep in TDI, the arrays a_i, b_i and c_i contain A^P, A^N and A^S, or A^P, A^E and A^W or A^P, A^H and A^L. The array r_i contains the source term S together with the contributions from the transposed terms. The order n corresponds to IMAX, JMAX or KMAX.

REFERENCES None

A.23 SUBROUTINE VISCOS

PURPOSE To calculate viscosity of combustion gas.

ARGUMENTS nspe, x, t, visc, amug

MAIN EQUATIONS

1. Viscosity of gas species i

$$\eta_i = 2.699 \times 10^{-6} F_i (MW_i T)^{1/2} / [\sigma_i^2 \Omega_i (T_i^*)]$$

2. Function F_i

$$F_i = 1 - 0.2756\, \omega_i + 0.059035\, \mu_{ri}^4 + \kappa_i$$

3. Collision integral

$$\Omega_i = \frac{1.16154}{(T_i^*)^{0.14874}} + 0.52487 \exp(-0.7732\, T_i^*) + 2.16178 \exp(-2.43787\, T_i^*)$$

4. Dimensionless temperature

$$T_i^* = kT/\epsilon_i$$

SUBROUTINES CALLED None

DESCRIPTION Subroutine VISCOS, called from CONDUCT, returns viscosities of CO_2, N_2, O_2, H_2O and SO_2. The data necessary to calculate viscosities are given in block data DATA2.

REFERENCE Reid, R. C., Prausnitz, J. M. and Poling, B. E., "The Properties of Gases and Liquids," p. 396, Fourth Edition, McGraw-Hill, 1987.

APPENDIX B. RADIATION PROPERTY SUBROUTINES

B.1 SUBROUTINE ABSGAS

PURPOSE To calculate absorption coefficient for gaseous species H_2O, CO_2 and CO.

ARGUMENTS vv, bl, t, ph2O, pCO2, pCO, pt, akh2O, akCO2, akCO, akgas

MAIN EQUATIONS

1. Absorption coefficient of band j in species i

$$\kappa_{\nu ij} = (s/d)_{ij}\rho_i/[1 + 2(s/d)_{ij}\rho_i L/(\beta_{ij}\rho_{ei})]^{1/2}$$

2. Mean intensity to line spacing

$$(\frac{s}{d})_{ij} = \frac{\alpha_{ij}}{\omega_{ij}} \exp(-2|\nu - \nu_{cij}|/\omega_{ij})$$

3. Effective broadening pressure

$$\rho_{ei} = [\frac{\rho}{\rho_0} + \frac{\rho_i}{\rho_0}(b_i - 1)]^{n_i}$$

4. Band width parameter

$$\omega_{ij} = \omega_{0ij}(T/T_0)^{1/2}$$

5. Absorption coefficient

$$\kappa_\nu = \sum_i \sum_j \kappa_{\nu_{ij}}$$

SUBROUTINES CALLED ALPBET (alph, bet, f, v, d, g, t, to, nm)

DATA

Vibrations ν_k, cm^{-1}	Bands $\delta_1, \delta_2, \ldots$	n	Spectral Location ν_c, cm^{-1}	ν_u, cm^{-1}	Band Absorption Parameters α_0, cm^{-1}/gm m^{-2}	β_0	ω_0, cm^{-1}
1. H_2O							
m = 3	(1) Rotational						
ν_1 = 3652		1	140		10400.0	0.14311	57.1

ν_2 = 1595	0,0,0						
ν_3 = 3756	(2) 6.3 μm		1600		41.2	0.094.27	56.4
g_1 = 1	0,1,0	1					
g_2 = 1	(3) 2.7 μm						
g_3 = 1	0,2,0				0.19		
	1,0,0	1	3760		2.30	0.07361	60.0
	0,0,1				22.40		
	(4) 1.87 μm	1	5350		3.0	0.08169	43.1
	0,1,1						
	(5) 1.38 μm	1	7250		2.5	0.11628	32.0
	1,0,1						
2. CO_2							
m = 3	(1) 15 μm						
ν_1 = 1351	0,1,0	0.7	667		19.0	0.06157	12.7
ν_2 = 667	(2) 10.4 μm						
ν_3 = 2396	-1,0,1	0.8	960		2.47×10^{-9}	0.04017	13.4
g_1 = 1	(3) 9.4 μm						
g_2 = 2	0,-2,1	0.8	1060		2.48×10^{-9}	0.11888	10.1
g_3 = 1	(4) 4.3 μm						
	0,0,1	0.8		2410	110.0	0.24723	11.2
	(5) 2.7 μm						
	1,0,1	0.65	3660		4.0	0.13341	23.5
	(6) 2.0 μm						
	2,0,1	0.65	5200		0.066	0.39305	34.5
3. CO							
m = 1	(1) 4.7 μm						
ν_1 = 2143	1	0.8	2143		20.9	0.07506	25.5
g_1 = 1	(2) 2.35 μm						
	2	0.8	4260		0.14	0.167.58	20.0

$b_{H2O} = 8.6\ (T_0/T)^{1/2} + 0.5$

$b_{CO2} = 1.3$

$b_{CO} = 1.1$ for 4.7 μm $b_{CO} = 1.0$ for 2.35 μm

DESCRIPTION

Exponential wide band model developed by Edwards and Balakrishnan is employed for estimating the absorption coefficients of H_2O, CO_2 and CO molecules. The overall procedure involves determining the individual contribution to absorption at a given wavelength from the 6.3, 2.7, 1.87 and 1.38 μm bands of H_2O, 15, 10.4, 9.4, 4.3, 2.7 and 2.0 μm bands of CO_2, and 4.7 and 2.35 μm bands of CO. The individual contribution from each band in gaseous species is linearly added to obtain gas absorption coefficient. Subroutine ALPBET is called for evaluating $(\alpha/\alpha_0)_{ij}$ and $(\beta/\beta_0)_{ij}$.

REFERENCES

Edwards, D. K. and Balakrishnan, A., "Thermal Radiation by Combustion Gases," Int. J. Heat Mass Transfer, Vol. 16, p. 25, 1973.

B.2 SUBROUTINE ALPBET

PURPOSE To calculate the band intensity α and the broadening parameter β.

ARGUMENTS alph, bet, f, v, d, g, t, to, nm

MAIN EQUATIONS 1. Band intensity

$$\left(\frac{\alpha}{\alpha_0}\right)_{ij} = \frac{[1 - \exp(-\sum_{k=1}^{m} u_k\delta_k)]\ \Psi_{ij}(T)}{[1 - \exp(-\sum_{k=1}^{m} u_{0k}\delta_k)]\ \Psi_{ij}(T_0)}$$

2. Broadening parameter

$$(\beta/\beta_0)_{ij} = (T/T_0)^{1/2}\Phi_{ij}(T)/\Phi_{ij}(T_0)$$

SUBROUTINES CALLED PHIPSY (psy, phi, t, f, v, d, g, nm)

DESCRIPTION Subroutine ALPBET, called from ABSGAS, returns $(\alpha/\alpha_0)_{ij}$ and $(\beta/\beta_0)_{ij}$ for specified values of f, υ_k, δ_k, T and T_0. It calls PHIPSY for calculating functions $\Psi_{ij}(T)$, $\Psi_{ij}(T_0)$, $\Phi_{ij}(T)$ and $\Phi_{ij}(T_0)$.

REFERENCES Edwards, D. K. and Balakrishnan, A., "Thermal Radiation by Combustion Gases," Int. J. Heat Mass Transfer, Vol. 16, p. 25, 1973.

B.3 SUBROUTINE FCTRL

PURPOSE	To compute factorials of three numbers.
ARGUMENTS	n1, n2, n3, r1, r2, r3
MAIN EQUATIONS	1. $r_1 = n_1!$
	2. $r_2 = n_2!$
	3. $r_3 = n_3!$
SUBROUTINES CALLED	None
DESCRIPTION	This subroutine, called from PHIPSY, computes factorials of three integers passed through argument and returns three real numbers.
REFERENCES	None

B.4 SUBROUTINE MIE

PURPOSE

To calculate the efficiency factors for extinction and scattering as functions of particle size parameter and complex refractive index.

ARGUMENTS

x, refre, refim, qext, qsca

MAIN EQUATIONS

1. Size parameter

$$x = 2\pi r/\lambda$$

2. Complex refractive index

$$m = n_R - in_I$$

3. Efficiency factor for extinction

$$Q_{ext} = \frac{2}{x^2} \sum (2n+1)\mathrm{Re}(a_n + b_n)$$

4. Efficiency factor for scattering

$$Q_{sca} = \frac{2}{x^2} \sum (2n+1)\left(|a_n|^2 + |b_n|^2\right)$$

5. Coefficients a_n and b_n

$$a_n = \frac{m\psi_n(mx)\psi_n'(x) - \psi_n(x)\psi_n'(mx)}{m\psi_n(mx)\xi'(x) - \xi_n(x)\psi_n'(mx)}$$

$$b_n = \frac{\psi_n(mx)\psi_n'(x) - m\psi_n(x)\psi_n'(mx)}{\psi_n(mx)\xi'(x) - m\xi(x)\psi_n'(mx)}$$

6. Riccati-Bessel functions

$$\psi_n(\rho) = \rho j_n(\rho)$$

$$\xi_n(\rho) = \psi_n(\rho) - i\chi_n(\rho)$$

SUBROUTINES CALLED

None

DESCRIPTION

The radiation cross-section calculations are based on application of Mie theory to interaction of electromagnetic waves with homogeneous spherical particles. The efficiency factors for absorption and scattering are expressed in terms

of the Riccati-Bessel functions. Both ψ_n and ξ_n satisfy

$$\psi_{n+1}(x) = \frac{2n+1}{x}\,\psi_n(x) - \psi_{n-1}(x)$$

and are computed by this upward recurrence relation beginning with

$$\psi_{-1}(x) = \cos x, \quad \psi(x) = \sin x$$
$$\chi_{-1} = -\sin x, \; \chi_0(x) = \cos x$$

The series summations in Q_{ext} and Q_{sca} are terminated after NSTOP terms, where NSTOP is the integer closest to $x + 4x^{1/3} + 2$. Subroutine MIE has been adapted from BHMIE with some minor modifications.

REFERENCES

Bohren, C. F. and Huffman, D. R., Absorption and Scattering of Light by Small Particles, John Wiley and Sons, New York, 1983.

B.5 SUBROUTINE OPT

PURPOSE

To calculate spectral absorption coefficients and scattering albedos.

ARGUMENTS

nsize, anum, ph20, pco2, pco, pg, nfrq, v, nmax, incl, yash, tg, bl, omega, beta

MAIN EQUATIONS

$$\beta_i = \kappa_{gi} + \pi \sum r_j^2 Q_{ext}(i,j) N_j$$

$$\sigma_i = \pi \sum r_j^2 Q_{sca}(i,j) N_j$$

$$\beta = \sum_{i=0}^{20} \beta_i \Delta\nu_i / \sum_{i=1}^{20} \Delta\nu_i$$

$$\sigma = \sum_{i=1}^{20} \sigma_i \Delta\nu_i / \sum_{i=1}^{20} \Delta\nu_i$$

$$\omega = \sigma/\beta$$

SUBROUTINES CALLED

ABSGAS (vnu, bl, tg, ph20, pco2, pco, pg, akh2o, akco2, akco, akg)

DESCRIPTION

OPT first calculates the contributions of the gaseous species, CO_2, H_2O and CO, to the absorption coefficient. For this purpose, each waveband is subdivided into 20 intervals, and subroutine ABSGAS is called at each interval. Subintegration is performed by summing over the 20 intervals to obtain the average absorption of the gas over the waveband. Next, particle extinction and scattering cross-sections are determined by integrating the corresponding efficiency factors for ash, soot and char over the particle size spectra and weighting over geometric cross-sections and number density. Finally, the particle cross-sections are combined with gas absorption coefficients to generate gas-particle mixture absorption coefficients and scattering albedo over each of the 37 wavebands considered.

REFERENCES

None

B.6 SUBROUTINE OPTASH

PURPOSE To calculate complex refractive indices of ash for specified composition.

ARGUMENTS wavl, yash, t, tefre, refim

MAIN EQUATIONS Equations (2.7) - (2.19)

DATA Section (2.5)

SUBROUTINES CALLED SIO2 (wavl, asio2)

DESCRIPTION The complex refractive indices of ash are calculated using the procedure outlined in Section (2.5). In the short wavelength region, $\lambda < 8\ \mu m$, a mixture rule is employed for calculating the contributions of SiO_2, CaO, Fe_2O_3 and MgO. Iron is the primary absorber for $\lambda < 4\ \mu m$ and silica for $4\ \mu m < \lambda < 8\ \mu m$. In the intermediate wavelength region, $8\ \mu m < \lambda < 13\ \mu m$, the complex indices are determined by the Restrahlen band of silica. In the long wavelength region, $\lambda > 13\ \mu m$, the optical constants are determined from the data for Restrahlen bands of alumina and magnesia.

REFERENCES

1. Goodwin, D. G., "Infrered Optical Constants of Coal Slag," HTGL Report No. T-255, Stanford, CA, 1986.

2. Im, K. H. and Ahluwalia, R. K., "Radiation Properties of Combustion Products," ANL/FE-91/2, 1991.

B.7 SUBROUTINE OPTCHAR

PURPOSE To calculate the complex refractive indices of char particles.

ARGUMENTS wavl, dummy1, dummy2, refre, refim

MAIN EQUATIONS Equations (2.5) - (2.6)

DATA Table (2.1)

SUBROUTINES CALLED None

DESCRIPTION The oscillator model used in calculating the optical constants of char is derived from a least-square fit analysis of efficiency-factor measurements of Brewster and Kunitomo on chars produced from Australian coals.

REFERENCES

1. Im, K. H. and Ahluwalia, R. K., "Radiation Properties of Combustion Products," ANL/FE-91/2, 1991.

2. Brewster, M. Q. and Kunitomo, T., "The Optical Constants of Coal, Char and Limestone," Journal of Heat Transfer, Vol. 106, p. 678, 1984.

B.8 SUBROUTINE OPTDRV

PURPOSE

To calculate extinction coefficients and scattering albedos and to assign solution indices for spectral radiation transport equation (RTE).

ARGUMENTS

None

MAIN EQUATIONS

None

SUBROUTINES CALLED

OPTPROP (nsize, nfrq, incl, r, anum, yash, tg, ph2o, pco2, pco, pg, bl, dfrq, beta, omega)

DESCRIPTION

OPTDRV is a driver module that calls OPTPROP for radiation cross-section at different frequency bands, gas temperatures, and gas compositions reflective of psd's in furnace zones. The RTE solution indices are assigned according to the following criteria

ipl(ifrq) = 1 if $\beta > \beta_{max}$ everywhere

is4(ifrq) = 1 if $\beta < \beta_{min}$ anywhere

ipl(ifrq) = 0 and is4(ifrq) = 0 if $\beta_{min} < \beta < \beta_{max}$ everywhere

ifrq = 1,2,...nfrq

The discrete ordinate method is used if is4 = 1, modified differential approximation if is4 = 0 and ipl = 0, and P_1 approximation if ipl = 1.

REFERENCES

None

B.9 SUBROUTINE OPTPROP

PURPOSE To determine extinction coefficients and scattering albedos for particle laden combustion gas.

ARGUMENTS nsize, nfrq, incl, r, anum, yash, tg, ph2o, pco2, pco, pg, dfrq, beta, omega

MAIN EQUATIONS None

SUBROUTINES CALLED

QEFF (iunit, optcon, nsize, r, l, nfrq, v, nmax, yash, tg)
OPT (nsize, r, anum, ph2o, pco2, pco, pg, nfrq, v, nmax, incl, yash, tg, omega, beta)

DESCRIPTION OPTPROP works internally with three files called qash, qsoot and qchar. Names of these files are read as input data. If the values of indices, incl(1), incl(2) and incl(3) read as input, are 2, files are opened with status unknown and efficiency factors are calculated and stored in the files by making calls to subroutine QEFF. Next, subroutine OPT is called to calculate the spectral absorption coefficients and scattering albedos of the gas-particle mixture. Finally, if the index nfrq is unity, the optical properties are averaged over the infrared spectrum by weighting over the Planck function.

REFERENCES None

B.10 SUBROUTINE OPTSOOT

PURPOSE To calculate the optical constants of soot particles.

ARGUMENTS wavl, dummy, t, refre, refim

MAIN EQUATIONS Equations (2.5) and (2.6) with $n_\infty = 1$

$$\gamma(T) = \gamma(T_0)(T/T_0)^{1/2}, \; T_0 = 1450K$$

DATA Table (2.2)

SUBROUTINES CALLED None

DESCRIPTION OPTSOOT uses dispersion constants recommended by Lee and Tien for hydrocarbon fuels. The data of Habib and Vervisch can also be used by removing the comments on the Fortran statements in the subroutine.

REFERENCES

1. Lee, S. C. and Tien, C. L., "Optical Constants of Soot in Hydrocarbon Flames," 18th Symposium (International) on Combustion, p. 1159, 1981.

2. Habib, Z. G. and Vervisch, P., "On the Refractive Index of Soot at Flame Temperature," Combustion Science and Technology, Vol. 59, p. 121, 1988.

B.11 SUBROUTINE PHIPSY

PURPOSE To calculate functions Ψ and Φ

ARGUMENTS psy, phi, t, f, v, d, g, nm

MAIN EQUATIONS

1. Function Ψ

$$\Psi(T) = \frac{\prod_{k=1}^{m} \sum_{\upsilon_k=\upsilon_{0k}}^{\infty} H_k(\upsilon_k)}{\prod_{k=1}^{m} \sum_{\upsilon_k=0}^{\infty} H_k(\upsilon_k)}$$

$$H_k(\upsilon_k) = \frac{(\upsilon_k + g_k + |\delta_k| - 1)!}{(g_k - 1)!\ \upsilon_k!} \exp(-u_k \upsilon_k)$$

2. Function Φ

$$\Phi(T) = \frac{\{\prod_{k=1}^{m} [\sum_{\upsilon_k=\upsilon_{0k}}^{\infty} G_k(\upsilon_k)]^{1/2}\}^2}{\prod_{k=1}^{m} \sum_{\upsilon_k=\upsilon_{0k}}^{\infty} G_k(\upsilon_k)}$$

$$G_k(\upsilon_k) = \frac{(\upsilon_k + g_k + |\delta_k| - 1)!}{(g_k - 1)!\ \upsilon_k!} \exp(-u_k \upsilon_k)$$

$$\upsilon_{0k} = 0 \quad \text{if} \quad \delta_k > 0$$

$$\upsilon_{0k} = |\delta_k| \quad \text{if} \quad \delta_k < 0$$

$$u_k = f\nu_k/T$$

SUBROUTINES CALLED FCTRL (n1, n2, n3, r1, r2, r3)

DESCRIPTION The factorials appearing in the equations Ψ and Φ are evaluated in subroutine FCTRL.

REFERENCES

Edwards, D. K. and Balakrishnan, A., "Thermal Radiation by Combustion Gases," Int. J. Heat Mass Transfer, Vol. 16, p. 25, 1973.

B.12 SUBROUTINE QEFF

PURPOSE	To calculate the efficiency factors for scattering and extinction by combustion particles.
ARGUMENTS	iunit, optcon, nsize, r, l, nfrq, v, nmax, yash, tg
MAIN EQUATIONS	None
SUBROUTINES CALLED	OPTCON (wavl, yash, tg, refre, refim) MIE (x, refre, refim, qext, qsca)
DESCRIPTION	QEFF calls OPTCON for spectral complex refractive indices of ash, soot or char. Next, MIE is called to calculate the efficiency factors for extinction and scattering as functions of particle size and frequency. For later reference, the results are stored in fields specified by the logical unit iunit.
REFERENCES	None

B.13 SUBROUTINE SIO2

PURPOSE	To obtain the spectral value of the absorption index for fused silica.
ARGUMENTS	wavl, asio2
MAIN EQUATIONS	None
SUBROUTINES CALLED	None
DATA	Table (2.4)
DESCRIPTION	The absorption indices of fused silica are available at discrete wavelengths. Linear interpolation is used to estimate the absorption index at wavelenth, wavl, passed to the subroutine as an argument.
REFERENCE	Phillip, H. R., "Silicon Oxides (Glass)," Handbook of Optical Constants of Solids, Ed. E. D. Palik, 1985.

APPENDIX C. I/O SUBROUTINES

C.1 BLOCK DATA DATA1

PURPOSE To initialize some variables appearing in Common Blocks.

ARGUMENTS None

MAIN EQUATIONS None

SUBROUTINES CALLED None

DATA

1. Number of ash, soot and char particle size grids: npt(1) = npt(2) = npt(3) = 40.
2. Frequency band centers: frq(37). See Table 3.2.
3. Frequency band widths: dfrq(37). See Table 3.2.
4. Ash particle size grid. See Table 3.3.
5. Soot particle size grid. See Table 3.3.
6. Char particle size grid. See Table 3.3.
7. Directional cosines for S_4 solution: xnu(24), yxi(24), and zet(24). See Eqs. (2.34) and (2.36).
8. Directional weights for S_4 solution: wt(24). See Eqs. (2.34) and (2.35).
9. Direction indices: ixnu(24), iyxi(24), and izet(24).

REFERENCES None

C.2 BLOCK DATA DATA2

PURPOSE To initialize variables pertaining to physical, thermodynamic, transport and reaction kinetic data.

ARGUMENTS None

MAIN EQUATIONS None

SUBROUTINES CALLED None

DATA

1. Molecular weight (MW), normal boiling point (T_b), critical temperature (T_c), critical pressure (P_c), critical volume (V_c), accentric factor (ω) and dipole moment (δ) of CO_2, N_2, O_2, H_2O, and SO_2. See description for subroutines CONDUC, DIFFUS and VISCOS.

2. Constants for calculating specific heats of CO_2, H_2, O_2, H_2O and SO_2: ac_p, bc_p, cc_p and dc_p. See description for subroutine CONDUC.

3. Pre-exponential factors (A and A_c), activation energies (E and E_c), burning mode parameter (α), swelling factor ($\mathfrak{w}$), and reaction order (n). See description for subroutine BURNOUT.

REFERENCES

1. Reid, R. C., Prausnitz, J. M., and Polling, B. E., The Properties of Gases and Liquids, Fourth Edition, Chapter 10, McGraw-Hill Book Company, 1987.

2. Hurt, R. H. and Hardesty, D. R., 'Rates and Mechanisms of Pulverized Coal Char Combustion,' Seventh Annual Coal Preparation, Utilization, and Environmental Control Contractor Conference Proceedings, Pittsburgh, PA, July 1991.

C.3 SUBROUTINE INPUT

PURPOSE To read input data.

ARGUMENTS None

MAIN EQUATIONS None

SUBROUTINES CALLED None

DATA None

DESCRIPTION Input reads twenty-eight items of data. Each item consists of a title followed by free-formatted numeric or alphanumeric data. The title must be enclosed in quotation marks and can be up to 80 characters long. Data items are specified in the following order:

1. Problem title
2. Debug indices
3. Number of frequencies
4. Cut-off extinction coefficients
5. Number of iterations
6. Nonlinear solver parameters
7. Finite difference grid
8. Convective heat transfer coefficients
9. Spectral surface emissivities
10. Spectral anisotropic scattering factors
11. Over-relaxation parameter for G_m equation
12. Furnace dimensions
13. Wall temperatures
14. Ultimate analysis of coal
15. Proximate analysis of coal
16. Air composition and excess air
17. Fractional gas recirculations
18. Fractional heat losses

19. Inlet temperatures
20. High heating value and furnace rating
21. Ash composition
22. Particle inclusion indices
23. Cumulative ash size distribution
24. Cumulative soot size distribution
25. Cumulative char size distribution
26. Material densities of ash, soot and char
27. File names for ash, soot and char efficiency factors
28. Furnace pressure and reference temperatures

REFERENCES None

C.4 SUBROUTINE OUTPF

PURPOSE To print out final results.

ARGUMENTS None

MAIN EQUATIONS None

SUBROUTINES CALLED None

DESCRIPTION OUTPF prints the following sets of results:

1. Ash, soot and char particle size distributions in first, second and last control volumes.
2. Average ash, soot and char loading, and partial pressures of CO_2, H_2O and CO_2 in first, second and last control volumes.
3. Spectral extinction coefficients and scattering albedos in first, second and last control volumes; and the RTE solution method index for every band.
4. Spectral heat transfer rates in every control volume
5. Heat transfer rates, heat fluxes and heat release rates in every control volume.
6. Summary output

   Column No. 1 = variable names

   Column No. 2 = temperatures (K)

   Column No. 3 = flow rates (kg/s)

   Column No. 4 = enthalpy (J/kg)

   Column No. 5 = enthalpy entering control volume (J/kg)

   Column No. 6 = enthalpy leaving control volume (J/kg)

   Column No. 7 = heat transfer rate from control volume (W)

   CPU time spent in various subroutines

REFERENCES None

C.5 SUBROUTINE OUTPUT

PURPOSE To produce detailed outputs of different variables.

ARGUMENTS nout

MAIN EQUATIONS None

SUBROUTINES CALLED None

DESCRIPTION Depending upon the value of nout, different variables listed below are printed. No output is generated if the associated index iout (nout) has a value of zero.

iout	Variable to be printed
1	Combustion gas composition, fuel flow rate, air flow rate, flue gas recirculation and combustion gas recirculation
3	Wall heat flux distribution due to G_s
4	Incident radiation field, G_s
5	Incident radiation field, G_m
6	Total wall heat flux distribution
7	Distribution of divergence of heat flux
8	Temperature field

APPENDIX D: PROGRAM LISTING

```
      program furn3d
c-----------------------------------------------------------c
c                                                           c
c     FURN3D VERSION 1.0                                    c
c     DATE OF RELEASE 9-3-92                                c
c                                                           c
c-----------------------------------------------------------c
      implicit real*8 (a-h,o-z)
      include 'furn3d.h'
      real*4  dtime, time(2)
      data tgs, tgm, tpl, ttg /4*0.d0/

c-----input data
      call input

c---- initiate clock timing
      tstart = dtime(time)

c---- initialization
      call init

c ----grid system
      call grid

c---- gas composition
      call compsn
      call output(1)

c---- combustion module
      call combdrv

c-----optical properties module
      call optdrv
      topt   = dtime(time)

c---- frequency loop for  Gs
      do 10 ifrq=1,nfrq

c----    skip if beta = 0 everywhere

         if(ibeta(ifrq) .eq. 0) goto 10

c----    skip if S4 or P1 approximation
         if (ipl(ifrq)+is4(ifrq) .gt. 0) goto 10

c----    S4 solution of I and Gs for MDA
         call sn(ifrq)

   10 continue

      call output(2)
      call output(3)
      call output(4)

   15 continue
      tgs = tgs + dtime(time)

c---- temperature iteration loop
      do 30 itry = 1, maxcal

c----    load gas temperatures: tg(ivol)-->t(i,j,k)
         call tfield

c----    frequency loop for Gm
```

```
      do 20 ifrq=1,nfrq

c----     skip if beta = 0 everywhere
          if(ibeta(ifrq) .eq. 0) goto 20

c----     Planck function at gas temperature
          call planckg(ifrq)
          tpl = tpl + dtime(time)

          if (is4(ifrq) .eq. 0) then
c----        coefficients of Gm equation
             call coeff(ifrq)

c----        Gm field from tdi
             call tdi(ifrq)
             tgm = tgm + dtime(time)

          else

c----        S4 solution of I and G (=Gs+Gm)
             call sn(ifrq)
             tgs = tgs + dtime(time)

          end if

c----     div(Qr): cumulative (w.r.t. frequency) summation.
          call diverq(ifrq)

   20   continue

c----   energy equation
        call energy(itry)

c----   non-linear equations solver
        call fsolvg(tg,hres,tgl,tgu,acc,deltg,nvol,ntry,
     1              maxcal,iout(14),rwork)
        if (ntry .ge. 1000) go to 40

   30 continue
      write(6,*) 'no convergence in temperature iteration loop '
   40 continue

      call output(5)

c---- wall heat flux
      call qflux
      call output(6)
      call output(7)
      call output(8)

c---- final summary output
      call outpf

c---- timing test
      write(6,2000)
      write(6,2003) 'time spent in optical props  ', topt,' secs'
      write(6,2003) 'time spent in Gs computation ', tgs ,' secs'
      write(6,2003) 'time spent in Gm computation ', tgm ,' secs'
      write(6,2003) 'time spent in Planck Function', tpl ,' secs'


 2000 format(1h1)
 2003 format(10x, a,1pe12.3,a)
```

```
      end


      subroutine burnout(nsize,anumc,rc,akg,diffo2,tg,tp,amcf,
     1                   po2,rhochar,rhoc,dtm)
c-----------------------------------------------------------------c
c     SUBROUTINE BURNOUT                                          c
c-----------------------------------------------------------------c
      implicit real*8(a-h,o-z)
      parameter(nsz=40)

      dimension amcf(nsize), anumc(nsize), rc(nsize), tp(nsize)

      common /comb/ order , aoxid  , aprod , eoxid, eprod, parmod,parswl

      data  hco   ,  hco2   , ru    , amwc  , amwo2 , pi        , anu
     1  /9.283e+6 , 3.280e+7, 8.314 , 0.012 , 0.032 , 3.14159265, 2.0/

      data   pconv
     1  / 1.01325e+5/

      do 40 i = 1, nsize

c----     skip if m = 0.0
          if (amcf(i).eq.0.0) then
              tp(i) = tg
              goto 40
          end if

c----     char particle diameter
          aa = (1.-parmod)/3.
          d  = 2.*rc(i)*amcf(i)**aa

c----     iteration loop for particle temperature
          tp(i) = tg+0.1
          iter  = 0

   10     iter = iter + 1

c----     oxidation rate constant, kg/m**2.s
          aks  = aoxid*exp(-eoxid/(ru*tp(i)))

c----     mole fraction ratio of reaction products ,co/co2
          fco  = aprod*exp(-eprod/(ru*tp(i)))

c----     heat of reaction per kg of carbon
          hc  = (hco2 + hco*fco)/(1. + fco)

c----     heat flux from a burning char partcle
          qflux = anu*akg/d*(tp(i)-tg)

c----     oxygen pressure at particle surface
          gradyo2 = ru*tg/amwc/pconv*d/(2.*diffo2)*(1.+fco)/(1.+2.*fco)
          po2s    = po2 - gradyo2*qflux/hc

c----     if po2s < 0 then set po2s = 0
          po2s = max(po2s,0.d0)

c----     characteristic oxidation rate, (kg of carbon)/m**2.s
          ratec = aks*po2s**order

c----     equation to be solved
          fx = 1. - ratec*hc/(qflux+1.e-40)
```

```
         if(abs(fx) .lt. 1.e-04) goto 30

         if(iter .gt. 200) then
            write(6,*) 'Failed in finding Tp'
            write(6,*) i , tp(i) , fx
            if(iter.gt.250) goto 30
         end if

         if(iter .gt. 2) goto 20

c-----   set up bounding values for bisection method
         if(iter .eq. 1) then
            xa    = tp(i)
            fa    = fx
            tpmax = tg + 0.9999*po2*hc/gradyo2*d/(anu*akg)
            tp(i) = tpmax
            goto 10

         else
            xb    = tp(i)
            fb    = fx
            tp(i) = 0.5*(xa+xb)
            goto 10
         endif

  20     continue


c------  bisection method

         if(fx*fa .lt. 0.0) then
            xb = tp(i)
            fb = fx

         else if(fx*fb .lt. 0.0) then
            xa = tp(i)
            fa = fx

         else
            write(6,*) 'Failed in finding Tp'
            write(6,*) 'iter=',iter, 'i=',i, 'Tp(i)=',tp(i), 'fx=',fx
            stop

         end if

         tp(i) = 0.5*(xa+xb)

         goto 10

c-----   completed tp calculation
  30     continue

c----    fractional carborn burnout, m(i)/m0(i)
         aa = (1.+2.*parmod)/3.
         t1 = amcf(i)**aa - 3.*aa*parswl**2/(rhoc*rc(i))*ratec*dtm
         t1 = max(t1,0.d0)
         amcf(i) = t1**(1./aa)

  40  continue


c---- remaining char concentration, (kg of char)/m**3
      t1  = 0.0
      do 60 i = 1, nsize
```

```
         t1  = t1 + rc(i)**3*amcf(i)*anumc(i)
   60  continue
       drhochr = rhochar - 4.*pi/3.*rhoc*t1
       rhochar = 4.*pi/3.*rhoc*t1

c---- oxygen partial pressure, atm
       po2 = po2 - drhochr/amwc*ru*tg/pconv


       end


       subroutine coeff(ifrq)

c-----------------------------------------------------------------------c
c          SUBROUTINE COEFF(ifrq)                                       c
c-----------------------------------------------------------------------c

       implicit real*8 (a-h,o-z)
       include 'furn3d.h'

c---- calculate coefficients of finite difference equation for Gm
c---- calculate Al,As,Aw,Ap,Ae,An,Ah, and S. beta is function of k only.

       do 20 k = 1, kmax

          if (k .eq. 1) then
             betahm = beta1(k,ifrq)
          else
             betahm = 0.5*(beta1(k,ifrq)+beta1(k-1,ifrq))
          end if

          if (k .eq. kmax) then
             betahp = beta1(k,ifrq)
          else
             betahp = 0.5*(beta1(k,ifrq)+beta1(k+1,ifrq))
          end if

          do 10 j = 1, jmax
          do 10 i = 1, imax

          al(i,j,k) = dx(i)*dy(j)/(betahm*delzm(k))
          as(i,j,k) = dx(i)*dz(k)/(beta1(k,ifrq)*delym(j))
          aw(i,j,k) = dy(j)*dz(k)/(beta1(k,ifrq)*delxm(i))
          ae(i,j,k) = dy(j)*dz(k)/(beta1(k,ifrq)*delxp(i))
          an(i,j,k) = dx(i)*dz(k)/(beta1(k,ifrq)*delyp(j))
          ah(i,j,k) = dx(i)*dy(j)/(betahp*delzp(k))

          ap(i,j,k) =-al(i,j,k) - ah(i,j,k) - ae(i,j,k) - aw(i,j,k)
     1              -an(i,j,k) - as(i,j,k) - 3.*(1.-omeg(k,ifrq))
     2              *beta(k,ifrq)*dx(i)*dy(j)*dz(k)

          s(i,j,k)  =-12.*pi*(1.-omeg(k,ifrq))
     1              *beta(k,ifrq)*ebg(i,j,k)*dx(i)*dy(j)*dz(k)
     2              -3.*omeg(k,ifrq)*beta(k,ifrq)*gs(i,j,k,ifrq)
     3              *(1.+a1(k,ifrq)/(3.-a1(k,ifrq)*omeg(k,ifrq)))
     3              *dx(i)*dy(j)*dz(k)

         if (k .eq. 1) then

            gam  = (2./(3.*beta1(k,ifrq)))*(2./ew(k,ifrq)-1.)
            upzo = gam/dz(k)-0.5
            dozo = gam/dz(k)+0.5
            alzo = upzo/dozo
```

```
      bezo = 4.*pi*ipl(ifrq)*ebwzm(i,j,ifrq)/dozo
      gazo = gam*beta(1,ifrq)*al(1,ifrq)
1            *omeg(1,ifrq)*qzm(i,j,ifrq)/(dozo*dx(i)*dy(j))

      ap(i,j,k)  = ap(i,j,k)+al(i,j,k)*alzo
      s(i,j,k)   = s(i,j,k)-al(i,j,k)*(bezo+gazo)
      al(i,j,k)  = 0.0

    end if

    if (k .eq. kmax) then

      gam    = (2./(3.*betal(k,ifrq)))*(2./ew(k,ifrq)-1.)
      upzmax = gam/dz(k)-0.5
      dozmax = gam/dz(k)+0.5
      alzmax = upzmax/dozmax
      bezmax = 4.*pi*ipl(ifrq)*ebwzp(i,j,ifrq)/dozmax
      gazmax = gam*beta(k,ifrq)*al(k,ifrq)
1              *omeg(k,ifrq)*qzp(i,j,ifrq)/(dozmax*dx(i)*dy(j))

      ap(i,j,k)  = ap(i,j,k)+ah(i,j,k)*alzmax
      s(i,j,k)   = s(i,j,k)-ah(i,j,k)*(bezmax+gazmax)
      ah(i,j,k)  = 0.0

    end if

    if (j .eq. 1) then

      gam  = (2./(3.*betal(k,ifrq)))*(2./ew(k,ifrq)-1.)
      upyo = gam/dy(j)-0.5
      doyo = gam/dy(j)+0.5
      alyo = upyo/doyo
      beyo = 4.*pi*ipl(ifrq)*ebwym(i,k,ifrq)/doyo
      gayo = gam*beta(k,ifrq)*al(k,ifrq)
1            *omeg(k,ifrq)*qym(i,k,ifrq)/(doyo*dx(i)*dz(k))

      ap(i,j,k)  = ap(i,j,k)+as(i,j,k)*alyo
      s(i,j,k)   = s(i,j,k)-as(i,j,k)*(beyo+gayo)
      as(i,j,k)  = 0.0

    end if

    if (j .eq. jmax) then

      gam    = (2./(3.*betal(k,ifrq)))*(2./ew(k,ifrq)-1.)
      upymax = gam/dy(j)-0.5
      doymax = gam/dy(j)+0.5
      alymax = upymax/doymax
      beymax = 4.*pi*ipl(ifrq)*ebwyp(i,k,ifrq)/doymax
      gaymax = gam*beta(k,ifrq)*al(k,ifrq)
1              *omeg(k,ifrq)*qyp(i,k,ifrq)/(doymax*dx(i)*dz(k))

      ap(i,j,k)  = ap(i,j,k)+an(i,j,k)*alymax
      s(i,j,k)   = s(i,j,k)-an(i,j,k)*(beymax+gaymax)
      an(i,j,k)  = 0.0

    end if

    if (i .eq. 1) then

      gam  = (2./(3.*betal(k,ifrq)))*(2./ew(k,ifrq)-1.)
      upxo = gam/dx(i)-0.5
      doxo = gam/dx(i)+0.5
      alxo = upxo/doxo
```

```
            bexo = 4.*pi*ipl(ifrq)*ebwxm(j,k,ifrq)/doxo
            gaxo = gam*beta(k,ifrq)*al(k,ifrq)
     1              *omeg(k,ifrq)*qxm(j,k,ifrq)/(doxo*dy(j)*dz(k))
            ap(i,j,k)  = ap(i,j,k)+aw(i,j,k)*alxo
            s(i,j,k)   = s(i,j,k)-aw(i,j,k)*(bexo+gaxo)
            aw(i,j,k)  = 0.0

         end if

         if (i .eq. imax) then

            gam    = (2./(3.*betal(k,ifrq)))*(2./ew(k,ifrq)-1.)
            upxmax = gam/dx(i)-0.5
            doxmax = gam/dx(i)+0.5
            alxmax = upxmax/doxmax
            bexmax = 4.*pi*ipl(ifrq)*ebwxp(j,k,ifrq)/doxmax
            gaxmax = gam*beta(k,ifrq)*al(k,ifrq)
     1               *omeg(k,ifrq)*qxp(j,k,ifrq)/(doxmax*dy(j)*dz(k))

            ap(i,j,k)  = ap(i,j,k)+ae(i,j,k)*alxmax
            s(i,j,k)   = s(i,j,k)-ae(i,j,k)*(bexmax+gaxmax)
            ae(i,j,k)  = 0.0

         end if

   10    continue
   20 continue

      end


      subroutine combdrv
c-----------------------------------------------------------------------c
c     SUBROUTINE COMBDRV                                                c
c-----------------------------------------------------------------------c
      implicit real*8(a-h,o-z)
      parameter(nsz=40,nsp=5)
      include 'furn3d.h'

      common /comb/ order, aoxid  , aprod , eoxid, eprod, parmod,parswl

      common /critc/ amw(nsp), tb (nsp), tc  (nsp), pc(nsp), vc(nsp),
     1               ome(nsp), dip(nsp)
      common /heatc/ acp(nsp), bcp(nsp), ccp (nsp), dcp(nsp)

      dimension amcf(nsz), anumc(nsz), rc(nsz), tp(nsz), xg(nsp)

      data (amcf(i), i = 1 , nsz)
     1  / nsz*1.d0   /

      data  pi        , pconv     ,  ru    ,  tpyro  ,  dtm   , nspe
     1 /    3.14159265, 1.01325e+5,  8.314 ,  40.e-3 ,  5.e-3 ,   5 /

      pi43  = 4.*pi/3.
      nsize = nsz
      ivol  = 2
      tgas  = trad(ivol)

c---- char concentration
      ychar    = fuel(9)*flow(1)/(flow(1)+flow(2)+flow(3))
      rhogr    = pgas*1.01325e+05/(8314.0/amwg*tgas)

      t1 = 0.0
      do 10 i = 1, nsize
```

```
         anumc(i)  = pdist(3,i,2)
         rc(i)     = rpt(3,i)
         if(anumc(i).lt.1.) amcf(i) = 0.0
         t1       = t1 + rc(i)**3*anumc(i)
   10  continue
       rhochar = pi43*rhopt(3)*t1

c---   theoretical oxygen pressure
       po2th = rhochar/0.012*ru*tgas/pconv

       do 20 ig = 1, nsp
         xg(ig) = gas(ig)*amwg/amw(ig)
   20  continue

c----  gas volocity
       area = xmax*ymax
       velg = (flow(1)+flow(2)+flow(3))/(rhogr*area)
       write(6,100) 'average gas velocity =',velg,' m/s'
       write(6,100) 'residence time       =',zmax/velg,' s'

c----  air to fuel ratio
       af = flow(2)/flow(1)

c----  oxygen  due to excess air
       yo2   = (air(1)*air(4)*af + gas(5)*fracr(1)*(1.+af))
     1       /((1.+af)*(1.+fracr(1)))
       po2ex = amwg/12.*yo2*pgas

c----  starting value of oxygen partial pressure for char burnout
       po2 = po2th + po2ex

c----  fraction of heat released from volatile matter
       hc   = 3.280e+7
       qcha = fuel(9)*flow(1)*hc
       qvol = qfurn - qcha

c----  initialize fraction of heat released in control volume
       do 30 ivl =  1, nvol
         qfrac(ivl) = 0.0
   30  continue

c----  control volume size
       zvol  = (kvol(ivol)-kvol(ivol-1))*zmax/kmax

c----  char burnout calculation
       time    = tpyro
       rhochao = rhochar

   40  time  = time + dtm

       z       = velg*time
       tgas    = trad(ivol)

c----  oxygen diffusivity
       call diffus(5,nsp,xg,tgas,pgas,diffo2)

c----  thermal conductivity
       call conduc(nsp,xg,tgas,akg)

c----  char burnout
       call burnout(nsize,anumc,rc,akg,diffo2,tgas,tp,amcf,po2,rhochar,
     1              rhopt(3),dtm )

c---   fraction burned
```

```
      yfrac = rhochar/(ychar*rhogr)

      if(z .ge. zvol .or. yfrac .le. 1.d-3) then

c----     heat release fraction in ivol
          qfrac(ivol) = (rhochao-rhochar)/(ychar*rhogr)*qcha/qfurn

c----     update size distribution for heat transfer calculation
          do 45 i = 1, nsize
             pdist(3,i,ivol) = 0.5*(anumc(i) + amcf(i)*pdist(3,i,2))
             anumc(i)        = amcf(i)*pdist(3,i,2)
  45      continue

          zvol    = zvol+(kvol(ivol)-kvol(ivol-1))*zmax/kmax
          rhochao = rhochar
          ivol    = ivol + 1

      end if

      if(yfrac .le. 1.d-3) goto 50

      goto 40

  50  continue

c---- volatiles are released in volume 2
      qfrac(2) = qfrac(2)+qvol/qfurn


 100  format(//,5x,a,1x,1pe10.3,1x,a)

      end


      subroutine compsn
c-----------------------------------------------------------------c
c     SUBROUTINE COMPSN                                           c
c-----------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- fuel heating value
      hv    = hhv*(1.-aloss(1)-aloss(2)-aloss(3))
     1        -fuel(6)*2.417422e+06

c---- fuel flow rate
      flow(1)  = qfurn/hhv

c---- theoretical oxygen/unit mass of fuel
      flowox    = fuel(1)*32./12.+fuel(2)*16./2.+fuel(3)*32./32.
     1            -fuel(5)

c---- wet air flow rate
      flowair   = flowox*(1.+air(4))/((1.-air(3))*air(1))
      flow(2)   = flowair*flow(1)

c---- gas composition:co2,h2o,so2,n2,o2,carbon,ash
      gas(1)    = fuel(1)*(1.-aloss(1))*44./12.
      gas(2)    = fuel(2)*18./2.+fuel(6)+flowair*air(3)
      gas(3)    = fuel(3)*64./32.
      gas(4)    = fuel(4)+flowair*(1.-air(3))*air(2)
      gas(5)    = flowox*air(4)+aloss(1)*fuel(1)*32./12.
      gas(6)    = aloss(1)*fuel(1)
```

```
      gas(7)    = fuel(7)
      t1        = gas(1)+gas(2)+gas(3)+gas(4)+gas(5)+gas(6)+gas(7)
      do 10 ig = 1, 7
         gas(ig) = gas(ig)/t1
   10 continue

c---- gas recirculation:3-->flue gas, 4-->combustion gas
      flow(3)   = fracr(1)*(flow(1)+flow(2))
      flow(4)   = fracr(2)*(flow(1)+flow(2))

c---- combustion gas molecular weight
      t1        = gas(1)/44.+gas(2)/18.+gas(3)/64.+gas(4)/28.+gas(5)/32.
      amwg      = 1./t1

c---- partial prassures of co2, h20, co
      pco2      = gas(1)/44.*amwg*pgas
      ph2o      = gas(2)/18.*amwg*pgas
      pco       = 0.

c---- ash size distribution: volume 1
      ivol      = 1
      yashp     = gas(7)
      pi43      = 3./(4.*pi)
      rhogr     = pgas*1.01325e+05/(8317.0/amwg*trad(ivol))
      fac       = pi43*rhogr/rhopt(1)*yashp
      pdist(1,1,ivol) = fac*ypt(1,1)/rpt(1,1)**3
      do 20 n  = 2, npt(1)
         pdist(1,n,1) = fac*(ypt(1,n)-ypt(1,n-1))/rpt(1,n)**3
   20 continue

c---- ash size distribution: volumes 2 to nvol
      do 28 ivol = 2, nvol
         rhogr    = pgas*1.01325e+05/(8317.0/amwg*trad(ivol))
         fac      = pi43*rhogr/rhopt(1)*yashp
         pdist(1,1,ivol) = fac*ypt(1,1)/rpt(1,1)**3
         do 25 n  = 2, npt(1)
            pdist(1,n,ivol) = fac*(ypt(1,n)-ypt(1,n-1))/rpt(1,n)**3
   25    continue
   28 continue

c---- soot size distribution: in volume 2 only
      ivol      = 2
      ysoot     = fuel(8)*fuel(10)*flow(1)/(flow(1)+flow(2)+flow(3))
      rhogr     = pgas*1.01325e+05/(8317.0/amwg*trad(ivol))
      fac       = pi43*rhogr/rhopt(2)*ysoot
      pdist(2,1,ivol) = fac*ypt(2,1)/rpt(2,1)**3
      do 30 n  = 2, npt(2)
         pdist(2,n,ivol) = fac*(ypt(2,n)-ypt(2,n-1))/rpt(2,n)**3
   30 continue

c---- char size distribution
      ivol      = 2
      ychar     = fuel(9)*flow(1)/(flow(1)+flow(2)+flow(3))
      rhogr     = pgas*1.01325e+05/(8317.0/amwg*trad(ivol))
      fac       = pi43*rhogr/rhopt(3)*ychar
      pdist(3,1,ivol) = fac*ypt(3,1)/rpt(3,1)**3
      do 40 n  = 2, npt(3)
         pdist(3,n,ivol) = fac*(ypt(3,n)-ypt(3,n-1))/rpt(3,n)**3
   40 continue


      end

      subroutine conduc(nspe,x,t,akg)
```

```
c-----------------------------------------------------------------------c
c     SUBROUTINE CONDUC                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      parameter (nsp=5)

      dimension cond(nsp), cp(nsp) , visc(nsp), x(nspe)

      common /critc/ amw(nsp), tb (nsp), tc  (nsp), pc (nsp), vc(nsp) ,
     1               ome(nsp), dip(nsp)
      common /heatc/ acp(nsp), bcp(nsp), ccp (nsp), dcp(nsp)

      ru  = 8.314

c---  specific heat
      do 10 i=1,nspe
         cp(i) = acp(i) +bcp(i)*t + ccp(i)*t*t + dcp(i)*t**3
  10  continue


c---  viscosity of individual species
      call viscos(nspe,x,t,visc,amug)

c---  thermal conductivity of individual species in terms of viscosity

      do 20 i = 1, nspe

         cv   = cp(i) - ru
         alpa = cv/ru-3./2.

         if(dip(i) .eq. 0.0) then
            beta = 0.762-0.7109*ome(i)+1.3168*ome(i)**2
         else
            beta = 0.758
         end if

         z    = 2. + 10.5*(t/tc(i))**2
         psi  = 1. + alpa*(0.215+0.28288*alpa-1.061*beta+0.26665*z)
     @          /(0.6366+beta*z+1.061*alpa*beta)
         cond(i)= 3750.*ru/amw(i)*psi*visc(i)

  20 continue


c--   thermal conductivity of gas mixture
      akg = 0.0

      do 40 i = 1, nspe
         sum2 = 0.0
         do 30 j = 1, nspe
            aij  = (1.+sqrt(visc(i)/visc(j))
     @               *(amw(j)/amw(i))**0.25)**2
     @              /sqrt(8.*(1.+amw(i)/amw(j)))
            sum2 = sum2 + x(j)*aij

 30      continue
         akg = akg + x(i)*cond(i)/sum2

 40   continue


      end
```

```
      subroutine diffus(n,nspe,x,t,p,dv)
c-----------------------------------------------------------------------c
c     SUBROUTINE DIFFUS                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)

      dimension x(nspe)
      parameter (nsp=5)
      common /critc/ amw(nsp), tb (nsp), tc  (nsp), pc(nsp) , vc(nsp) ,
     1               ome(nsp), dip(nsp)

      vb   = 0.285*vc(n)**1.048
      dipa = 1.94d+03*dip(n)**2/(vb*tb(n))
      eka  = 1.18*(1.0+1.3*dipa**2)*tb(n)
      siga =(1.585*vb/(1.0+1.3*dipa**2))**(1./3)
      amwa = amw(n)
      suml = 0.0

      do 10 i = 1, nspe
         if(i.eq.n) goto 10
         vb  = 0.285*vc(i)**1.048
         dipi = 1.94d+03*dip(i)**2/(vb*tb(i))
         eki  = 1.18*(1.0+1.3*dipi**2)*tb(i)
         sigi =(1.585*vb/(1.0+1.3*dipi**2))**(1./3.)
         ek   = sqrt(eka*eki)
         sig  = sqrt(siga*sigi)
         tsta = t/ek
         am   = 2.*amwa*amw(i)/(amwa+amw(i))
         dipm = sqrt(dipa*dipi)
         omega= 1.06036/tsta**0.1561+0.1930*exp(-0.47635*tsta)
     1         +1.03587*exp(-1.52996*tsta)
     2         +1.76474*exp(-3.9411*tsta)
     2         +0.19*dipm**2/tsta

c--      binary diffusion coefficient(m**2/s)
         dai = 2.66d-07*t**1.5/(p*am*sig**2*omega)
         suml = suml +x(i)/dai
   10 continue

c--   diffusion coefficient of species n in gas mixture
      dv = 1./suml

      end


      subroutine diverq(ifrq)
c-----------------------------------------------------------------------c
c     SUBROUTINE  DIVERQ(ifrq)                                          c
c-----------------------------------------------------------------------c


      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

      if (ifrq .eq. 1) then
         do 10 k = 1, kmax
         do 10 j = 1, jmax
         do 10 i = 1, imax
            divq(i,j,k) = 0.0
   10    continue
      end if

      do 20 k = 1,kmax
```

```
      do 20 j = 1,jmax
      do 20 i = 1,imax
         divq(i,j,k) = divq(i,j,k)
     1          +dfrq(ifrq)*4.*pi*(1.-omeg(k,ifrq))*beta(k,ifrq)*
     2          (ebg(i,j,k)-(gm(i,j,k,ifrq)+gs(i,j,k,ifrq))/(4.*pi))
   20 continue


      end


      subroutine energy(itry)
c-----------------------------------------------------------------------c
c     SUBROUTINE ENERGY                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- fuel/air/gas enthalpy at inlet temperature
      if (itry .eq. 1) then
         hfag(1)  = hfuel(temp(1),cp)
         hfag(2)  = hair(temp(2),air,cp)
         hfag(3)  = hgas(temp(3),gas,cp)
      end if

c---- gas enthalpy
      do 10 ivol = 1, nvol
         enth(ivol) = hgas(tg(ivol),gas,cp)
   10 continue

c---- integrate divq(i,j,k) over control volume
      do 50 ivol = 1, nvol
         divqv(ivol) = 0.
         if (ivol .eq. 1) then
            klow = 1
         else
            klow = kvol(ivol-1) + 1
         end if
         khigh   = kvol(ivol)
         do 40 i = 1,imax
            do 30 j = 1,jmax
               do 20 k = klow, khigh
                  vol   = dx(i)*dy(j)*dz(k)
                  divqv(ivol) = divqv(ivol) + divq(i,j,k)*vol
  20          continue
  30       continue
  40    continue
  50 continue

c---  convective heat transfer
      do 55 ivol = 1, nvol
         qconv(ivol) = xwall(ivol)*hcoef(ivol)*( tg(ivol) - txm )
     1               + xwall(ivol)*hcoef(ivol)*( tg(ivol) - txp )
     2               + ywall(ivol)*hcoef(ivol)*( tg(ivol) - tym )
     3               + ywall(ivol)*hcoef(ivol)*( tg(ivol) - typ )
  55 continue

c---- residual enthalpy in volume 1
      hres(1)  = flow(3)*(hfag(3)-enth(1))+flow(4)*(enth(2)-enth(1))
     1         - qconv(1)  - divqv(1)

c---- residual enthalpy in volume 2
      hres(2)  = flow(1)*(hfag(1)+hv*qfrac(2)-enth(2))
```

```
     1          +flow(2)*(hfag(2)-enth(2))
     2          +(flow(3)+flow(4))*(enth(1)-enth(2))
     3         - qconv(2)  - divqv(2)

c---- residual enthalpy in volumes 3 through nvol
      sumf     = flow(1)+flow(2)+flow(3)
      do 60 ivol = 3, nvol
         hres(ivol) = flow(1)*hv*qfrac(ivol)
     1               +sumf*(enth(ivol-1)-enth(ivol))
     2               -qconv(ivol)  - divqv(ivol)

   60 continue

      end


      function frac(v1,v2)
c-----------------------------------------------------------------------c
c     FUNCTION FRAC                                                     c
c-----------------------------------------------------------------------c

      implicit real*8(a-h,o-z)
      fct(n,a,c) = c**n/n**4*((a*n)**3 + 3.*a*a*n*n + 6.*a*n + 6.)

      sum1 = 1./0.153989734
      if( v1 .eq. 0.0) goto 20

      sum1 = 0.0
      cc   = exp(-v1)
      do 10 n = 1, 20
         t1 = fct(n,v1,cc)
         sum1 = sum1 + t1
         if(t1 .lt. 1.d-04) goto 20
  10  continue

  20  continue
      sum2 = 0.0
      if( v2 .gt. 1.d6) goto 40

      cc   = exp(-v2)
      do 30 n = 1, 20
         t1 = fct(n,v2,cc)
         sum2 = sum2 + t1
         if(t1 .lt. 1.d-04) goto 40
  30  continue

  40  continue
      frac = 0.153989734*(sum1 - sum2)

      end


      subroutine grid
c-----------------------------------------------------------------------c
c     SUBROUTINE GRID                                                   c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- generate the grid system (nonuniform)
      do 10 i = 1,imax
         dx(i) = xmax/imax
```

```
   10 continue

      do 20 j = 1,jmax
         dy(j) = ymax/jmax
   20 continue

      do 30 k = 1,kmax
         dz(k) = zmax/kmax
   30 continue

c---- position of each cell

      px(1) = 0.5*dx(1)
      do 15 i = 2,imax
         px(i) = px(i-1)+(dx(i-1)+dx(i))/2.
   15 continue

      py(1) = 0.5*dy(1)
      do 25 j = 2,jmax
         py(j) = py(j-1)+(dy(j-1)+dy(j))/2.
   25 continue

      pz(1) = 0.5*dz(1)
      do 35 k = 2,kmax
         pz(k) = pz(k-1)+(dz(k-1)+dz(k))/2.
   35 continue

      do 40 k = 1,kmax
         if(k.ne.kmax) delzp(k) = 0.5*(dz(k)+dz(k+1))
         if(k.ne.1)    delzm(k) = 0.5*(dz(k)+dz(k-1))
         if(k.eq.kmax) delzp(k) = dz(kmax)
         if(k.eq.1)    delzm(k) = dz(1)
   40 continue

      do 50 j = 1,jmax
         if(j.ne.jmax) delyp(j) = 0.5*(dy(j)+dy(j+1))
         if(j.ne.1)    delym(j) = 0.5*(dy(j)+dy(j-1))
         if(j.eq.jmax) delyp(j) = dy(jmax)
         if(j.eq.1)    delym(j) = dy(1)
   50 continue

      do 60 i = 1,imax
         if(i.ne.imax) delxp(i) = 0.5*(dx(i)+dx(i+1))
         if(i.ne.1)    delxm(i) = 0.5*(dx(i)+dx(i-1))
         if(i.eq.imax) delxp(i) = dx(imax)
         if(i.eq.1)    delxm(i) = dx(1)
   60 continue

c---- surface areas

      do 62 ivol = 1, nvol
         xwall(ivol) = 0.0
         ywall(ivol) = 0.0
  62  continue

      do 80 j = 1, jmax
         ks   = 1
         ivol = 0

  65     ivol = ivol + 1
         do 70 k = ks, kvol(ivol)
            xwall(ivol) = xwall(ivol) + dy(j)*dz(k)
  70     continue
         ks = kvol(ivol)+1
```

```
         if(ivol .lt. nvol) goto 65

  80  continue


      do 110 i = 1, imax
         ks   = 1
         ivol = 0

  90     ivol = ivol + 1
         do 100 k = ks, kvol(ivol)
            ywall(ivol) = ywall(ivol) + dx(i)*dz(k)
 100     continue
         ks = kvol(ivol)+1
         if(ivol .lt. nvol) goto 90

 110  continue

      zwall = 0.0
      do 140 i = 1, imax
      do 140 j = 1, jmax
         zwall = zwall + dx(i)*dy(j)
 140  continue


      end


      function hair(t,air,cp)
c-------------------------------------------------------------c
c     FUNCTION HAIR                                           c
c-------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      dimension air(4), amw(8), comp(3), cp(8,7,2), index(3)
      data amw /
     1   0.044011,  0.018016,  0.064000,  0.028016,  0.032000,
     2   0.012000,  0.012000,  0.012000   /

c---- oxygen
      index(1) = 5
      comp(1)  = (1.-air(3))*air(1)

c---- nitrogen
      index(2) = 4
      comp(2)  = (1.-air(3))*air(2)

c---- moisture
      index(3) = 2
      comp(3)  = air(3)

c---- air enthalpy
      hair     = 0.
      tr       = 298.0
      if (t .gt. 1000.) then
         n2 = 1
      else
         n2 = 2
      end if
      do 10 is = 1, 3
         n     = index(is)
         hr    = ((((cp(n,5,2)/5.)*tr+cp(n,4,2)/4.)*tr
     1              +cp(n,3,2)/3.)*tr+cp(n,2,2)/2.)*tr
     2              +cp(n,1,2)+cp(n,6,2)/tr
```

```
         h      = ((((cp(n,5,n2)/5.)*t+cp(n,4,n2)/4.)*t
     1               +cp(n,3,n2)/3.)*t+cp(n,2,n2)/2.)*t
     2               +cp(n,1,n2)+cp(n,6,n2)/t
         hg     = 8.317/amw(n) * (t*h -tr*hr)
         hair   = hair+comp(is)*hg
   10 continue

      end


      function hfuel(t,cp)
c-----------------------------------------------------------------------c
c     FUNCTION HFUEL                                                    c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      dimension amw(8), cp(8,7,2)
      data amw /
     1   0.044011,  0.018016,  0.064000,  0.028016,  0.032000,
     2   0.012000,  0.012000,  0.012000   /

c---- fuel sensible enthalpy
      tr     = 298.0
      if (t .gt. 1000.) then
         n2 = 1
      else
         n2 = 2
      end if
      hr     = ((((cp(8,5,2)/5.)*tr+cp(8,4,2)/4.)*tr
     1            +cp(8,3,2)/3.)*tr+cp(8,2,2)/2.)*tr
     2            +cp(8,1,2)+cp(8,6,2)/tr
      h      = ((((cp(8,5,n2)/5.)*t+cp(8,4,n2)/4.)*t
     1            +cp(8,3,n2)/3.)*t+cp(8,2,n2)/2.)*t
     2            +cp(8,1,n2)+cp(8,6,n2)/t
      hfuel = 8.317/amw(8) * (t*h -tr*hr)


      end



      function hgas(t,gas,cp)
c-----------------------------------------------------------------------c
c     FUNCTION HGAS                                                     c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      dimension amw(8), gas(7), cp(8,7,2)
      data amw /
     1   0.044011,  0.018016,  0.064000,  0.028016,  0.032000,
     2   0.012000,  0.012000,  0.012000   /

c---- combustion gas enthalpy
      tr     = 298.0
      if (t .gt. 1000.) then
         n2 = 1
      else
         n2 = 2
      end if
      hgas     = 0.
      do 10 is = 1, 7
         hr     = ((((cp(is,5,2)/5.)*tr+cp(is,4,2)/4.)*tr
     1              +cp(is,3,2)/3.)*tr+cp(is,2,2)/2.)*tr
     2              +cp(is,1,2)+cp(is,6,2)/tr
```

```
        h      = ((((cp(is,5,n2)/5.)*t+cp(is,4,n2)/4.)*t
     1               +cp(is,3,n2)/3.)*t+cp(is,2,n2)/2.)*t
     2               +cp(is,1,n2)+cp(is,6,n2)/t
        hg     = 8.317/amw(is) * (t*h -tr*hr)
        hgas   = hgas+gas(is)*hg
   10 continue

      end


      subroutine init
c-----------------------------------------------------------------------c
c     SUBROUTINE INIT                                                   c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- initialization
      do 20 i = 1, imax
      do 20 j = 1, jmax
      do 20 k = 1, kmax

c----    ebg: Planck function at gas temperature
         ebg(i,j,k) = 0.

c----    qt: total heat flux
         qxmt(j,k) = 0.
         qxpt(j,k) = 0.
         qymt(i,k) = 0.
         qypt(i,k) = 0.
         qzmt(i,j) = 0.
         qzpt(i,j) = 0.

c----    divq: divergence of heat flux
         divq(i,j,k) = 0.

         do 10 ifrq = 1, nfrq

            ebg(i,j,k) = 0.

            ebwxm(j,k,ifrq) = 0.
            ebwxp(j,k,ifrq) = 0.
            ebwym(i,k,ifrq) = 0.
            ebwyp(i,k,ifrq) = 0.
            ebwzm(i,j,ifrq) = 0.
            ebwzp(i,j,ifrq) = 0.

c----       q: spectral heat flux
            qxm(j,k,ifrq)   = 0.
            qxp(j,k,ifrq)   = 0.
            qym(i,k,ifrq)   = 0.
            qyp(i,k,ifrq)   = 0.
            qzm(i,j,ifrq)   = 0.
            qzp(i,j,ifrq)   = 0.

c----       gm: medium-originated irradiation
            gm(i,j,k,ifrq)  = 0.

c----       gs: surface-originated irradiation
            gs(i,j,k,ifrq)  = 0.

   10    continue
```

```
   20 continue

c---- initialize imax2, jmax2, kmax2
      imax2   = imax + 2
      jmax2   = jmax + 2
      kmax2   = kmax + 2

      do 30 mu = 1, mumax
      do 30 k  = 1, kmax2
      do 30 j  = 1, jmax2
      do 30 i  = 1, imax2
         ri(i,j,k,mu) = 0.0
   30 continue


c---- Planck function at wall temperature
      call planckw

c---- mean beam length
      beam = 1.7*xmax*ymax*zmax/(xmax*ymax+xmax*zmax+ymax*zmax)

c---- temperature limits for non-linear equation solver
      do 40  ivol  = 1, nvol
         tg(ivol)  = trad(ivol)
         tgl(ivol) = 273.0
         tgu(ivol) = 3500.0
   40 continue

      end


      subroutine planckg(ifrq)
c-----------------------------------------------------------------------c
c     SUBROUTINE PLANCKG(ifrq)                                          c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- radiation constants
      data      sig,       c1     ,   c2
     1  /   5.669e-08, 1.1908e-08, 1.43883 /

c---- planck function at gas temperature
      do 10 k = 1,kmax
      do 10 j = 1,jmax
      do 10 i = 1,imax
         ebg(i,j,k) = sig*t(i,j,k)**4/pi
  10  continue

      if(nfrq .eq. 1) return

c---- spectral calculation
      dfreq = dfrq(ifrq)
      v1    = c2*(frq(ifrq) - 0.5*dfreq)
      v2    = c2*(frq(ifrq) + 0.5*dfreq)

      if( ifrq .eq. nfrq) then
          v2 = 1.d+20
      else if (ifrq .eq. 1) then
          v1 = 0.d0
      end if

      do 20 k = 1, kmax
```

```
      do 20 j = 1, jmax
      do 20 i = 1, imax
         f1          = v1/t(i,j,k)
         f2          = v2/t(i,j,k)
         ebg(i,j,k) = frac(f1,f2)*ebg(i,j,k)/dfreq
   20 continue

      end


      subroutine planckw
c-----------------------------------------------------------------------c
c     SUBROUTINE PLANCKW                                                c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- radiation constants
      data      sig,       c1     ,    c2
     1  /   5.669e-08, 1.1908e-08, 1.43883 /

c---- planck function at wall temperatures
      do 20 j = 1, jmax
      do 20 i = 1, imax
         ebwzp(i,j,1) = sig*tzp**4/pi
         ezp          = ebwzp(i,j,1)
   20 continue

      do 21 j = 1, jmax
      do 21 i = 1, imax
         ebwzm(i,j,1) = sig*tzm**4/pi
         ezp          = ebwzp(i,j,1)
   21 continue

      do 22 k = 1, kmax
      do 22 i = 1, imax
         ebwyp(i,k,1) = sig*typ**4/pi
         eyp          = ebwyp(i,k,1)
   22 continue

      do 23 k = 1, kmax
      do 23 i = 1, imax
         ebwym(i,k,1) = sig*tym**4/pi
         eym          =  ebwym(i,k,1)
   23 continue

      do 24 k = 1, kmax
      do 24 j = 1, jmax
         ebwxp(j,k,1) = sig*txp**4/pi
         exp          = ebwxp(j,k,1)
   24 continue

      do 25 k = 1, kmax
      do 25 j = 1, jmax
         ebwxm(j,k,1) = sig*txm**4/pi
         exm          = ebwxm(j,k,1)
   25 continue
      if( nfrq .eq. 1) return

c---- spectral calculation
      do 130 ifrq = 1, nfrq
         dfreq = dfrq(ifrq)
         v1 = c2*(frq(ifrq) - 0.5*dfreq)
```

```
        v2 = c2*(frq(ifrq) + 0.5*dfreq)

        if( ifrq .eq. nfrq) then
            v2 = 1.d+20
        else if (ifrq .eq. 1) then
            v1 = 0.d0
        end if

        do 30 j = 1, jmax
        do 30 i = 1, imax
           f1 = v1/tzp
           f2 = v2/tzp
           ebwzp(i,j,ifrq) = frac(f1,f2)*ezp/dfreq
   30   continue

        do 31 j = 1, jmax
        do 31 i = 1, imax
           f1 = v1/tzm
           f2 = v2/tzm
           ebwzm(i,j,ifrq) =  frac(f1,f2)*ezm/dfreq
   31   continue

        do 32 k = 1, kmax
        do 32 i = 1, imax
           f1 = v1/typ
           f2 = v2/typ
           ebwyp(i,k,ifrq) = frac(f1,f2)*eyp/dfreq
   32   continue

        do 33 k = 1, kmax
        do 33 i = 1, imax
           f1 = v1/tym
           f2 = v2/tym
           ebwym(i,k,ifrq) = frac(f1,f2)*eym/dfreq
   33   continue

        do 34 k = 1, kmax
        do 34 j = 1, jmax
           f1 = v1/txp
           f2 = v2/txp
           ebwxp(j,k,ifrq) = frac(f1,f2)*exp/dfreq
   34   continue

        do 35 k = 1, kmax
        do 35 j = 1, jmax
           f1 = v1/txm
           f2 = v2/txm
           ebwxm(j,k,ifrq) = frac(f1,f2)*exm/dfreq
   35   continue
  130 continue

      end


      subroutine qflux
c-----------------------------------------------------------------------c
c     SUBROUTINE QFLUX                                                  c
c-------------------------------- ------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- this subroutine calculates  heat flux contributed by the
c---- radiation originated from the gas medium and adds it to the
```

```
c---- cntribution from the surface orginated radiation if the
c---- MDA is the soulution method.

      do 40 ifrq=1 , nfrq

         if(is4(ifrq) .eq. 1 .or. ibeta(ifrq) .eq. 0) goto 40

         do 10 j = 1 , jmax
         do 10 i = 1 , imax
            upzo = (2./(3.*beta1(1,ifrq)))*(2./ew(1,ifrq)-1.)/dz(1)-0.5
            dozo = (2./(3.*beta1(1,ifrq)))*(2./ew(1,ifrq)-1.)/dz(1)+0.5
            alzo = upzo/dozo
            bezo = 4.*pi*ip1(ifrq)*ebwzm(i,j,ifrq)/dozo

            gazo = (2./(3.*beta1(1,ifrq)))
     1            *(2./ew(1,ifrq)-1.)*beta(1,ifrq)*a1(1,ifrq)
     1            *omeg(1,ifrq)*qzm(i,j,ifrq)/(dozo*dx(i)*dy(j))

            gij0   = alzo*gm(i,j,1,ifrq)+bezo+gazo
            gijhlf = 0.5*(gij0+gm(i,j,1,ifrq))

            qzm(i,j,ifrq) = qzm(i,j,ifrq)
     1                     -dx(i)*dy(j)*(4.*pi*ip1(ifrq)*ebwzm(i,j,ifrq)
     1                     -gijhlf)/(2.*(2./ew(1,ifrq)-1.))

            upzmax = (2./(3.*beta1(kmax,ifrq)))
     1               *(2./ew(kmax,ifrq)-1.)/dz(kmax)-0.5
            dozmax = (2./(3.*beta1(kmax,ifrq)))
     1               *(2./ew(kmax,ifrq)-1.)/dz(kmax)+0.5
            alzmax = upzmax/dozmax
            bezmax = 4.*pi*ip1(ifrq)*ebwzp(i,j,ifrq)/dozmax

            gazmax = (2./(3.*beta1(kmax,ifrq)))
     1               *(2./ew(kmax,ifrq)-1.)*beta(kmax,ifrq)
     1               *a1(kmax,ifrq)
     1               *omeg(kmax,ifrq)*qzp(i,j,ifrq)/(dozmax*dx(i)*dy(j))

            gijkmxp = alzmax*gm(i,j,kmax,ifrq)+bezmax+gazmax
            gijkmxh = 0.5*(gijkmxp+gm(i,j,kmax,ifrq))

            qzp(i,j,ifrq) = qzp(i,j,ifrq)
     1                     -dx(i)*dy(j)*(4.*pi*ip1(ifrq)*ebwzp(i,j,ifrq)
     1                     -gijkmxh)/(2.*(2./ew(kmax,ifrq)-1.))
10      continue

         do 20 k = 1 , kmax
         do 20 i = 1 , imax
            upyo = (2./(3.*beta1(k,ifrq)))*(2./ew(k,ifrq)-1.)/dy(1)-0.5
            doyo = (2./(3.*beta1(k,ifrq)))*(2./ew(k,ifrq)-1.)/dy(1)+0.5
            alyo = upyo/doyo

            beyo = 4.*pi*ip1(ifrq)*ebwym(i,k,ifrq)/doyo
            gayo = (2./(3.*beta1(k,ifrq)))*(2./ew(k,ifrq)-1.)
     1            *beta(k,ifrq)*a1(k,ifrq)
     1            *omeg(k,ifrq)*qym(i,k,ifrq)/(doyo*dx(i)*dz(k))

            gi0k    = alyo*gm(i,1,k,ifrq)+beyo+gayo
            gihalfk = 0.5*(gi0k+gm(i,1,k,ifrq))

            qym(i,k,ifrq) = qym(i,k,ifrq)
     1                    -dx(i)*dz(k)*(4.*pi*ip1(ifrq)*ebwym(i,k,ifrq)
     1                    -gihalfk)/(2.*(2./ew(k,ifrq)-1.))

            upymax = (2./(3.*beta1(k,ifrq)))
```

```
     1                *(2./ew(k,ifrq)-1.)/dy(jmax)-0.5
            doymax = (2./(3.*beta1(k,ifrq)))
     1                *(2./ew(k,ifrq)-1.)/dy(jmax)+0.5
            alymax = upymax/doymax

            beymax = 4.*pi*ipl(ifrq)*ebwyp(i,k,ifrq)/doymax
            gaymax = (2./(3.*beta1(k,ifrq)))
     1                *(2./ew(k,ifrq)-1.)*beta(k,ifrq)*al(k,ifrq)
     1                *omeg(k,ifrq)*qyp(i,k,ifrq)/(doymax*dx(i)*dz(k))

            gijmxpk = alymax*gm(i,jmax,k,ifrq)+beymax+gaymax
            gijmxhk = 0.5*(gijmxpk+gm(i,jmax,k,ifrq))

            qyp(i,k,ifrq) = qyp(i,k,ifrq)
     1                     -dx(i)*dz(k)*(4.*pi*ipl(ifrq)*ebwyp(i,k,ifrq)
     1                     -gijmxhk)/(2.*(2./ew(k,ifrq)-1.))
   20     continue

          do 30 k = 1 , kmax
          do 30 j = 1 , jmax
            upxo = (2./(3.*beta1(k,ifrq)))*(2./ew(k,ifrq)-1.)/dx(1)-0.5
            doxo = (2./(3.*beta1(k,ifrq)))*(2./ew(k,ifrq)-1.)/dx(1)+0.5
            alxo = upxo/doxo

            bexo = 4.*pi*ipl(ifrq)*ebwxm(j,k,ifrq)/doxo
            gaxo = (2./(3.*beta1(k,ifrq)))
     1            *(2./ew(k,ifrq)-1.)*beta(k,ifrq)*al(k,ifrq)
     1            *omeg(k,ifrq)*qxm(j,k,ifrq)/(doxo*dy(j)*dz(k))

            g0jk    = alxo*gm(1,j,k,ifrq)+bexo+gaxo
            ghalfjk = 0.5*(g0jk+gm(1,j,k,ifrq))

            qxm(j,k,ifrq) = qxm(j,k,ifrq)
     1                     -dy(j)*dz(k)*(4.*pi*ipl(ifrq)*ebwxm(j,k,ifrq)
     1                     -ghalfjk)/(2.*(2./ew(k,ifrq)-1.))

            upxmax = (2./(3.*beta1(k,ifrq)))
     1              *(2./ew(k,ifrq)-1.)/dx(imax)-0.5
            doxmax = (2./(3.*beta1(k,ifrq)))
     1              *(2./ew(k,ifrq)-1.)/dx(imax)+0.5
            alxmax = upxmax/doxmax

            bexmax = 4.*pi*ipl(ifrq)*ebwxp(j,k,ifrq)/doxmax
            gaxmax = (2./(3.*beta1(k,ifrq)))
     1              *(2./ew(k,ifrq)-1.)*beta(k,ifrq)*al(k,ifrq)
     1              *omeg(k,ifrq)*qxp(j,k,ifrq)/(doxmax*dy(j)*dz(k))

            gimxpjk = alxmax*gm(imax,j,k,ifrq)+bexmax+gaxmax
            gimxhjk = 0.5*(gimxpjk+gm(imax,j,k,ifrq))

            qxp(j,k,ifrq) = qxp(j,k,ifrq)
     1                    -dy(j)*dz(k)*(4.*pi*ipl(ifrq)*ebwxp(j,k,ifrq)
     1                    -gimxhjk)/(2.*(2./ew(k,ifrq)-1.))
   30     continue

   40  continue

c---   add contributions from all frequencies.

       do 80 ifrq = 1 , nfrq

          do 50 i = 1 , imax
          do 50 j = 1 , jmax
             qzpt(i,j) = qzpt(i,j)+qzp(i,j,ifrq)*dfrq(ifrq)
```

```
            qzmt(i,j) = qzmt(i,j)+qzm(i,j,ifrq)*dfrq(ifrq)
 50      continue

         do 60 i = 1 , imax
         do 60 k = 1 , kmax
            qypt(i,k) = qypt(i,k)+qyp(i,k,ifrq)*dfrq(ifrq)
            qymt(i,k) = qymt(i,k)+qym(i,k,ifrq)*dfrq(ifrq)
 60      continue

         do 70 k = 1 , kmax
         do 70 j = 1 , jmax
            qxpt(j,k) = qxpt(j,k)+qxp(j,k,ifrq)*dfrq(ifrq)
            qxmt(j,k) = qxmt(j,k)+qxm(j,k,ifrq)*dfrq(ifrq)
 70      continue

 80   continue


      end


      subroutine sn(ifrq)
c-----------------------------------------------------------------------c
c     SUBROUTINE SN(ifrq)                                               c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'
      dimension
     1 ebwxml(jmx2,kmx2),  ebwxpl(jmx2,kmx2),  ebwyml(imx2,kmx2),
     2 ebwypl(imx2,kmx2),  ebwzml(imx2,jmx2),  ebwzpl(imx2,jmx2),
     3 error(mumax)      ,  ewl(kmx2)         ,
     3 riyr(imx2)        ,  rizr(imx2,jmx2)   ,  riold(imx2,jmx2,kmx2)

c---- initialize arrays
      do 10 i = 1, imax2
      do 10 j = 1, jmax2
      do 10 k = 1, kmax2
         ebwxml(j,k) = ebwxm(1,1,ifrq)
         ebwxpl(j,k) = ebwxp(1,1,ifrq)
         ebwyml(i,k) = ebwym(1,1,ifrq)
         ebwypl(i,k) = ebwyp(1,1,ifrq)
         ebwzml(i,j) = ebwzm(1,1,ifrq)
         ebwzpl(i,j) = ebwzp(1,1,ifrq)
         riold(i,j,k)= 0.0
   10 continue

c---- initialize ewl arrays
      ewl(1)        = ew(1,ifrq)
      ewl(kmax2)    = ew(kmax,ifrq)
      do 20 k = 1, kmax
         ewl(k+1)   = ew(k,ifrq)
   20 continue

c---- interpolation parameter alph
      alpha1 = 1./alpha

c---- start of iteration
      iter = 0
  999 iter = iter+1

c---- negative intensity counter
      nzero = 0
```

```
      do 260 mu = 1, mumax

      if(iter .gt. 1) then
         do 25 i = 1, imax2
         do 25 j = 1, jmax2
         do 25 k = 1, kmax2
            riold(i,j,k) = ri(i,j,k,mu)
  25     continue
      end if

c---- radiation intensity leaving x=0 wall
      if (ixnu(mu).gt.0) then
         do 40 k = 1,kmax2
         do 40 j = 1,jmax2
            sum=0.0
            do 30 imu = 1, mumax
               if (ixnu(imu) .gt. 0) go to 30
               sum = sum+wt(imu)*abs(xnu(imu))*ri(1,j,k,imu)
  30        continue
            ri(1,j,k,mu) = ewl(k)*ebwxml(j,k)
     1                        +(1.-ewl(k))*sum/pi
  40    continue
      end if

c---- radiation intensity leaving  y=0 wall
      if (iyxi(mu) .gt. 0) then
         do 60 k = 1, kmax2
         do 60 i = 1, imax2
            sum    = 0.0
            do 50 imu = 1, mumax
               if (iyxi(imu) .ge. 0) go to 50
               sum = sum+wt(imu)*abs(yxi(imu))*ri(i,1,k,imu)
  50        continue
            ri(i,1,k,mu) = ewl(k)*ebwyml(i,k)
     1                        +(1.-ewl(k))*sum/pi
  60    continue
      end if

c---- radiation intensity leaving z=0 wall
      if (izet(mu) .gt. 0) then
         do 80 j = 1, jmax2
         do 80 i = 1, imax2
            sum    = 0.0
            do 70 imu=1,mumax
               if (izet(imu) .ge. 0) go to 70
               sum = sum+wt(imu)*abs(zet(imu))*ri(i,j,1,imu)
  70        continue
            ri(i,j,1,mu) = ewl(1)*ebwzml(i,j)
     1                        +(1.-ewl(1))*sum/pi
  80    continue
      end if

c---- radiation intensity leaving x=xmax wall
      if (ixnu(mu) .lt. 0) then
         do 100 k = 1, kmax2
         do 100 j = 1, jmax2
            sum    = 0.0
            do 90 imu = 1, mumax
               if (ixnu(imu) .lt. 0) go to 90
               sum = sum+wt(imu)*abs(xnu(imu))*ri(imax2,j,k,imu)
  90        continue
            ri(imax2,j,k,mu) = ewl(k)*ebwxpl(j,k)
     1                           +(1.-ewl(k))*sum/pi
 100    continue
```

```
      end if

c---- radiation intensity leaving y=ymax wall
      if (iyxi(mu) .lt. 0) then
         do 120 k = 1, kmax2
         do 120 i = 1, imax2
            sum    = 0.0
            do 110 imu = 1, mumax
               if (iyxi(imu) .lt. 0) go to 110
               sum = sum+wt(imu)*abs(yxi(imu))*ri(i,jmax2,k,imu)
  110       continue
            ri(i,jmax2,k,mu) = ewl(k)*ebwypl(i,k)
     1                          +(1.-ewl(k))*sum/pi
  120    continue
      end if

c---- radiation intensity leaving z=zmax wall
      if (izet(mu) .lt. 0) then
         do 140 j = 1, jmax2
         do 140 i = 1, imax2
            sum    = 0.0
            do 130 imu = 1, mumax
               if(izet(imu) .lt. 0) go to 130
               sum = sum+wt(imu)*abs(zet(imu))*ri(i,j,kmax2,imu)
  130       continue
            ri(i,j,kmax2,mu) = ewl(kmax2)*ebwzpl(i,j)
     1                          +(1.-ewl(kmax2))*sum/pi
  140    continue
      end if

c---- radiation intensity at x-y wall
      do 150 i = 2, imax+1
      do 150 j = 2, jmax+1
         if(izet(mu) .gt. 0) then
            rizr(i,j) = ri(i,j,1,mu)
         else
            rizr(i,j) = ri(i,j,kmax2,mu)
         end if
  150 continue

      do 230 kk = 2, kmax+1
         if (izet(mu) .gt. 0) then
            k = kk
         else
            k = kmax+3-kk
         end if

c----    radiation intensity at x-z wall
         do 160 i = 2, imax+1
            if(iyxi(mu) .gt. 0) then
               riyr(i) = ri(i,1,k,mu)
            else
               riyr(i) = ri(i,jmax2,k,mu)
            end if
  160    continue

      do 200 jj = 2, jmax+1
         if (iyxi(mu) .gt. 0) then
            j = jj
         else
            j = jmax+3-jj
         end if

c----    radiation intensity at y-z wall
```

```
         if(ixnu(mu) .gt. 0) then
            rixr = ri(1,j,k,mu)
         else
            rixr = ri(imax2,j,k,mu)
         end if

      do 180 ii = 2, imax+1
         if (ixnu(mu) .gt. 0) then
            i = ii
         else
            i = imax+3-ii
         end if

         aa  = dy(j-1)*dz(k-1)
         ba  = dx(i-1)*dz(k-1)
         ca  = dx(i-1)*dy(j-1)
         vol = dx(i-1)*dy(j-1)*dz(k-1)

c---     check numerical stability
         rixr      = max(0.d0,rixr)
         riyr(i)   = max(0.d0,riyr(i))
         rizr(i,j) = max(0.d0,rizr(i,j))
         if (rixr*riyr(i)*rizr(i,j) .eq. 0.0) then
            nzero = nzero +1
         end if

         den = abs(xnu(mu))*aa+abs(yxi(mu))*ba+abs(zet(mu))*ca
     1       + alpha*beta(k-1,ifrq)*vol


         rnum = abs(xnu(mu))*aa*rixr+abs(yxi(mu))*ba*riyr(i)
     1        + abs(zet(mu))*ca*rizr(i,j)

c---     add radiation source term
         if(is4(ifrq) .eq. 1) then

            sum=0.0
            do 170 imu=1,mumax
               phase=1.+al(k-1,ifrq)*(xnu(mu)*xnu(imu)
     1              +yxi(mu)*yxi(imu)+zet(mu)*zet(imu))
               sum=sum+wt(imu)*phase*ri(i,j,k,imu)
  170       continue

            scat = alpha*vol*omeg(k-1,ifrq)*beta(k-1,ifrq)*sum/(4.*pi)

            rnum = rnum + alpha*vol*(1.-omeg(k-1,ifrq))*beta(k-1,ifrq)
     1            *ebg(i-1,j-1,k-1) + scat
         end if

         ri(i,j,k,mu)=rnum/den

c----    radiation intensity at face (x+dx/2,y,z)
         rixr = alpha1*ri(i,j,k,mu) - (alpha1-1.)*rixr

  180    continue

c----    radiation intensity at face (x,y+dy/2,z)
         do 190 i = 2, imax+1
            riyr(i) = alpha1*ri(i,j,k,mu) - (alpha1-1.)*riyr(i)
  190    continue

c----    radiation intensity arriving at x = 0 & x = xmax walls
         if (ixnu(mu) .gt. 0) then
             ri(imax+2,j,k,mu) = rixr
```

```
         else
             ri(1,j,k,mu) = rixr
         end if

  200    continue

c----    radiation intensity at  face (x,y,z+dz/2)
         do 210 i = 2, imax+1
         do 210 j = 2, jmax+1
            rizr(i,j) = alpha1*ri(i,j,k,mu)-(alpha1-1.)*rizr(i,j)
  210    continue

c----    radiation intensity arriving at y = 0 & y = ymax walls
         do 220 i = 2, imax+1
            if (iyxi(mu) .gt. 0) then
               ri(i,jmax+2,k,mu) = riyr(i)
            else
               ri(i,1,k,mu) = riyr(i)
            end if
  220    continue

  230    continue

c----    radiation intensity arriving at z = 0 & z = zmax walls
         do 240 j = 2, jmax+1
         do 240 i = 2, imax+1
            if (izet(mu) .gt. 0) then
                ri(i,j,kmax+2,mu) = rizr(i,j)
             else
                ri(i,j,1,mu) = rizr(i,j)
            end if
  240    continue
         error(mu) = 0.0
         do 250 k  = 2, kmax+1
         do 250 j  = 2, jmax+1
         do 250 i  = 2, imax+1
            absri  = abs(ri(i,j,k,mu))
            if (absri .eq. 0.0) goto 250
            error(mu) = error(mu)+abs(ri(i,j,k,mu)-riold(i,j,k))/absri
  250    continue

  260 continue

c---- convergence test
      sum = 0.0
      do 270 mu = 1, mumax
         sum = sum + error(mu)
 270  continue
      sum = sum/(imax*jmax*kmax*mumax)

      if(sum .gt. 2.d-07 .and. iter .lt. niterj) go to 999

c---- print non-convergence

      if (iter .ge. niterj ) then
         write(6,*) 'no convergence in S4 for ifrq = ',ifrq
      end if

c---- calculate (Gs) by summing over discrete angles
      do 300 k = 1, kmax
      do 300 j = 1, jmax
      do 300 i = 1, imax

         gs(i,j,k,ifrq)  = 0.0
```

```
         do 280 mu = 1, mumax
            gs(i,j,k,ifrq) = gs(i,j,k,ifrq)+wt(mu)*ri(i+1,j+1,k+1,mu)
  280    continue

  300 continue

c---- Heat Flux Calculation
      do 320 j = 1,jmax
      do 320 i = 1,imax
         qzm(i,j,ifrq) = 0.0
         qzp(i,j,ifrq) = 0.0
         do 310 mu = 1,mumax
            qzm(i,j,ifrq) = qzm(i,j,ifrq)
     1              -wt(mu)*zet(mu)*ri(i+1,j+1,1,mu)*dx(i)*dy(j)
            qzp(i,j,ifrq) = qzp(i,j,ifrq)
     1              +wt(mu)*zet(mu)*ri(i+1,j+1,kmax2,mu)*dx(i)*dy(j)
  310    continue
  320 continue

      do 340 k = 1, kmax
      do 340 i = 1, imax
         qym(i,k,ifrq) = 0.0
         qyp(i,k,ifrq) = 0.0
         do 330 mu = 1, mumax
            qym(i,k,ifrq) = qym(i,k,ifrq)
     1                  -wt(mu)*yxi(mu)*ri(i+1,1,k+1,mu)*dx(i)*dz(k)
            qyp(i,k,ifrq) = qyp(i,k,ifrq)
     1              +wt(mu)*yxi(mu)*ri(i+1,jmax2,k+1,mu)*dx(i)*dz(k)
  330    continue
  340 continue

      do 360 k = 1, kmax
      do 360 j = 1, jmax
         qxm(j,k,ifrq) = 0.0
         qxp(j,k,ifrq) = 0.0
         do 350 mu = 1, mumax
            qxm(j,k,ifrq) = qxm(j,k,ifrq)
     1              -wt(mu)*xnu(mu)*ri(1,j+1,k+1,mu)*dy(j)*dz(k)
            qxp(j,k,ifrq) = qxp(j,k,ifrq)
     1              +wt(mu)*xnu(mu)*ri(imax2,j+1,k+1,mu)*dy(j)*dz(k)
  350    continue
  360 continue


      if(iout(9) .eq. 1) then
         write(6,2100) 'ifrq =' ,ifrq,'is4=',is4(ifrq),'iter =',iter,
     1                 'nzero =',nzero,'error =',sum
         return
      end if

c---- BEGIN  ACCURACY CHECK(Divergence Theorem)
c---- total heat transfer
      qtot   = 0.
      do 370 j = 1, jmax
      do 370 k = 1, kmax
         qtot   = qtot + qxm(j,k,ifrq) + qxp(j,k,ifrq)
  370 continue

      do 380 i = 1, imax
      do 380 k = 1, kmax
         qtot   = qtot + qym(i,k,ifrq) + qyp(i,k,ifrq)
  380 continue

      do 390 i = 1, imax
```

```
      do 390 j = 1, jmax
         qtot    = qtot + qzm(i,j,ifrq) + qzp(i,j,ifrq)
 390  continue

c---- total divergence of heat flux due to gs or gs+gm if S4
      divqt      = 0.
      do 400 i = 1, imax
      do 400 j = 1, jmax
      do 400 k = 1, kmax
         vol     = dx(i)*dy(j)*dz(k)
         t1      = (1.-omeg(k,ifrq)*is4(ifrq))*beta(k,ifrq)*
     1             (4.*pi*is4(ifrq)*ebg(i,j,k)-gs(i,j,k,ifrq))
         divqt   = divqt + t1*vol
 400  continue

      if(iout(10). eq. 1) then
         write(6,2000) 'iter =',iter,'nzero =',nzero,'error =',sum,
     1                 'qtot =',qtot,'divqt =',divqt
      end if

c---- END  ACCURACY CHECK

 2000 format(2x,a,i3,3x,a,i7,4 (3x,a,1pe10.3))
 2100 format(2x,3(a,i3,3x),a,i7,4 (3x,a,1pe10.3))

      end


      subroutine tdi(ifrq)
c-----------------------------------------------------------------------c
c     SUBROUTINE TDI(IFRQ)                                              c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'
      dimension a(100),b(100),c(100),utd(100),r(100)
      dimension phi(imx,jmx,kmx),phio(imx,jmx,kmx)

c---- load phi and phio
      do 10 k = 1,kmax
      do 10 j = 1,jmax
      do 10 i = 1,imax
         phi(i,j,k) = gm(i,j,k,ifrq)
         phio(i,j,k) = 0.0
  10  continue

c---- successive overrelaxation with the relaxation parameter omega
      iter=0

  15  continue
      iter = iter+1
      omeg0 = omegag*exp(-0.11*iter) + 1.7*(1. - exp(-0.11*iter))

      do 40 k = 1,kmax
      do 40 j = 1,jmax

         do 20 i = 1,imax
            a(i) = aw(i,j,k)
            b(i) = ap(i,j,k)
            c(i) = ae(i,j,k)
            r(i) = s(i,j,k)

            if(k.ne.1)     r(i) = r(i)-al(i,j,k)*phi(i,j,k-1)
            if(j.ne.1)     r(i) = r(i)-as(i,j,k)*phi(i,j-1,k)
```

```
            if(k.ne.kmax) r(i) = r(i)-ah(i,j,k)*phi(i,j,k+1)
            if(j.ne.jmax) r(i) = r(i)-an(i,j,k)*phi(i,j+1,k)

   20    continue

         call tridag(a,b,c,r,utd,imax)

         do 30 i = 1,imax
           phi(i,j,k) = phi(i,j,k)+omeg0*(utd(i)-phi(i,j,k))
   30    continue

   40 continue

      do 70 k = 1,kmax
      do 70 i = 1,imax

         do 50 j = 1,jmax
            a(j) = as(i,j,k)
            b(j) = ap(i,j,k)
            c(j) = an(i,j,k)
            r(j) = s(i,j,k)

            if(k.ne.1)     r(j) = r(j)-al(i,j,k)*phi(i,j,k-1)
            if(i.ne.1)     r(j) = r(j)-aw(i,j,k)*phi(i-1,j,k)
            if(k.ne.kmax) r(j) = r(j)-ah(i,j,k)*phi(i,j,k+1)
            if(i.ne.imax) r(j) = r(j)-ae(i,j,k)*phi(i+1,j,k)

   50    continue

         call tridag(a,b,c,r,utd,jmax)

         do 60 j=1,jmax
            phi(i,j,k) = phi(i,j,k)+omeg0*(utd(j)-phi(i,j,k))
   60    continue

   70 continue

      do 100 j = 1,jmax
      do 100 i = 1,imax

         do 80 k = 1,kmax
            a(k) = al(i,j,k)
            b(k) = ap(i,j,k)
            c(k) = ah(i,j,k)
            r(k) = s(i,j,k)

            if(j.ne.1)     r(k) = r(k)-as(i,j,k)*phi(i,j-1,k)
            if(i.ne.1)     r(k) = r(k)-aw(i,j,k)*phi(i-1,j,k)
            if(j.ne.jmax) r(k) = r(k)-an(i,j,k)*phi(i,j+1,k)
            if(i.ne.imax) r(k) = r(k)-ae(i,j,k)*phi(i+1,j,k)

   80    continue

         call tridag(a,b,c,r,utd,kmax)

         do 90 k = 1,kmax
            phi(i,j,k) = phi(i,j,k)+omeg0*(utd(k)-phi(i,j,k))
   90    continue

  100 continue

c---- convergence test
      error = 0.0
      do 110 j = 1,jmax
```

```
      do 110 i = 1,imax
         error = error+abs((phi(i,j,1)-phio(i,j,1))/phi(i,j,1))
         error = error+abs((phi(i,j,kmax)-phio(i,j,kmax))/phi(i,j,kmax))
  110 continue

      do 120 k = 1,kmax
      do 120 i = 1,imax
         error = error+abs((phi(i,1,k)-phio(i,1,k))/phi(i,1,k))
         error = error+abs((phi(i,jmax,k)-phio(i,jmax,k))/phi(i,jmax,k))
  120 continue

      do 130 k = 1,kmax
      do 130 j = 1,jmax
         error = error+abs((phi(1,j,k)-phio(1,j,k))/phi(1,j,k))
         error = error+abs((phi(imax,j,k)-phio(imax,j,k))/phi(imax,j,k))
  130 continue

      do 140 k = 1,kmax
      do 140 j = 1,jmax
      do 140 i = 1,imax
         phio(i,j,k) = phi(i,j,k)
  140 continue

      error = error/(2.*imax*jmax+2.*jmax*kmax+2.*imax*kmax)

      if(iter .lt. nitgmmn) go to 15

      if(error .gt. 1.e-7 .and. iter .lt. nitergm) go to 15

c---- print non-convergence
      if (iter .ge. nitergm .and. iout(10) .eq. 1) then
         write(6,*) 'no convergence in Gm for ifrq = ',ifrq,
     1              '  error =',error
      end if

c---- load gm(i,j,k,ifrq)
      do 150 k = 1,kmax
      do 150 j = 1,jmax
      do 150 i = 1,imax
         gm(i,j,k,ifrq) = phi(i,j,k)
  150 continue


      end


      subroutine tfield
c-----------------------------------------------------------------------c
c     SUBROUTINE TFIELD                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- load gas temperatures: tg(ivol) --> t(i,j,k)
      do 40 ivol = 1, nvol

         if (ivol .eq. 1) then
            klow = 1

         else
            klow = kvol(ivol-1) + 1
         end if
```

```
         khigh   = kvol(ivol)
         do 30 i = 1, imax
            do 20 j = 1, jmax
               do 10 k = klow, khigh
                  t(i,j,k) = tg(ivol)
  10          continue
  20       continue
  30    continue

  40  continue


      end


      subroutine tridag(a,b,c,r,u,n)
c-----------------------------------------------------------------------c
c     SUBROUTINE TRIDAG(a,b,c,r,u,n)                                    c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      dimension gam(100),a(n),b(n),c(n),r(n),u(n)

      if (b(1) .eq. 0.) then
         write(6,*) 'Stopped in tridag'
         stop
      end if
      bet  = b(1)
      u(1) = r(1)/bet

      do 10 j = 2, n
         gam(j) = c(j-1)/bet
         bet    = b(j)-a(j)*gam(j)
         if (bet .eq. 0.) then
            write(6,*) 'Stopped in tridag'
            stop
         end if
         u(j)   = (r(j)-a(j)*u(j-1))/bet
   10 continue

      do 20 j = n-1,1,-1
         u(j) = u(j)-gam(j+1)*u(j+1)
   20 continue


      end


      subroutine viscos(nspe,x,t,visc,amug)
c-----------------------------------------------------------------------c
c     SUBROUTINE VISCOS                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)

      parameter (nsp=5)
      dimension  akap(nsp)  , ek(nsp)  , ekij (nsp,nsp), sig(nsp),
     1           visc(nspe) , x(nspe)  , sigij(nsp,nsp)

      common /critc/ amw(nsp), tb(nsp) , tc(nsp) , pc(nsp) , vc(nsp),
     1               ome(nsp), dip(nsp)

c--   visc  : viscosity of single component in pa.s
c--   amug  : viscosity of gas mixture in pa.s
```

```
c--   t      : gas temperature in  k
c--   x      : mole fraction

c--   function statement for collision integral
      omega(tstr) = 1.16145/tstr**0.14874
     @            + 0.52487*exp(-0.77320*tstr)
     @            + 2.16178*exp(-2.43787*tstr)

c--   sig : lennard-jones potential parameter in angstrom
c--   ek  : e/k  in k

      do 10 i=1,nspe
         akap(i) = 0.0682
         dipr    = 131.3*dip(i)/sqrt(vc(i)*tc(i))
         fc      = 1.-0.2756*ome(i)+0.059035*dipr**4+akap(i)
         sig(i)  = 0.809*vc(i)**(1./3.)
         ek(i)   = 0.79409196*tc(i)
         ts      = t/ek(i)
         visc(i) = 2.699e-06*fc*sqrt(amw(i)*t)/ (sig(i)**2*omega(ts))
   10 continue

c--   the rest of program is to calculate viscosity of gas mixture


c--   combining rules


      do 30 i = 1, nspe
         do 20 j = 1, nspe
            sigij(i,j) = sqrt(sig(i)*sig(j))
            ekij(i,j)  = sqrt(ek(i)*ek(j))
   20    continue
   30 continue

c--   potential parameters of mixutre
      sum1  = 0.0
      sigm3 = 0.0
      do 45 i = 1, nspe
         do 40 j = 1, nspe
            sigm3 = sigm3 + x(i)*x(j)*sigij(i,j)**3
            sum1  = sum1 + x(i)*x(j)*sigij(i,j)**3*ekij(i,j)
  40     continue
  45  continue

      sigm = sigm3**(1./3.)
      ekm  = sum1/sigm3

c--   mixture rule for reduced mass, accentricity factor,
c--   dipole moments and association factor

      sum1 = 0.0
      sum2 = 0.0
      sum3 = 0.0
      sum4 = 0.0
      do 55 i = 1, nspe
         do 50 j = 1, nspe
            amij = 2.*amw(i)*amw(j)/(amw(i)+amw(j))
            xij  = x(i)*x(j)
            sum1 = sum1 + xij*ekij(i,j)*sigij(i,j)**2*sqrt(amij)
            sum2 = sum2 + xij*0.5*(ome(i)+ome(j))*sigij(i,j)**3
            sum3 = sum3 + xij*(dip(i)*dip(j))**2/sigij(i,j)**3
            sum4 = sum4 + xij*sqrt(akap(i)*akap(j))
   50    continue
   55 continue
```

```
      amwm   = (sum1/(ekm*sigm**2))**2
      omem   = sum2/sigm3
      dipmx  = (sigm3*sum3)**0.25
      akapm  = sum4

c--   mixture rule of critical temperature and volume

      tcm = 1.2593*ekm
      vcm = (sigm/0.809)**3
      dipm = 131.3*dipmx/sqrt(vcm*tcm)
      fcm  = 1.-0.275*omem+0.059035*dipm**4 + akapm
      ts   = t/ekm

c--   viscosity of gas mixture, pa.s

      amug = 2.669e¬06*fcm*sqrt(amwm*t)/(sigm**2*omega(ts))

      end


      subroutine fsolvg(x,f,bl,bu,acc,del,n,it,maxit,print,a)
c-----------------------------------------------------------------c
c     SUBROUTINE FSOLVG                                           c
c-----------------------------------------------------------------c

      real*8 x(*), f(*), bl(*), bu(*), a(*), acc, del, t1,t2,t3
      integer n, it, maxit, print
      integer i,nb,ndx,ndf,nxs,nfs,nh,
     *   nhs,nxsc,nfsc,nmu,nmi,nhi,nit,nbi,nw1,nw2
      nb=1
      nbi=nb+n*n
      ndx=nbi+n*n
      ndf=ndx+n
      nxs=ndf+n
      nfs=nxs+n
      nfsc=nfs+n
      nxsc=nfsc+n
      nw1=nxsc+n
      nw2=nw1+n
      nh=nw2+n
      nhs=nh+1
      nmu=nhs+1
      nhi=nmu+1
      nmi=nhi+1
      nit=nmi+1
      if (it.eq.0) then
         if (a(nit) .ne.0 .and. del.lt.0.) then
            a(nit)=n+1
            a(nmu)=0.
            a(nmi)=0.
            a(nhs)=0.
            do 10 i=1, n
               a(nfs+i-1) = f(i)/a(nfsc+i-1)
               a(nhs) =a(nhs)+ a(nfs+i-1)*a(nfs+i-1)
 10         continue
            a(nhi)=a(nhs)
         else
            a(nit)=0
         endif
      else
         a(nit)=a(nit)+1
      endif
```

```
      t1=0.0
      do 20 i=1, n
         t1=t1+f(i)*f(i)
 20   continue
      t1=dsqrt(t1)
      if (print.ge.1 .and. (a(nit).eq.0 .or. a(nit).gt.n)) then
         write(6,1000) it,t1
 1000    format(/'solvg n=',i4,' f=',e12.4)
         write(6,1010) (x(i),i=1,n)
 1010    format('  x=',10e12.4)
         write(6,1020) (f(i),i=1,n)
 1020    format('  c=',10e12.4)
      endif
      if (t1.lt.acc) then
         it=1000
         return
      endif
      if (it.ge.maxit-1) then
         write(6,1030)
 1030    format(/'maximun iterations exceeded in solvg')
         it=2000
         return
      endif
      if (a(nit) .le.n) then
         call jacob(x,f,bl,bu,a(nxs),a(nfs),a(nxsc),a(nfsc),
     @     a(nb),a(nbi),a(nit),del,t1,n,it,print)
         a(nh)=t1
         a(nhs)=t1
         a(nhi)=t1
         if (a(nit).lt.n .or. it.eq.5000) return
      else
         it=it+1
         a(nh)=0.0
         do 30 i=1, n
            x(i)=x(i)*a(nxsc+i-1)
            f(i)=f(i)/a(nfsc+i-1)
            a(nh)=a(nh)+f(i)*f(i)
 30      continue
         if (a(nh).lt.a(nhs)) then
            a(nhs)=a(nh)
            do 40 i=1, n
               t1=x(i)
               x(i)=a(nxs+i-1)
               a(nxs+i-1)=t1
               t1=f(i)
               f(i)=a(nfs+i-1)
               a(nfs+i-1)=t1
 40         continue
         endif
         if (a(nh).gt.a(nhs)) then
            a(nmu)=a(nmu)+1
         else
            a(nmu)=a(nmu)-1
            a(nmu)=dmax1(0.0,a(nmu))
         endif
         if (a(nmu).ge.a(nmi)+3.0.and.a(nhi).ge.a(nhs)
     @     .and.a(nh).gt.a(nhs)) then
            a(nit)= -1.0
            do 50 i=1, n
               x(i)=a(nxs+i-1)/a(nxsc+i-1)
 50         continue
            return
         endif
         if (a(nhs) .ne.a(nhi))
```

```
     @      call update(x,f,a(ndx),a(ndf),a(nxs),a(nfs),a(nw1),a(nw2),
     @        a(nb),a(nbi),n)
      endif
      call steps(a(nw1),a(nw2),a(nfs),a(nb),a(nbi),t1,t2,n)
      if (a(nit).eq.n)  then
         a(nmu)=dmax1(0.0,dlog(t1/a(nhs))/log(2.0e0))
         a(nmi)=a(nmu)
      endif
      if (print.ge.2) then
         t3=0.0
         do 60 i=1, n
           t3 = t3+a(nw1+i-1)*a(nw2+i-1)
 60      continue
         t3=t3/sqrt(t1*t2)
         write(6,1040) a(nh),a(nhs),a(nmu),t1,t2,t3
1040     format('  h=',e11.4,' hs=',e11.4,' mu=',e7.2,' n='
     @     ,e7.2,' s=',e7.2,' a=',e8.2)
      endif
      call newx(x,bl,bu,a(nw1),a(nw2),a(nxs),a(ndx),a(nxsc),a(nb),
     @  a(nmu),n,it,print)
      end

      subroutine jacob(x,f,bl,bu,xs,fs,xsc,fsc,b,bi,ait,del,t1,n,
     @  it,print)
      real*8 x(*), f(*), bl(*), bu(*), xs(*), fs(*),
     @    xsc(*), fsc(*), b(*), bi(*), ait, del, t1, t2
      integer n, it, print, i, j, id
      id= ait+1
      if (id.eq.1) then
         it=it+1
         do 10 i=1, n
            xs(i)=x(i)
            fs(i)=f(i)
 10       continue
      else
         do 20 i=1, n
            b((i-1)*n+id-1)=(f(i)-fs(i))/(x(id-1)-xs(id-1))
 20      continue
         x(id-1)=xs(id-1)
      endif
      if (id.le.n) then
         t1=dabs(del*x(id))
         t2=dabs(del*(bu(id)-bl(id)))
         if (t1.lt.1e-10*t2 .or. t1.gt.t2)  t1=t2
         x(id)=xs(id)+t1
         return
      endif
      do 30 i=1, n
         xsc(i)=0.0
         do 40 j=1, n
           xsc(i)=dmax1(xsc(i), dabs(b((j-1)*n+i)))
 40      continue
         if (xsc(i).eq.0.0) then
            write(6,1000) i
1000        format(/'no equation depends on variable ',i3,
     @        ' in task solvg')
            it=5000
            xsc(i)=1.0
         endif
C        test line
         xsc(i)=1.0
         xs(i)=xs(i)*xsc(i)
         x(i)=xs(i)
         do 50 j=1, n
```

```
            b((j-1)*n+i)=b((j-1)*n+i)/xsc(i)
 50       continue
 30    continue
       t1=0.0
       do 60 i=1, n
          t2=fsc(i)
          fsc(i)=0.0
          do 70 j=1, n
             fsc(i)=dmax1(fsc(i), dabs(b((i-1)*n+j)) )
 70       continue
          if (fsc(i).eq.0.0) then
             write(6,1010) i
1010         format(/'constraint ',i3,
     @          'is independent of all variables in solvg ')
             it=5000
             fsc(i)=1.0
          endif
          if (it.gt.1) fsc(i)=dmin1(t2, fsc(i))
C   test line
          fsc(i)=1.0
          fs(i)=fs(i)/fsc(i)
          f(i)=fs(i)
          do 80 j=1, n
             b((i-1)*n+j)=b((i-1)*n+j)/fsc(i)
 80       continue
          t1=t1+fs(i)*fs(i)
 60    continue
       if (it.eq.5000)  return
       j=n*n
       do 90 i=1, j
          bi(i)=b(i)
 90    continue
       call invt(bi,n,n,t2)
       end

       subroutine update(x,f,dx,df,xs,fs,w1,w2,b,bi,n)
       real*8 x(*), f(*), dx(*), df(*), xs(*), fs(*), w1(*),
     @   w2(*), b(*), bi(*), t1, t2, t3
       integer i, j, n
       do 10 i=1, n
          dx(i)=x(i)-xs(i)
          df(i)=f(i)-fs(i)
 10    continue
       do 20 i=1, n
          w1(i)=df(i)
          w2(i)=dx(i)
          do 30 j=1, n
             w1(i)=w1(i)-b((i-1)*n+j)*dx(j)
             w2(i)=w2(i)-bi((i-1)*n+j)*df(j)
 30       continue
 20    continue
       t1=0.0
       t2=0.0
       do 40 i=1, n
          t3=0.0
          do 50 j=1, n
             t3=t3+bi((j-1)*n+i)*dx(j)
 50       continue
          t1=t1+dx(i)*dx(i)
          t2=t2+t3*df(i)
          df(i)=t3
 40    continue
       if (dabs(t2).lt.0.1*t1) then
          t3=0.8
```

```
      else
         t3=1.0
      endif
      t2=t3/(t3*t2+(1.0-t3)*t1)
      t1=t3/t1
      do 60 i=1, n
         do 70 j=1, n
            b((i-1)*n+j)=b((i-1)*n+j)+t1*w1(i)*dx(j)
            bi((i-1)*n+j)=bi((i-1)*n+j)+t2*w2(i)*df(j)
 70      continue
 60   continue
      end

      subroutine steps(w1,w2,fs,b,bi,t1,t2,n)
      real*8 w1(*), w2(*), fs(*), b(*), bi(*),d2,d3,t1,t2
      integer i, j, n
      t1=0.0
      t2=0.0
      do 10 i=1, n
         w1(i)=0.0
         w2(i)=0.0
         do 20 j=1, n
            w1(i)=w1(i)-bi((i-1)*n+j)*fs(j)
            w2(i)=w2(i)-b((j-1)*n+i)*fs(j)
 20      continue
       t1=t1+w1(i)*w1(i)
       t2=t2+w2(i)*w2(i)
 10   continue
      d2=0.0
      do 30 i=1, n
         d3=0.0
         do 40 j=1, n
            d3 = d3+b((i-1)*n+j)*w2(j)
 40      continue
         d2 = d2+d3*d3
 30   continue
      d2=t2/d2
      t2=0.0
      do 50 i=1, n
         w2(i)=d2*w2(i)
         t2 = t2+w2(i)*w2(i)
 50   continue
      end

      subroutine newx(x,bl,bu,w1,w2,xs,dx,xsc,b,amu,n,it,print)
      real*8 x(*), bl(*), bu(*), w1(*), w2(*), xs(*),
     @  dx(*), xsc(*), b(*),amu,t1
      integer n, it, print
      integer i, j
 10   continue
      do 20 i=1 , n
        dx(i)=2.0**(-amu)*(w1(i)+amu*w2(i))
 20   continue
      t1=0.0
      j= 0
      do 30 i=1, n
         t1=dmax1(t1,dabs(dx(i))/xsc(i))
         x(i)=(xs(i)+dx(i))/xsc(i)
         if (x(i).gt.bu(i) .or. x(i).lt.bl(i)) j=i
 30   continue
      if (j.gt.0) then
         amu=amu+1
         if (t1.lt.1e-12) then
            write(6,1000) j
```

```
1000        format(/'hitting bound on variable ',i3,' in solvg')
            it=6000
            return
         endif
         if (print.ge.2) write(6,1005) j
1005       format('b=',i3)
      endif
      if (j.gt.0) goto 10
      if (t1.lt.1e-15) then
         if (amu.gt.10) then
            write(6,1010)
1010        format(/'unable, find an improved point in solvg')
            it=3000
            return
         endif
         if (print.ge.2) then
            write(6,1020)
1020        format(/'convergence of independent variables in solvg')
            it=4000
            return
         endif
      endif
      end

      subroutine invt(a,n,m,det)
      real*8 a(*), det, s, t, r, rm
      integer n, m, rno(100), cno(100), i, j, k, js, im, jm, l
      det=1.0
      do 10 i=1, n
 10      rno(i)= -1
      do 20 i=1, m
 20      cno(i)= -1
      do 30 k=1, n
         rm=0.0
         do 40 i=1, n
            if (rno(i).gt.-1) goto 40
            js= -1
            s=0.0
            t=0.0
            do 50 j=1, n
               r=dabs( a((i-1)*m+j) )
               if (cno(j).gt.-1 .or. r.lt.t) goto 50
               t=r
               if (r.lt.s) goto 50
               t=s
               s=r
               js=j
 50         continue
            if (s.eq.0.0) then
               det= 0
               write(6,1000) js
1000           format(/'determinant zero, variable=',i3)
               return
            endif
            if (t.eq.0.0)  t=1.0e-20*s
            r=s/t
            if (r.lt.rm) goto 40
            rm=r
            im=i
            jm=js
 40      continue
         cno(jm)=im
         rno(im)=jm
         t=a((im-1)*m+jm)
```

```
         s=1.0/t
         a((im-1)*m+jm)=1.0
         do 60 j=1, m
            a((im-1)*m+j)=a((im-1)*m+j)*s
 60      continue
         do 70 i=1, n
            if (i.eq.im) goto 70
            t=a((i-1)*m+jm)
            a((i-1)*m+jm)=0.0
            do 80 j=1, m
               a((i-1)*m+j)=a((i-1)*m+j)-t*a((im-1)*m+j)
 80         continue
 70      continue
 30   continue
      do 90 i=1, n
         k= cno(i)
         if (k.eq.i) goto 90
         do 100 j=1, m
            r=a((i-1)*m+j)
            a((i-1)*m+j)=a((k-1)*m+j)
            a((k-1)*m+j)=r
 100     continue
         l= rno(i)
         do 110 j=1, n
            s=a((j-1)*m+i)
            a((j-1)*m+i)=a((j-1)*m+l)
            a((j-1)*m+l)=s
 110     continue
         rno(k)=l
         cno(l)=k
 90   continue
      end



      subroutine optdrv
c-----------------------------------------------------------------------c
c     SUBROUTINE OPTDRV                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'
      dimension bet(37), om(37)

c---- flame zone: no ash particles, ivol = 2
      ivol = 2
      do 20 iknd = 1, 3
         do 10 n = 1, npt(iknd)
            anum(iknd,n) = pdist(iknd,n,ivol)
   10    continue
   20 continue

      call optprop(npt,nfrq,incl,rpt,anum,yash,trad(ivol),ph2o,pco2,
     1             pco,pgas,beam,dfrq,bet,om)
      do 35 k = kvol(1)+1, kvol(2)
         do 30 ifrq = 1, nfrq
            beta(k,ifrq)    = bet(ifrq)
            omeg(k,ifrq)    = om(ifrq)
            beta1(k,ifrq)   = beta(k,ifrq)*(1.-a1(k,ifrq)*om(ifrq)/3.)
   30    continue
   35 continue

c---- non-flame zones: no char/soot particles, ivol = 1
```

```
      ivol = 1
      do 50 iknd = 1, 3
         do 40 n = 1, npt(iknd)
            anum(iknd,n) = pdist(iknd,n,ivol)
   40    continue
   50 continue

      call optprop(npt,nfrq,incl,rpt,anum,yash,trad(ivol),ph2o,pco2,
     1             pco,pgas,beam,dfrq,bet,om)
      do 70 k = 1, kvol(1)
         do 60 ifrq = 1, nfrq
            beta(k,ifrq)    = bet(ifrq)
            omeg(k,ifrq)    = om(ifrq)
            beta1(k,ifrq)   = beta(k,ifrq)*(1.-a1(k,ifrq)*om(ifrq)/3.)
   60    continue
   70 continue

c---- non-flame zones: no char/soot particles, ivol = 3 to nvol
      do 100 ivol = 3, nvol
         do 80 iknd = 1, 3
            do 75 n = 1, npt(iknd)
               anum(iknd,n) = pdist(iknd,n,ivol)
   75       continue
   80    continue

         call optprop(npt,nfrq,incl,rpt,anum,yash,trad(ivol),ph2o,pco2,
     1             pco,pgas,beam,dfrq,bet,om)
         do 90 k = kvol(ivol-1)+1, kvol(ivol)
            do 85 ifrq = 1, nfrq
               beta(k,ifrq)    = bet(ifrq)
               omeg(k,ifrq)    = om(ifrq)
               beta1(k,ifrq)   = beta(k,ifrq)*(1.-a1(k,ifrq)*om(ifrq)/3.)
   85       continue
   90    continue
  100 continue

c---- modify dfrq(1) for gray body computation
      if (nfrq .eq. 1) dfrq(1) = 1.

c---- if beta < betmin everywhre skip calculation
      betmin = 5.e-05

c---- set method index
      do 120 ifrq = 1, nfrq

c----    MDA
         ip1(ifrq)    = 0
         is4(ifrq)    = 0

         ic = 0
         jc = 0

         do 110 ivol = 1, nvol
            k = kvol(ivol)

            if(beta(k,ifrq).lt.betmin) then
              jc = jc + 1

            else if(beta(k,ifrq).le.betamn ) then
c---           solve by S4
               is4(ifrq) = 1

            else if(beta(k,ifrq) .ge. betamx) then
               ic = ic + 1
```

```
            end if

  110     continue

c---      P1-Approximation
          if(ic .eq. nvol) ip1(ifrq) = 1

          ibeta(ifrq) = 1
c---      skip calculation
          if(jc .eq. nvol) ibeta(ifrq) = 0

  120 continue
c     write(6,200) (is4(i),i=1,nfrq)
c     write(6,200) (ip1(i),i=1,nfrq)
c     write(6,200) (ibeta(i),i=1,nfrq)

  200 format(20(i3))
      end


      subroutine mie( x,refre,refim,qext,qsca)
c-----------------------------------------------------------------------c
c     SUBROUTINE MIE                                                    c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)

      dimension amu(100) , theta(100), pi(100)  , tau(100) ,
     1          pi0(100) , pi1(100)

      complex   d(3000)  , y          , refrel   , xi       ,
     1          xi0      , xi1        , an       , bn       ,
     1          s1(200)  , s2(200)

      refrel= cmplx(refre,refim)
      nang  = 1
      dx    = x
      y     = x*refrel

c--   series terminated after nstop terms
      xstop = x + 4.*x**0.3333 + 2.0
      nstop = xstop
      ymod  = cabs(y)
      nmx   = max(xstop,ymod) + 15
      dang  = 0.0
      if(nang.gt.1) dang  = 1.570796327 / float(nang-1)
      do 10 j=1,nang
         theta(j) = (float(j)-1.)*dang
         amu(j)   = cos(theta(j))
   10 continue

c--   logarithmic derivative d(j) calculted by downward
c--   recurence beginning with initial value 0.0 + i*0.0 at j=nmx
      d(nmx)  = cmplx(0.0,0.0)
      nn      = nmx-1
      do 20 n=1,nn
         rn        = nmx-n+1
         d(nmx-n) = (rn/y) - (1./(d(nmx-n+1)+rn/y))
   20 continue

      do 30 j=1,nang
         pi0(j)  = 0.0
         pi1(j)  = 1.0
```

```
   30 continue

      nn  = 2*nang - 1
      do 40 j=1,nn
         s1(j)  = cmplx(0.0,0.0)
         s2(j)  = cmplx(0.0,0.0)
   40 continue

c--   riccati-bessel functions with real argument x by upward recurence
      psi0  = dcos(dx)
      psi1  = dsin(dx)
      chi0  =-sin(x)
      chi1  = cos(x)
      apsi0 = psi0
      apsi1 = psi1
      xi0   = cmplx(apsi0,-chi0)
      xi1   = cmplx(apsi1,-chi1)
      qsca  = 0.0
      n     = 1

c--   main loop begins
   50 dn    = n
      rn    = n
      fn    = (2.*rn+1.) / (rn*(rn+1.))
      psi   = (2.*dn-1.)*psi1/dx - psi0
      apsi  = psi
      chi   = (2.*dn-1.)*chi1/x - chi0
      xi    = cmplx(apsi,-chi)
      an    = ((d(n)/refrel+rn/x)*apsi - apsi1)
     1       / ((d(n)/refrel+rn/x)*xi - xi1)
      bn    = ((refrel*d(n)+rn/x)*apsi - apsi1)
     1       /((refrel*d(n)+rn/x)*xi - xi1)
      qsca  = qsca + (2.*rn+1.)*(cabs(an)*cabs(an)+cabs(bn)*cabs(bn))

      do 60 j=1,nang
         jj     = 2*nang - j
         pi(j)  = pi1(j)
         tau(j) = rn*amu(j)*pi(j) - (rn+1.)*pi0(j)
         p      = (-1.)**(n-1)
         s1(j)  = s1(j) + fn*(an*pi(j)+bn*tau(j))
         t      = (-1.)**n
         s2(j)  = s2(j) + fn*(an*tau(j)+bn*pi(j))
         if (j.eq.jj) go to 60
         s1(jj) = s1(jj) + fn*(an*pi(j)*p+bn*tau(j)*t)
         s2(jj) = s2(jj) + fn*(an*tau(j)*t+bn*pi(j)*p)
   60 continue

      psi0  = psi1
      psi1  = psi
      apsi1 = psi1
      chi0  = chi1
      chi1  = chi
      xi1   = cmplx(apsi1,-chi1)
      n     = n + 1
      rn    = n

      do 70 j=1,nang
         pi1(j) = ((2.*rn-1.)*amu(j)*pi(j) - rn*pi0(j))/(rn-1.)
         pi0(j) = pi(j)
   70 continue

      if (n-1-nstop) 50,80,80

c---- loop branching point
```

```
   80 qsca = (2./(x*x))*qsca
      qext = (4./(x*x))*real(s1(1))

      end


      subroutine optprop(nsize,igray,incl,r,anum,yash,tg,ph2o,pco2,
     1                   pco,pg,bl,dfrq,beta,omega)
c-----------------------------------------------------------------------c
c     SUBROUTINE OPTPROP                                                c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      character*15  qash, qsoot, qchar

       common /files/
     1 qash           , qsoot         , qchar

c-----------------------------------------------------------------------c
c    nsize(i)   : number of partcle size(1=ash,2=soot,3=char)           c
c    incl(i)    : switch index                                          c
c                 0 = do not include in calculation                     c
c                 1 = include without updating efficiecy factor          c
c                 2 = update and include                                c
c    yash(i)    : ash composition(1=SiO2,2=Al2O3,3=CaO,4=Fe2O3,5=MgO)  c
c    ph2o,pco2,pco: partial pressure in atm                             c
c    pg         : gas pressure in atm                                   c
c    tg         : reference gas temperature in K                        c
c    bl         : mean beam length in m                                 c
c    r(l,i)     : particle radius in m                                  c
c    anum(l,i)  : number density in #/m**3                              c
c    dfrq(ifrq): band width in cm-1                                     c
c-----------------------------------------------------------------------c
      dimension  v(100) , beta(37), omega(37), r(3,40) , anum(3,40),
     1           yash(5), dfrq(37), incl(3)  , nsize(3)

      external optash, optsoot, optchar

c---- function statement of Planck function
      pf(t,frq) = 1.1908e-08*frq**3/(exp(1.43883*frq/t)-1.)

      nfrq       = 37
      vi         = 200.
      do 10 ifrq = 1, nfrq
         v(ifrq) = vi+dfrq(ifrq)
         vi      = v(ifrq)
  10  continue

      nmax = 20

      if(incl(1).eq.2) then
         open(unit=8,status='unknown',file=qash)
         call qeff(8,optash,nsize(1),r,1,nfrq,v,nmax,yash,tg)
         close(8)
      end if

      if(incl(2).eq.2) then
         open(unit=9,status='unknown',file=qsoot)
         call qeff(9,optsoot,nsize(2),r,2,nfrq,v,nmax,yash,tg)
         close(9)
      end if

      if(incl(3).eq.2) then
         open(unit=10,status='unknown',file=qchar)
```

```
         call qeff(10,optchar,nsize(3),r,3,nfrq,v,nmax,yash,tg)
         close(10)
      end if


c---- open files to read efficiency factors
      open(unit=8,status='old',file=qash)
      open(unit=9,status='old',file=qsoot)
      open(unit=10,status='old',file=qchar)

c---- optical properties
      call opt(nsize,r,anum,ph2o,pco2,pco,pg,nfrq,v,nmax,incl,
     1         yash,tg,bl,omega,beta)

c---- close files
      close(8)
      close(9)
      close(10)

c---- gray body averaging
      if (igray .ne. 1) return
      frq   = 200.+0.5*dfrq(1)
      betas = beta(1)*pf(tg,frq)*dfrq(1)
      omegs = beta(1)*omega(1)*pf(tg,frq)*dfrq(1)
      do 20 ifrq = 2, nfrq
         frq   = frq + 0.5*(dfrq(ifrq-1)+dfrq(ifrq))
         betas = betas + beta(ifrq)*pf(tg,frq)*dfrq(ifrq)
         omegs = omegs + beta(ifrq)*omega(ifrq)*pf(tg,frq)*dfrq(ifrq)
   20 continue

c---- grey body planck function
      pfs = 5.669e-08*tg**4/3.14159265

c---- Planck mean of beta and omega
      beta(igray)  = betas/pfs
      omega(igray) = omegs/betas

      end


      subroutine opt(nsize,r,anum,ph2o,pco2,pco,pg,nfrq,v,nmx,incl,
     1               yash,tg,bl,omega,beta)
c-----------------------------------------------------------------c
c     SUBROUTINE OPT                                              c
c-----------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      dimension r(3,40)     , anum(3,40), v(100) , beta(37),
     1          omega(37), yash(5)    , cext(3) , csca(3)    ,
     2          qe(40)     , qs(40)     , iunit(3), nsize(3)   ,
     3          incl(3)


      data iunit/8,9,10/

      pi   = 3.14159265

      vi = 200.

      do 40 ifrq = 1, nfrq

         akbnd = 0.0
         if(pho2+pco2.gt.0.0) then
            nmax= nmx
```

```
            dv  = (v(ifrq)-vi)/float(nmax)
            vf  = dv/(v(ifrq)-vi)
            vnu = vi -0.5*dv
            do 10 iv = 1, nmax
               vnu  = vnu + dv
               wavl = 1.d+04/vnu
               call absgas(vnu,bl,tg,ph2o,pco2,pco,pg,akh2o,
     1                     akco2,akco,akg)
               akbnd = akbnd + akg*vf
   10       continue
            vi = v(ifrq)
         end if

         cex = akbnd + 1.d-20
         csc = 0.0

         do 30 l = 1, 3

            cext(l) = 0.0
            csca(l) = 0.0

            if(incl(l).eq.0) goto 30

            iounit = iunit(l)
            read(iounit,*) (qe(i),i=1,nsize(l)),(qs(i),i=1,nsize(l))

            do 20 i = 1, nsize(l)
               crss    = pi*r(l,i)**2*anum(l,i)
               cext(l) = cext(l) + crss*qe(i)
               csca(l) = csca(l) + crss*qs(i)
   20       continue

            cex = cex + cext(l)
            csc = csc + csca(l)

   30    continue

         beta(ifrq) = cex
         omega(ifrq)= csc/cex

   40 continue

      end


      subroutine qeff(iunit,optcon,nsize,r,l,nfrq,v,nmx,yash,tg)
c-----------------------------------------------------------------------c
c     SUBROUTINE QEFF                                                   c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      dimension r(3,nsize), v(37), qe(40), qs(40), yash(5)

      pi = 3.14159265
      vi = 200.

      do 40 ifrq = 1, nfrq

         nmax= nmx
         dv  = (v(ifrq)-vi)/float(nmax)
         vf  = dv/(v(ifrq)-vi)
         vnu = vi - 0.5*dv

         do 10 i = 1, nsize
```

```
            qe(i) = 0.0
            qs(i) = 0.0
   10     continue

          do 30 iv = 1, nmax

            vnu  = vnu + dv
            wavl = 1.d+04/vnu
            call optcon(wavl,yash,tg,refre,refim)

            do 20 i = 1, nsize
               rad = 1.d+06*r(l,i)
               x   = 2.*pi*rad/wavl
               call mie(x,refre,refim,qext,qsca)
               qe(i) = qe(i) + qext*vf
               qs(i) = qs(i) + qsca*vf
   20       continue

   30     continue

          write(iunit,200) (qe(i),i=1,nsize),(qs(i),i=1,nsize)

          vi  = v(ifrq)

   40 continue

  200 format(4(1x,1pe23.16))

      end


      subroutine optash(wavl,yash,t,refre,refim)
      implicit real*8 (a-h,o-z)

c-----------------------------------------------------------------------c
c     this subroutine calculates optical constants of ash.              c
c     ref. David G. Goodwin                                             c
c     Infrared Optical Constants of Coal Slags,                         c
c     High Temperarture Gasdynamics Laboratoty                          c
c     Stanford University, Topical Report T-255 July 1986.              c
c                                                                       c
c     wavl: wavelength (micrometer)                                     c
c     t   : temperature(k)                                              c
c     yash: weight fraction of ash component                            c
c      species numbering convention ;                                   c
c            SiO2 = 1     Al2O3 = 2   CaO = 3  Fe2O3 =4  MgO =5.       c
c     refre,refim: real and imaginary part of complex refractive index  c
c                                                                       c
c     Ref. D. G. Goodwin and M. Mitchiner, "Infrared Optical Constants ofc
c     Coal Slag: Dependence on Chemical Composition", j. Thermophysics  c
c     vol 3,N0. 1, pp 53, 1989.                                         c
c-----------------------------------------------------------------------c
      dimension yash(5)

      dimension a(6) , b(6) , c(6) , d(6),
     1          a1(6), b1(6), c1(6),
     2          a2(3), b2(3), c2(3),
     3          a3(4), b3(4), c3(4),
     4          a4(2), b4(2), c4(2)

c--   statement function ref(refractive index).
      ref(aa,bb) = 0.7071067*sqrt(aa+sqrt(aa*aa+bb*bb))

c--   rhol : specific gravity of ash.
```

```
      rhol  = 2.542+0.978*yash(4)

c--   vnu  : wave number (cm-1).
      vnu   = 1./(1.e-04*wavl)
      if (wavl .ge. 8.) go to 200

c   -------------------------------------------------------
c     refractive index for the wavelength  wavl < 8.
c   -------------------------------------------------------

c--   refractive index is calculated from mixture rule.

      data ( a(i)   ,  b(i)   ,  c(i)   ,  d(i)     ,i=1,5)/
     1      0.9389  ,  53.0   ,  5.011  ,  420.0    ,
     2      1.914   , 174.0   , 10.36   , 1633.8    ,
     3      4.250   , 827.7   , 16.63   , 6102.3    ,
     4      1.647   ,   0.0   , 11.36   ,    0.0    ,
     5      1.278   , 136.9   ,  7.433  , 1200.9    /

      tl  = 0.0
      do 10 i = 1, 5
         f  = (a(i)*wavl*wavl-b(i))/(c(i)*wavl*wavl-d(i))
         tl = tl+yash(i)*f
   10 continue

      refre = sqrt((2.*rhol*tl + 1.)/(1.-rhol*tl))
      if(wavl.gt.4.3) go to 100
c
c   ---------------------------------------------------------
c     absorption index for  wavl< 4.
c   ---------------------------------------------------------
c
c--   gf - function is curve fitted (see appendix b of goodwin).
c--
      data ( al(i) , bl(i) , cl(i) ,i=1,6)/
     1      5.50   , 1.1   , 2.5   ,
     2     -1.3529 , 1.54  , 2.18  ,
     3      0.7778 , 1.9   , 2.46  ,
     4     -0.9150 , 2.3   , 2.094 ,
     5     -0.6533 , 2.6   , 1.898 ,
     6      0.1877 , 4.3   , 2.153 /

      gf = 0.3
      if(wavl.lt.0.7) goto 25

      do 20 i = 1, 6
         if (wavl .le. bl(i)) then
            gf = al(i)*(wavl-bl(i))+cl(i)
            go to 25
         end if
  20  continue

  25  gf = gf*1.e-04
c--
c--   fe2p : molal concentration of fe2+
c--   fe3p : molal concentration of fe3+ (mole/litre)
c--   assume that the fraction of fe2+ is 0.77 as sugested in ref.
c--          r2 = (fe2+)/((fe2+) + (fe3+)) = 0.77
c--   wfe2o3: molecular weight of fe2o3.
c--   (fe)  : mole / litre of iron element.
c--
      r2    = 0.77
      aa1   = 3.61e-03*rhol**2*r2*(1.-r2)*yash(4)**2
      aa2   = rhol*yash(4)*(9.63+11.*rhol*r2*yash(4))
```

```
      refim = aa1*exp(1.75/wavl) + aa2*gf
      go to 400
c--
c--   absorption index for  wavelength between 4 and 8.
c--   for this range absorption index is calculated from silica glass.
c--   ref. H.R. Philipp 'Silicon Oxide(sio2)(glass)',
c--   Handbook of Optical Constants of Solids
c--   Ed. by E.D Palik 1985.
c--
  100 call sio2(wavl,asio2)
      rsio2 = 2.190
      refim = rhol/rsio2*yash(1)*asio2
      go to 400
  200 if(wavl .gt.13.) goto 300
c
c   ------------------------------------------------------------
c     absorption and refractive indeces for  8 < wavl < 13
c   ------------------------------------------------------------
c
c--   complex refractive index is calculated from oscillator model
c--   for wavelength between 8 and 13.
c--   species contributing the most is SiO2.
c--   the following table is for the Reststrahlen band obtained
c--   from the Table 4.15 of Goodwin.
c--
c       oxide     wavl      comments        ref.
c    ------------------------------------------------------------
c       sio2       9.1     fused silica       1
c       al2o3     15.7     sapphire           2
c       cao       33.9                        3
c       mgo       24.9                        4
c    ------------------------------------------------------------
c--
c--   Ref. D. G. Goodwin and M. Mitchiner, "Infrared Optical Constants of
c--   Coal Slag: Dependence on Chemical Composition", j. Thermophysics vol 3,
c--   N0. 1, pp 53, 1989.
c--   a2(i) = wp**2(cm-2), b2(i) = wj(cm-1), c2(i) = gam(cm-1)
c--
      data (    b2(i) ,  c2(i) ,i=1,3)/
     1         1062.8 , 164.7  ,
     2          955.8 ,  79.1  ,
     3          762.2 ,  27.5  /
c--
c--   fn2mk2 = n**2-k**2 : real part of dielectric function
c--   f2nk   = 2*n*k     : imaginary part of dielectric function
c--

      fn2mk2 = 2.15
      f2nk   = 0.0

      a2(1) = (0.425-0.60*yash(4))*(yash(1)/0.52)*b2(1)**2
      a2(2) = (0.175+0.75*yash(4))*(yash(1)/0.52)*b2(2)**2
      a2(3) = 0.053*(yash(1)/0.52)*b2(3)**2

      do 30 i = 1, 3
         t1     = (b2(i)*b2(i)-vnu*vnu)**2+(c2(i)*vnu)**2
         fn2mk2 = fn2mk2+a2(i)*(b2(i)*b2(i)-vnu*vnu) / t1
         f2nk   = f2nk  +a2(i)*c2(i)*vnu / t1
   30 continue

      refre = ref(fn2mk2,f2nk)
      refim = 0.5*f2nk/refre
      goto 400
  300 continue
```

```
c
c   ---------------------------------------------------------------
c     absorption index for wavel > 13.
c   ---------------------------------------------------------------
c
c-- optical constants of Al2O3 ---Reststrahlen band obtained from
c--   O.B.Toon, J.B. Pollack and B.N. Khare
c--       'The Optical Constants of Atmospheric Aerosol Species:
c--        Ammonium Sulfate, Alumium Oxide and Sodium'
c--       J. Geophysical Research vol 18 no 33 p5733 1976
c--
c-- a(i) = (wp/wj)**2, b(i) = wj(cm-1) , c(i) = gam/wj
c--
      data (a3(i) , b3(i)  , c3(i)  ,i=1,4) /
     1      0.30  , 385.0  , 0.015  ,
     2      2.70  , 442.0  , 0.010  ,
     3      3.00  , 369.0  , 0.020  ,
     4      0.30  , 635.0  , 0.020  /

      fn2mk2 = 3.20
      f2nk   = 0.0

      do 40 i=1,4
         t1     = (b3(i)*b3(i)-vnu*vnu)**2+(c3(i)*b3(i)*vnu)**2
         fn2mk2 = fn2mk2 + a3(i)*b3(i)*b3(i)*(b3(i)*b3(i)-vnu*vnu) / t1
         f2nk   = f2nk   + a3(i)*b3(i)*b3(i)*c3(i)*b3(i)*vnu / t1
   40 continue

      ral2o3 = ref(fn2mk2,f2nk)
      refre  = ral2o3*yash(2)
      refim  = 0.5*f2nk/ral2o3
c--
c--   Reststrahlen region of MgO.
c--   ref. G.F. Bohren and D.R. Huffman
c--        Absorption and Scattering of Light by Small Particles
c--        p245 1983.
c--
c--   a(i) = wp(cm-1) , b(i) = wj(cm-1), c(i) = gam(cm-1)
c--
      data ( a4(i) , b4(i) , c4(i) ,i=1,2)/
     1      1030.2 , 401.  , 7.62  ,
     2       135.8 , 640.  , 102.4 /

      fn2mk2 = 3.01
      f2nk   = 0.0

      do 50 i = 1, 2
         t1     = (b4(i)*b4(i)-vnu*vnu)**2+(c4(i)*vnu)**2
         fn2mk2 = fn2mk2+a4(i)*a4(i)*(b4(i)*b4(i)-vnu*vnu) / t1
         f2nk   = f2nk +a4(i)*a4(i)*c4(i)*vnu / t1
   50 continue
      rmgo  = ref(fn2k2,f2nk)
      refre = refre + rmgo*yash(5)
      refim = refim + 0.5*f2nk/rmgo*yash(5)
      refre = max(1.0,refre)
  400 continue

c---- temperature correction
      if(wavl .gt. 4. .and. wavl .lt.8) then
         cc2   = 14388.
         refim = refim*(1. + 2./(exp(0.5*cc2/(wavl*t))-1.))
      end if
```

```
      end

      subroutine sio2(wavl,asio2)

c-----------------------------------------------------------------c
c     ref. H.R. Philipp 'Silicon Oxide(sio2)(glass)',             c
c     Handbook of Optical Constants of Solids                     c
c     ed. by E.D Palik 1985                                       c
c-----------------------------------------------------------------c

      implicit real*8(a-h,o-z)
      dimension w(34), ak(34)

      data w /
     1  4.000  , 4.082  , 4.167  , 4.255 , 4.348  ,
     2  4.396  , 4.444  , 4.494  , 4.545 , 4.651  ,
     3  4.762  , 4.878  , 5.000  , 5.063 , 5.128  ,
     4  5.263  , 5.333  , 5.405  , 5.556 , 5.882  ,
     5  6.061  , 6.154  , 6.250  , 6.452 , 6.667  ,
     6  6.897  , 7.143  , 7.407  , 7.692 , 7.752  ,
     7  7.813  , 7.874  , 7.937  , 8.000          /

      data ak /
     1  5.79e-05, 7.99e-05, 1.07e-04, 1.32e-04, 2.13e-04,
     2  2.65e-04, 2.84e-04, 2.84e-04, 2.56e-04, 2.62e-04,
     3  4.85e-04, 1.82e-03, 3.98e-03, 5.12e-03, 5.18e-03,
     3  5.49e-03, 5.69e-03, 5.72e-03, 5.63e-03, 5.94e-03,
     4  6.32e-03, 6.46e-03, 6.52e-03, 6.57e-03, 7.16e-03,
     5  8.51e-03, 1.06e-02, 1.48e-02, 3.72e-02, 4.74e-02,
     6  7.68e-02, 1.32e-01, 2.16e-01, 3.23e-01/

      if(wavl .le. w(1) ) then
         asio2 = ak(1)
         return
      end if

      do 10 i = 2, 34
         if(wavl .lt. w(i)) then
            slop  = (ak(i)-ak(i-1))/(w(i)-w(i-1))
            asio2 = slop*(wavl-w(i-1))+ak(i-1)
            return
         end if
   10 continue

      if(wavl .ge. w(34)) then
         asio2 = ak(34)
      else
         write(6,100) 'error in asio2'
      end if

  100 format(5x,a)


      end


      subroutine optsoot(wavl,dummy1,t,refre,refim)
c-----------------------------------------------------------------c
c     OPTICAL CONSTANTS OF SOOT                                   c
c     Ref.1 Z.G. Harbib and P. Vervisch, "On The Refractive       c
c     at Flame Temperature", Combust.Sci. and                     c
c     Index of Soot Tech. Vol.59,pp.121,1988                      c
c     Ref.2 S.c. Lee and C.L. Tien, "Optical Constants            c
c     of Soot in Hydrocarbon Flames",18th symp.(int.) on          c
```

```
c     Combustion pp.1159,1981                                           c
c-----------------------------------------------------------------------c
      implicit real*8(a-h,o-z)
      dimension a(2), b(2), c(2), dummy1(*)

c--   a(i)= wp(cm-1)    b(i)= wj(cm-1)   c(i)= gam(cm-1)
c-    wavl: wave length in micrometer
c-    vnu : wave number in cm-1

c-          Habib & Vervisch data
c-------------------------------------------------------------------
c      data ( a(i)   ,   b(i)    ,    c(i)   , i=1,2)/
c     1    7.690e+04 , 4.167e+04 , 2.333e+05 ,
c     2    2.545e+05 , 2.417e+05 , 2.417e+05 /
c
c      data   wpc    ,   gamc    /
c     1    2.112e+04 , 4.000e+04 /
c-----------------------------------------------------------------
c--         Lee and Tien data
c-----------------------------------------------------------------
      data ( a(i)   ,   b(i)    ,    c(i)   , i=1,2)/
     1    1.201e+05 , 4.167e+04 , 1.967e+05 ,
     2    3.979e+05 , 2.417e+05 , 1.867e+05 /

      data   wpc    ,   gamc    /
     3    5.049e+04 , 4.000e+04 /
c-----------------------------------------------------------------

      ref(f1,f2) = 0.7071*sqrt(f1+sqrt(f1*f1+f2*f2))


      vnu    = 6.283e+04/wavl
      tcor   = sqrt(t/1450.)

      fn2mk2 = 1.
      f2nk   = 0.

      do 10 i = 1, 2
         t1     = (b(i)**2 - vnu**2)**2+(c(i)*tcor*vnu)**2
         fn2mk2 = fn2mk2 + a(i)**2*(b(i)**2-vnu**2)/t1
         f2nk   = f2nk   + a(i)**2*vnu*c(i)*tcor/t1
  10  continue

      t2     = vnu*vnu + gamc*gamc*tcor
      fn2mk2 = fn2mk2 - wpc**2/t2
      f2nk   = f2nk   + wpc**2*gamc*tcor/(t2*vnu)
      refre  = ref(fn2mk2,f2nk)
      refim  = 0.5*f2nk/refre

      end

      subroutine optchar(wavl,dummy1,dummy2,refre,refim)
c-----------------------------------------------------------------------c
c-    OPTICAL CONSTANTS OF CHAR                                         c
c-----------------------------------------------------------------------c

      implicit real*8(a-h,o-z)
      dimension a(3), b(3), c(3), dummy1(*)

c--   a(i)= wp(cm-1)    b(i)= wj(cm-1)   c(i)= gam(cm-1)
c-    wavl: wave length in micrometer
c-    vnu : wave number in cm-1

            saraji coal char data
```

```
c-------------------------------------------------------------
c      data ( a(i)    ,    b(i)     ,     c(i)    , i=1,3)/
c     1    3.550e+04 , 1.357e+04 , 6.259e+03 ,
c     2    4.500e+03 , 3.597e+05 , 7.622e+05 ,
c     3    3.435e+04 , 7.593e+03 , 2.166e+04 /
c
c      data   wpc     ,    gamc     , refinf    /
c     1    1.371e+04 , 4.522e+00 , 2.046e-02 /
c-------------------------------------------------------------
c--          sufco coal char data
c      data ( a(i)    ,    b(i)     ,     c(i)    , i=1,3)/
c     1    2.252e+04 , 1.357e+04 , 9.869e+03 ,
c     2    4.506e+03 , 3.597e+05 , 7.622e+05 ,
c     3    3.950e+04 , 7.593e+03 , 3.896e+04 /
c
c      data   wpc     ,    gamc     , refinf    /
c     4    9.157e+03 , 5.187e+01 , 3.012e-02
c-------------------------------------------------------------
c-           west coal char data
c-------------------------------------------------------------
      data ( a(i)    ,    b(i)     ,     c(i)    , i=1,3)/
     1    3.542e+04 , 1.357e+04 , 3.418e+03 ,
     2    4.499e+03 , 3.597e+05 , 7.622e+05 ,
     3    3.450e+04 , 7.593e+03 , 1.964e+04 /

      data   wpc     ,    gamc     , refinf    /
     1    1.286e+04 , 1.548e-01 , 1.896e-02 /

c-------------------------------------------------------------

      ref(f1,f2) = 0.7071*sqrt(f1+sqrt(f1*f1+f2*f2))


      vnu    = 6.283e+04/wavl

      fn2mk2 = refinf**2
      f2nk   = 0.

      do 10 i = 1, 2
         t1     = (b(i)**2 - vnu**2)**2+(c(i)*vnu)**2
         fn2mk2 = fn2mk2 + a(i)**2*(b(i)**2-vnu**2)/t1
         f2nk   = f2nk   + a(i)**2*vnu*c(i)/t1
 10   continue

      t2     = vnu*vnu + gamc*gamc
      fn2mk2 = fn2mk2 - wpc**2/t2
      f2nk   = f2nk   + wpc**2*gamcr/(t2*vnu)
      refre  = ref(fn2mk2,f2nk)
      refim  = 0.5*f2nk/refre


      end


      subroutine absgas(vv,bl,t,ph2o,pco2,pco,pt,akh2o,akco2
     1                  ,akco,akgas)
c-------------------------------------------------------------------c
c      ref. j. heat mass transfer vol.16,pp25,1973                  c
c      bl     ,   radiation beam lenth  m                           c
c      vv     ,   wave number in 1/cm                               c
c      rhoh2o,  g/m**3                                              c
c      rhoco2,                                                      c
c      rhoco ,                                                      c
c      ph2o  ,  atm                                                 c
```

```
c      pco2  ,                                                          c
c      pco   ,                                                          c
c      pt,  atm                                                         c
c      akh2o  ,   wide band absorption coefficient in 1/m               c
c      akco2  ,                                                         c
c      akco   ,                                                         c
c      kgas  ,                                                          c
c      alph  ,  integrated band intensity                               c
c      bet   ,  line width parameter                                    c
c      w     ,  band width parameter                                    c
c      b     ,  pressure broadning parameter                            c
c      pe    ,  broadning pressure          c
c      soverd,  spectral band intensity over line spacing               c
c      f=1.43883027 /* cm.k*//*  h*c/kb    */                           c
c-----------------------------------------------------------------------c
      implicit real*8(a-h,o-z)

      real*8 v(3), al(3), be(3), h2ovk(3), co2vk(3), covk(1)

      real*8 h2oa0(7), h2ob0(5), h2ow0(5), h2ovc(5), h2on(1),
     1       co2a0(6), co2b0(6), co2w0(6), co2vc(6), co2n(6),
     2       coa0(2) , cob0(2) , cow0(2) , covc(2) , con(1)

      integer h2ogk(3), h2od1(3), h2od2(3), h2od3(9), h2od4(3),
     1        h2od5(3), co2gk(3), co2d1(3), co2d2(3), co2d3(3),
     2        co2d4(3), co2d5(3), co2d6(3), cod1 (2), cogk (1),
     3        d(3)    , g(3)

      data
     1   h2ovk /3652., 1595., 3756./,
     2   h2ogk /1, 1, 1/,
     3   h2od1 /0,0,0/,
     4   h2od2 /0,1,0/,
     5   h2od3 /0,2,0,1,0,0,0,0,1/,
     6   h2od4 /0,1,1/,
     7   h2od5 /1,0,1/,
     8   h2on  /1/,
     9   h2ovc /500.,1600.,3760.,5350.,7250./,
     @   h2oa0 /5200.,41.2,0.91,2.30, 22.40, 3.0, 2.5/,
     1   h2ob0 /0.14311, 0.09427, 0.13219, 0.08169, 0.11628/,
     2   h2ow0 /28.4, 56.4, 60.0, 43.1, 32. /

      data
     1   co2vk /1351., 667., 2396./,
     2   co2gk /1, 2, 1/,
     3   co2d1 /0,1,0/,
     4   co2d2 /-1,0,1/,
     5   co2d3 /0,-2,1/,
     6   co2d4 /0,0,1/,
     7   co2d5 /1,0,1/,
     8   co2d6 /2,0,1/,
     9   co2n  /0.7, 0.8, 0.8, 0.8, 0.65, 0.65/,
     @   co2vc /667., 960., 1060., 2350., 3660., 5200./,
     1   co2a0 /19., 2.47e-09, 2.48e-09, 110., 4., 0.066/,
     2   co2b0 /0.06157, 0.04017, 0.11888, 0.24723, 0.13341,0.39305/,
     3   co2w0 /12.7, 13.4, 10.1, 11.2, 23.5, 34.5/

      data
     1   covk /2143./,
     2   cogk /1/,
     3   cod1 /1,2/,
     4   con  /0.8/,
     5   covc /2143., 4260./,
     6   coa0 /20.9, 0.14/,
```

```
     7   cob0 /0.07506, 0.16758/,
     8   cow0 /25.5, 20./

c---- densities
      rhoh2o = 1.013e+05*ph2o*18./(8.3143*t)
      rhoco2 = 1.013e+05*pco2*44./(8.3143*t)
      rhoco  = 1.013e+05*pco*28./(8.3143*t)

      i     = 0
      t0    = 100.
      f     = 1.43883027d0
      akh2o = 0.0
      akco2 = 0.0
      akco  = 0.0

c--   H2O molecules
      if(ph2o .eq. 0.0) go to 45

      do 40 j = 1, 5
         if(abs(vv-h2ovc(j))/(h2ow0(j)*sqrt(t/t0)).gt.10.) go to 40
         nm = 3
         if(j.eq.3) go to 15

         if(j.eq.1) then
            alph = h2oa0(1)
            bet  = h2ob0(1)*sqrt(t/t0)

          else

            do 10 k = 1, 3
               v(k) = h2ovk(k)
               g(k) = h2ogk(k)
               go to (10,2,10,4,5) j

    2          d(k) = h2od2(k)
               go to 10

    4          d(k) = h2od4(k)
               go to 10

    5          d(k) = h2od5(k)
   10       continue

            nm=3
            call alpbet(alph,bet,f,v,d,g,t,t0,nm)

            if (i.gt.j) then
               jj = j+2

            else
               jj = j
            end if

            alph = h2oa0(jj)*alph
            bet  = h2ob0(j)*bet
         end if

   15    if(j.eq.3)then

          s1 = 0.0
          s2 = 0.0
          ks = 1
          i  = j-1
```

```
          do 30 kk = 1, 3
             k = 0
             i = i+1

             do 20 kl = ks, ks+2
                k    = k+1
                v(k) = h2ovk(k)
                g(k) = h2ogk(k)
                d(k) = h2od3(kl)
   20        continue

             call alpbet(alk,bek,f,v,d,g,t,t0,nm)
             al(kk) = h2oa0(i)*alk
             be(kk) = h2ob0(j)*bek
             ks     = ks+3
             sl     = sl+al(kk)
             s2     = s2+sqrt(al(kk)*be(kk))

   30     continue

          alph = sl
          bet  = s2*s2/sl

       end if

       b      = 8.6*sqrt(t0/t)+0.5
       pe     = (pt+ph2o*(b-1.))**h2on(1)
       w      = 1.2*h2ow0(j)*sqrt(t/t0)
       soverd = alph/w*exp(-2.*abs(vv-h2ovc(j))/w)
       akh2o  = akh2o+soverd*rhoh2o
     @          /sqrt(1.+soverd*rhoh2o*bl/(bet*pe))
   40 continue

c---- co2 molecules
   45 if(pco2.eq.0.0) go to 75

      do 70 j = 1, 6

         if(abs(vv-co2vc(j))/(co2w0(j)*sqrt(t/t0)).gt.10.) goto 70
         nm = 3

         do 60 k = 1, 3
            v(k) = co2vk(k)
            g(k) = co2gk(k)
            go to (51,52,53,54,55,56) j

  51        d(k) = co2d1(k)
            go to 60

  52        d(k) = co2d2(k)
            go to 60

  53        d(k) = co2d3(k)
            go to 60

  54        d(k) = co2d4(k)
            go to 60

  55        d(k) = co2d5(k)
            go to 60

  56        d(k) = co2d6(k)
  60    continue
```

```
      call alpbet(alph,bet,f,v,d,g,t,t0,nm)
      alph = co2a0(j)*alph
      bet  = co2b0(j)*bet
      b    = 1.3
      pe   = (pt+pco2*(b-1.))**co2n(j)
      w    = 1.2*co2w0(j)*sqrt(t/t0)
      soverd = alph/w*exp(-2.*abs(vv-co2vc(j))/w)
      akco2  = akco2+1.1*soverd*rhoco2
     @       /sqrt(1.+soverd*rhoco2*bl/(bet*pe))

   70 continue

c---- co gas
   75 if(pco.eq.0.0) goto 90

      nm =  1

      do 80 j = 1, 2

         if(abs(vv-covc(j))/(cow0(j)*sqrt(t/t0)).gt.10.) goto 80

         if(j.eq.1) then
            b = 1.1
         else
            b = 1.
         end if

         v(1) = covk(1)
         g(1) = cogk(1)
         d(1) = cod1(j)
         call alpbet(alph,bet,f,v,d,g,t,t0,nm)

         alph = coa0(j)*alph
         bet  = cob0(j)*bet
         pe   = (pt+pco*(b-1.))**con(1)
         w    = 1.2*cow0(j)*sqrt(t/t0)
         soverd = alph/w*exp(-2.*abs(vv-covc(j))/w)
         akco   = akco+soverd*rhoco
     @          /sqrt(1.+soverd*rhoco*bl/(bet*pe))

   80 continue

c---- absorption coefficient of gas mixutre

   90 akgas =akh2o+akco2+akco


      end

      subroutine alpbet(alph,bet,f,v,d,g,t,t0,nm)
c-----------------------------------------------------------------------c
c     SUBROUTINE ALPBET                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      real*8 v(*)
      integer d(*), g(*)

      s1 = 0.0
      s2 = 0.0

      do 10 k = 1, nm
         s1 = s1+f*v(k)*d(k)/t
         s2 = s2+f*v(k)*d(k)/t0
```

```
   10 continue

      call phipsy(psy,phi,t,f,v,d,g,nm)
      call phipsy(psy0,phi0,t0,f,v,d,g,nm)

      alph = (1.-exp(-s1))*psy/((1.-exp(-s2))*psy0)
      bet  = sqrt(t0/t)*phi/phi0

      end

      subroutine fctrl(n1,n2,n3,r1,r2,r3)
c-----------------------------------------------------------------------c
c     SUBROUTINE FCTRL                                                  c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)

      r1 = 1.0
      r2 = 1.0
      r3 = 1.0

      if(n1.gt.1) then
         do 10 i = 1, n1
            r1 = r1*i
   10    continue
      end if

      if(n2.gt.1) then
         do 20 i = 1, n2
            r2 = r2*i
   20    continue
      end if

      if(n3.gt.1) then
         do 30 i = 1, n3
            r3 = r3*i
   30    continue
      end if

      end

      subroutine phipsy(psy,phi,t,f,v,d,g,nm)
c-----------------------------------------------------------------------c
c     SUBROUTINE PHIPSY                                                 c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      real*8 v(*)
      integer d(*), g(*)

       t1 = 1.0
       t2 = 1.0
       t3 = 1.0

       do 30 k = 1, nm

          s1 = 0.0
          s2 = 0.0
          s3 = 0.0
          uk = f*v(k)/t
          expu = exp(-uk)

          if(d(k).gt.0) then
             is = 0
```

```
         else
            is = abs(d(k))
         end if

         do 10 iv = is, 30

            nd=abs(d(k))
            call fctrl(iv+g(k)+nd-1,g(k)-1,iv,r1,r2,r3)

            if(iv.eq.0) then
               f2 = 1.
            else
               f2 = expu**iv
            end if

            s1 = s1+r1*f2/(r2*r3)
            s2 = s2+sqrt(r1*f2/(r2*r3))
            if(f2.lt.1.d-06) go to 15

   10    continue

   15    t1 = t1*s1
         t2 = t2*s2

         do 20 iv = 0, 30
            call fctrl(iv+g(k)-1,g(k)-1,iv,r1,r2,r3)

            if(iv.eq.0) then
               f2 = 1.
            else
               f2=expu**iv
            end if

            s3 = s3+r1*f2/(r2*r3)
            if(f2.lt.1.d-06) go to 25
   20    continue

   25    t3 = t3*s3

   30 continue

      phi = t2**2/t1
      psy = t1/t3

      end


      subroutine output(nout)
c-----------------------------------------------------------------c
c     SUBROUTINE OUTPUT                                           c
c-----------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

      if (iout(nout) .eq. 0) return
      go to (10,20,30,40,50,60,70,80) nout

c---- gas composition
   10 continue
      write(6,501) 'combustion gas:CO2, H2O, SO2, N2, O2, CARB, ASH'
      write(6,503) (gas(n), n = 1,7)

c---- flow rates
```

```
      write(6,501) 'flow rates:fuel,air,flue and comb gas recirc'
      write(6,503) (flow(n), n = 1, 4)
      return

c---- radiosity field: ajxm(jmax,kmax,nf)
   20 continue
      return

c---- wall heat flux due to Gs: qxm(jmax,kmax,nf)
   30 continue
      write(6,501) 'qxm(jmax,kmax,nf) due to Gs'
      do 31 j = 1, jmax
      do 31 k = 1, kmax
         write(6,505) 'j = ',j,'k = ',k
         write(6,503) (qxm(j,k,ifrq), ifrq=1,nfrq)
   31 continue

c---- wall heat flux due to Gs: qym(imax,kmax,nf)
      write(6,501) 'qym(imax,kmax,nf) due to Gs'
      do 32 i = 1, imax
      do 32 k = 1, kmax
         write(6,505) 'i = ',i,'k = ',k
         write(6,503) (qym(i,k,ifrq), ifrq=1,nfrq)
   32 continue

c---- wall heat flux due to Gs: qzm(imax,jmax,nf)
      write(6,501) 'qzm(imax,jmax,nf) due to Gs'
      do 33 i = 1, imax
      do 33 j = 1, jmax
         write(6,505) 'i = ',i,'j = ',j
         write(6,503) (qzm(i,j,ifrq), ifrq=1,nfrq)
   33 continue
      return

c---- Gs field: gs(imax,jmax,kmax,nf)
   40 write(6,501) 'gs(imax,jmax,kmax,nf)'
      do 41 i = 1, imax
      do 41 j = 1, jmax
      do 41 k = 1, kmax
         write(6,505) 'i = ',i,'j = ',j,'k = ',k
         write(6,503) (gs(i,j,k,ifrq), ifrq=1,nfrq)
   41 continue
      return

c---- Gm field: gm(imax,jmax,kmax,nf)
   50 write(6,501) 'gm(imax,jmax,kmax,nf)'
      do 51 i = 1, imax
      do 51 j = 1, jmax
      do 51 k = 1, kmax
         write(6,505) 'i = ',i,'j = ',j,'k = ',k
         write(6,503) (gm(i,j,k,ifrq), ifrq=1,nfrq)
   51 continue
      return

c---- wall heat flux due to Gs and Gm: qxm(jmax,kmax,nf)
   60 continue
      write(6,501) 'qxm(jmax,kmax,nf) due to Gs and Gm'
      do 61 j = 1, jmax
      do 61 k = 1, kmax
         write(6,505) 'j = ',j,'k = ',k
         write(6,503) (qxm(j,k,ifrq), ifrq=1,nfrq)
   61 continue

c---- wall heat flux due to Gs and Gm: qym(imax,kmax,nf)
```

```
      write(6,501) 'qym(imax,kmax,nf) due to Gs and Gm'
      do 62 i = 1, imax
      do 62 k = 1, kmax
         write(6,505) 'i = ',i,'k = ',k
         write(6,503) (qym(i,k,ifrq), ifrq=1,nfrq)
   62 continue

c---- wall heat flux due to Gs and Gm: qzm(imax,jmax,nf)
      write(6,501) 'qzm(imax,jmax,nf) due to Gs and Gm'
      do 63 i = 1, imax
      do 63 j = 1, jmax
         write(6,505) 'i = ',i,'j = ',j
         write(6,503) (qzm(i,j,ifrq), ifrq=1,nfrq)
   63 continue
      return

c---- divergence field: divq(imax,jmax,kmax)
   70 write(6,501) 'divq(imax,jmax,kmax)'
      do 71 k = 1, kmax
      do 71 i = 1, imax
         write(6,505) 'k = ',k,'i = ',i
         write(6,503) (divq(i,j,k), j=1,jmax)
   71 continue
      return

c---- temperature field: t(imax,jmax,kmax)
   80 write(6,501) 't(imax,jmax,kmax)'
      do 81 k = 1, kmax
      do 81 i = 1, imax
         write(6,505) 'k = ',k,'i = ',i
         write(6,503) (t(i,j,k), j=1,jmax)
   81 continue
      return

c---- formats
  501 format(//10x,a,5x,a,i3,5x,a,1pe15.8)
  502 format(1x,a5,i3,1x,7 (1pe10.3),/8 (1pe10.3))
  503 format(8 (1pe10.3))
  504 format(/8 (3x,a,3x))
  505 format(/5x,10(a,i2,2x))

      end

      subroutine outpf
c-----------------------------------------------------------------------c
c     SUBROUTINE OUTPF                                                  c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'
      character head(nv)*7

      dimension  qwxmv(nv) , qwxpv(nv) ,  qwymv(nv)  ,  qwypv(nv) ,
     1           qwall(nv) , qwflux(nv),  qwv(nv)

      data (head(n),n=1,nv) /nv*'Vol No '/


c---- partial pressures and particle size spectrum: bottom zone
      write(6,501) 'ash/soot/char size spectrum in bottom zone'
      write(6,502) 'inum','rash','nash','rsot','nsot','rchr','nchr'
      write(6,503) '    ',' m  ','#/m3',' m  ','#/m3',' m  ','#/m3'
      nmx      = max(npt(1),npt(2),npt(3))
      t1       = 0.
```

```
      t2       = 0.
      t3       = 0.
      pi43     = 4./3.*pi

      do 10 n = 1, nmx
         t1    = t1+pi43*rpt(1,n)**3*pdist(1,n,1)*rhopt(1)
         t2    = t2+pi43*rpt(2,n)**3*pdist(2,n,1)*rhopt(2)
         t3    = t3+pi43*rpt(3,n)**3*pdist(3,n,1)*rhopt(3)
         write(6,504) n,rpt(1,n),pdist(1,n,1),rpt(2,n),pdist(2,n,1),
     1                rpt(3,n),pdist(3,n,1)
   10 continue

      write(6,507) 'average ash loading     =',t1,'kg/m**3'
      write(6,507) 'average soot loading    =',t2,'kg/m**3'
      write(6,507) 'average char loading    =',t3,'kg/m**3'
      write(6,507) 'partial pressure of CO2 =',pco2,'atm'
      write(6,507) 'partial pressure of H2O =',ph2o,'atm'
      write(6,507) 'partial pressure of CO  =',pco,'atm'

c---- partial pressures and particle size spectrum: flame zone
      write(6,501) 'ash/soot/char size spectrum in flame zone'
      write(6,502) 'inum','rash','nash','rsot','nsot','rchr','nchr'
      write(6,503) '    ',' m  ','#/m3',' m  ','#/m3',' m  ','#/m3'
      nmx      = max(npt(1),npt(2),npt(3))
      t1       = 0.
      t2       = 0.
      t3       = 0.
      pi43     = 4./3.*pi

      do 20 n = 1, nmx
         t1    = t1+pi43*rpt(1,n)**3*pdist(1,n,2)*rhopt(1)
         t2    = t2+pi43*rpt(2,n)**3*pdist(2,n,2)*rhopt(2)
         t3    = t3+pi43*rpt(3,n)**3*pdist(3,n,2)*rhopt(3)
         write(6,504) n,rpt(1,n),pdist(1,n,2),rpt(2,n),pdist(2,n,2),
     1                rpt(3,n),pdist(3,n,2)
   20  continue

      write(6,507) 'average ash loading     =',t1,'kg/m**3'
      write(6,507) 'average soot loading    =',t2,'kg/m**3'
      write(6,507) 'average char loading    =',t3,'kg/m**3'
      write(6,507) 'partial pressure of CO2 =',pco2,'atm'
      write(6,507) 'partial pressure of H2O =',ph2o,'atm'
      write(6,507) 'partial pressure of CO  =',pco,'atm'

c---- partial pressures and particle size spectrum: absorption zone
      write(6,501) 'ash/soot/char size spectrum in absorption zone'
      write(6,502) 'inum','rash','nash','rsot','nsot','rchr','nchr'
      write(6,503) '    ',' m  ','#/m3',' m  ','#/m3',' m  ','#/m3'
      nmx      = max(npt(1),npt(2),npt(3))
      t1       = 0.
      t2       = 0.
      t3       = 0.
      pi43     = 4./3.*pi

      do 30 n = 1, nmx
         t1    = t1+pi43*rpt(1,n)**3*pdist(1,n,3)*rhopt(1)
         t2    = t2+pi43*rpt(2,n)**3*pdist(2,n,3)*rhopt(2)
         t3    = t3+pi43*rpt(3,n)**3*pdist(3,n,3)*rhopt(3)
         write(6,504) n,rpt(1,n),pdist(1,n,3),rpt(2,n),pdist(2,n,3),
     1                rpt(3,n),pdist(3,n,3)
   30  continue

      write(6,507) 'average ash loading     =',t1,' kg/m**3'
      write(6,507) 'average soot loading    =',t2,' kg/m**3'
```

```
      write(6,507) 'average char loading    =',t3,' kg/m**3'
      write(6,507) 'partial pressure of CO2 =',pco2,' atm'
      write(6,507) 'partial pressure of H2O =',ph2o,' atm'
      write(6,507) 'partial pressure of CO  =',pco,' atm'

c---- optical properties
      write(6,501) 'Optical Properties of Combustion Gas'
      write(6,521) 'ifrq','bet1','omg1','bet2','omg2','bet3','omg3',
     1             ' ipl is4'
      write(6,503) '    ','m-1 ','    ','m-1 ','    ','m-1 ','    '
      k1          = kvol(1)
      k2          = kvol(2)
      k3          = kmax

      do 40 ifrq = 1, nfrq
         write(6,522) ifrq,beta(k1,ifrq),omeg(k1,ifrq),beta(k2,ifrq),
     1                omeg(k2,ifrq),beta(k3,ifrq),omeg(k3,ifrq),
     2                ipl(ifrq),is4(ifrq)
   40 continue

      write(6,501) 'Spectral Heat Transfer'
      write(6,511) 'ifrq',(ivol,ivol=1,nvol)

c---- initialize
      do 45 ivol = 1, nvol
         qwall(ivol)  = 0.0
         qwflux(ivol) = 0.0
  45  continue
      qwalzm   = 0.0
      qwalzp   = 0.0
      qwfluxm  = 0.0
      qwfluxp  = 0.0


      do 170 ifrq = 1, nfrq

c---     initialize the spectral quantities
         do 50 ivol = 1, nvol
            qwxmv(ivol) = 0.0
            qwxpv(ivol) = 0.0
            qwymv(ivol) = 0.0
            qwypv(ivol) = 0.0
   50    continue

         do 80 j  = 1, jmax

            ks   = 1
            ivol = 0

   60       ivol = ivol + 1
            kf   = kvol(ivol)

            do 70 k = ks , kf
               qwxmv(ivol) = qwxmv(ivol) + qxm(j,k,ifrq)*dfrq(ifrq)
               qwxpv(ivol) = qwxpv(ivol) + qxp(j,k,ifrq)*dfrq(ifrq)
   70       continue

            ks = kf + 1
            if(ivol.lt.nvol) goto 60

   80    continue

         do 120 i  = 1, imax
```

```
            ks   = 1
            ivol = 0

   90       ivol = ivol + 1
            kf   = kvol(ivol)

            do 110 k = ks , kf
               qwymv(ivol) = qwymv(ivol) + qym(i,k,ifrq)*dfrq(ifrq)
               qwypv(ivol) = qwypv(ivol) + qyp(i,k,ifrq)*dfrq(ifrq)
  110       continue

            ks = kf + 1
            if(ivol.lt.nvol) goto 90

  120    continue

         qwzmv = 0.0
         qwzpv = 0.0

         do 150 i = 1, imax
            do 140 j = 1, jmax
               qwzmv = qwzmv + qzm(i,j,ifrq)*dfrq(ifrq)
               qwzpv = qwzpv + qzp(i,j,ifrq)*dfrq(ifrq)
  140       continue
  150    continue

         do 155 ivol = 1, nvol
            qwv(ivol) = 0.5*(qwxmv(ivol)+qwxpv(ivol))/xwall(ivol)
     1                 +0.5*(qwymv(ivol)+qwypv(ivol))/ywall(ivol)
  155    continue

         write(6,512) ifrq,(qwv(ivol),ivol=1,nvol)

c----    summing ove frequency
         do 160 ivol = 1, nvol
            qwall(ivol) = qwall(ivol) + qwxmv(ivol) + qwxpv(ivol)
     1                  + qwymv(ivol) + qwypv(ivol) + qconv(ivol)/nfrq
            qwflux(ivol)= qwflux(ivol)
     1                  + 0.5*(qwxmv(ivol)+qwxpv(ivol))/xwall(ivol)
     2                  + 0.5*(qwymv(ivol)+qwypv(ivol))/ywall(ivol)
     3                  + 0.5*qconv(ivol)/(nfrq*(xwall(ivol)
     4                                     + ywall(ivol)))

  160    continue

         qwalzm   = qwalzm + qwzmv
         qwalzp   = qwalzp + qwzpv
         qwfluxm  = qwfluxm + qwzmv/zwall
         qwfluxp  = qwfluxp + qwzpv/zwall

  170  continue


      qtotal = qwalzm + qwalzp
      do 180 ivol = 1, nvol
         qtotal = qtotal + qwall(ivol)
  180 continue

      write(6,501) 'Wall Heat Flux  and Heat Transfer Rate Distribution'
      write(6,520) '     ','Qrate', 'Qflux',' Qrel'
      do 190 ivol = 1, nvol
         qrele = qfrac(ivol)*qfurn
         write(6,510) 'vol',ivol,qwall(ivol),qwflux(ivol),qrele
  190 continue
```

```
      write(6,513) 'bott ',qwalzm,qwfluxm
      write(6,513) 'top  ',qwalzp,qwfluxp
      write(6,513) 'totl ',qtotal

c---- heat balance
      write(6,501) 'summary output'
      write(6,502) '     ','temp','flow','enth','hin ','hout','divq'
      write(6,503) '     ',' K  ','kg/s','J/kg',' W  ',' W  ',' W  '

c---- fuel
      hinf    = flow(1)*(hhv+hfag(1))
      houtf   = flow(1)*(hv+hfag(1))
      write(6,505) 'fuel',temp(1),flow(1),hfag(1),hinf,houtf

c---- air
      hina    = flow(2)*hfag(2)
      write(6,505) 'air ',temp(2),flow(2),hfag(2),hina

c---- recirculating gas
      hinr    = flow(3)*hfag(3)
      write(6,505) 'recg',temp(3),flow(3),hfag(3),hinr

c---- furnace volume 1
      flow1   = flow(3)+flow(4)
      hin1    = flow(3)*hfag(3)+flow(4)*enth(2)
      hout1   = flow1*enth(1)
      write(6,505) 'vol1',tg(1),flow1,enth(1),hin1,hout1,divqv(1)

c---- furnace volume 2 .
      sumf    = flow(1)+flow(2)+flow(3)
      hin2    = houtf+hina+hout1
      hout2   = (sumf+flow(4))*enth(2)
      write(6,505) 'vol2',tg(2),sumf,enth(2),hin2,hout2,divqv(2)

c---- furnace volumes 3 through nv
      do 200 n = 3, nvol
         hin   = sumf*enth(n-1)
         hout  = sumf*enth(n)
         write(6,506) 'vol',n,tg(n),sumf,enth(n),hin,hout,divqv(n)
  200 continue

c---- furnace
      divqt   = 0.
      do 210 n = 1, nvol
         divqt = divqt+divqv(n) + qconv(n)
  210 continue
      hint    = houtf+hina+hinr
      houtt   = sumf*enth(nvol)
      write(6,505) 'furn',tg(nvol),sumf,enth(nvol),hint,houtt,divqt

c---- formats
  501 format('1',//20x,a//)
  502 format(10 (3x,a,4x))
  503 format(10 (3x,a,4x)/)
  504 format(3x,i3,4x,8 (1pe10.3,1x))
  505 format(3x,a4,4x,8 (1pe10.3,1x))
  506 format(3x,a3,i1,4x,6 (1pe10.3,1x))
  507 format(/,10x,a,1pe10.3,a)
  508 format(3x,i3,4x,6(1pe10.3,1x),2(3x,i3))
  509 format(/,a,8(1x,a,i1,1x))
  510 format(4x,a,i1,2x,4(2x,1pe10.3))
  511 format(/,a4,8(4x,i2,4x))
  512 format(1x,i3,8(1x,1pe9.2))
```

```
  513 format(4x,a,1x,4(2x,1pe10.3))
  520 format(1x,a5,5x,3(2x,a7,2x))
  521 format(6(3x,a,4x),3x,a,2x,2(a,1x))
  522 format(3x,i3,4x,6(1pe10.3,1x),2(1x,i2))


      end


      block data data1
c-----------------------------------------------------------------------c
c     BLOCK DATA DATA1                                                  c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'

c---- number of particle sizes
      data (npt(i), i= 1, 3) / 40,  40,  40 /

c---  band centers in 1/cm ( histogram )
      data (frq(n), n = 1, 37)  /
     1    285.0,   505.0,   755.0,  1055.0,  1310.0,  1630.0,  2020.0,
     2   2365.0,  2760.0,  3035.0,  3300.0,  3670.0,  3980.0,  4250.0,
     3   4600.0,  5000.0,  5415.0,  5730.0,  6225.0,  6565.0,  6890.0,
     4   7250.0,  7650.0,  7975.0,  8325.0,  8750.0,  9500.0, 10500.0,
     5  11500.0, 12500.0, 13500.0, 14500.0, 15500.0, 16500.0, 17500.0,
     6  18500.0, 19500.0          /

c---  band width
      data (dfrq(n), n = 1, 37)  /
     1   170.0,   270.0,   230.0,   370.0,   140.0,   500.0,   280.0,
     2   410.0,   380.0,   170.0,   360.0,   380.0,   240.0,   300.0,
     3   400.0,   400.0,   430.0,   470.0,   250.0,   430.0,   220.0,
     4   500.0,   300.0,   350.0,   350.0,   500.0,  1000.0,  1000.0,
     5  1000.0,  1000.0,  1000.0,  1000.0,  1000.0,  1000.0,  1000.0,
     6  1000.0,  1000.0   /

c---  Ash particle sizes
      data ((rpt(n1,n2), n2 = 1, 40),  n1 = 1, 1)   /
     1  0.10e-06,  0.25e-06,  0.50e-06,  0.75e-06,  1.00e-06,  1.25e-06,
     2  1.50e-06,  1.75e-06,  2.00e-06,  2.50e-06,  3.00e-06,  3.50e-06,
     3  4.00e-06,  4.50e-06,  5.00e-06,  6.00e-06,  7.00e-06,  8.00e-06,
     4  9.00e-06, 10.00e-06, 12.00e-06, 14.00e-06, 16.00e-06, 18.00e-06,
     5 20.00e-06, 22.00e-06, 24.00e-06, 26.00e-06, 28.00e-06, 30.00e-06,
     6 32.00e-06, 34.00e-06, 36.00e-06, 38.00e-06, 40.00e-06, 42.00e-06,
     7 44.00e-06, 46.00e-06, 48.00e-06, 50.00e-06   /

c---  Soot particle sizes
      data ((rpt(n1,n2), n2 = 1, 40),  n1 = 2, 2)   /
     1  0.01e-06,  0.02e-06,  0.03e-06,  0.04e-06,  0.05e-06,  0.06e-06,
     2  0.07e-06,  0.08e-06,  0.09e-06,  0.10e-06,  0.11e-06,  0.12e-06,
     3  0.13e-06,  0.14e-06,  0.15e-06,  0.16e-06,  0.17e-06,  0.18e-06,
     4  0.19e-06,  0.20e-06,  0.21e-06,  0.22e-06,  0.23e-06,  0.24e-06,
     5  0.25e-06,  0.26e-06,  0.27e-06,  0.28e-06,  0.29e-06,  0.30e-06,
     6  0.32e-06,  0.34e-06,  0.36e-06,  0.38e-06,  0.40e-06,  0.42e-06,
     7  0.44e-06,  0.46e-06,  0.48e-06,  0.50e-06   /


c----- Char particle sizes
      data ((rpt(n1,n2), n2 = 1, 40),  n1 = 3, 3)   /
     1  0.10e-06,  0.25e-06,  0.50e-06,  0.75e-06,  1.00e-06,  1.25e-06,
     2  1.50e-06,  1.75e-06,  2.00e-06,  2.50e-06,  3.00e-06,  3.50e-06,
     3  4.00e-06,  4.50e-06,  5.00e-06,  6.00e-06,  7.00e-06,  8.00e-06,
```

```
     4  9.00e-06, 10.00e-06, 12.00e-06, 14.00e-06, 16.00e-06, 18.00e-06,
     5 20.00e-06, 22.00e-06, 24.00e-06, 26.00e-06, 28.00e-06, 30.00e-06,
     6 32.00e-06, 34.00e-06, 36.00e-06, 38.00e-06, 40.00e-06, 42.00e-06,
     7 44.00e-06, 46.00e-06, 48.00e-06, 50.00e-06   /

c---- quadrature for s4

      data (xnu(i), i = 1 , 24)
     1 / 0.2958759,  0.9082483,  0.2958759,
     2   0.2958759,  0.9082483,  0.2958759,
     3   0.2958759,  0.9082483,  0.2958759,
     4   0.2958759,  0.9082483,  0.2958759,
     5  -0.2958759, -0.9082483, -0.2958759,
     6  -0.2958759, -0.9082483, -0.2958759,
     7  -0.2958759, -0.9082483, -0.2958759,
     8  -0.2958759, -0.9082483, -0.2958759 /

      data (yxi(i),i = 1 , 24)
     1 / 0.2958759,  0.2958759,  0.9082483,
     2  -0.2958759, -0.2958759, -0.9082483,
     3   0.2958759,  0.2958759,  0.9082483,
     4  -0.2958759, -0.2958759, -0.9082483,
     5   0.2958759,  0.2958759,  0.9082483,
     6  -0.2958759, -0.2958759, -0.9082483,
     7   0.2958759,  0.2958759,  0.9082483,
     8  -0.2958759, -0.2958759, -0.9082483/

      data (zet(i),i = 1 , 24)
     1 / 0.9082483,  0.2958759,  0.2958759,
     2   0.9082483,  0.2958759,  0.2958759,
     3  -0.9082483, -0.2958759, -0.2958759,
     4  -0.9082483, -0.2958759, -0.2958759,
     5   0.9082483,  0.2958759,  0.2958759,
     6   0.9082483,  0.2958759,  0.2958759,
     7  -0.9082483, -0.2958759, -0.2958759,
     8  -0.9082483, -0.2958759, -0.2958759/

      data (wt(i),i = 1, mumax)
     1 / mumax*0.523598776 /

c---  signs of direction cosines

      data (ixnu(i), i = 1 , 24)
     1 / 1,  1,  1,
     2   1,  1,  1,
     3   1,  1,  1,
     4   1,  1,  1,
     5  -1, -1, -1,
     6  -1, -1, -1,
     7  -1, -1, -1,
     8  -1, -1, -1 /

      data (iyxi(i),i = 1 , 24)
     1 / 1,  1,  1,
     2  -1, -1, -1,
     3   1,  1,  1,
     4  -1, -1, -1,
     5   1,  1,  1,
     6  -1, -1, -1,
     7   1,  1,  1,
     8  -1, -1, -1/

      data (izet(i),i = 1 , 24)
     1 / 1,  1,  1,
```

```
     2   1,  1,  1,
     3  -1, -1, -1,
     4  -1, -1, -1,
     5   1,  1,  1,
     6   1,  1,  1,
     7  -1, -1, -1,
     8  -1, -1, -1/


       end

      block data data2
c-----------------------------------------------------------------------c
c     BLOCK DATA2                                                       c
c-----------------------------------------------------------------------c

      implicit real*8(a-h,o-z)
      parameter(nsp=5)

      common /comb/ order , aoxid  , aprod , eoxid, eprod, parmod,parswl

      common /critc/ amw(nsp), tb (nsp), tc  (nsp), pc(nsp) , vc(nsp) ,
     1               ome(nsp), dip(nsp)
      common /heatc/ acp(nsp), bcp(nsp), ccp (nsp), dcp(nsp)

c---  CO2=1; N2=2; O2=3; H2O=4; SO2=5;

      data (amw(i), tb(i), tc(i), pc(i), vc(i), ome(i), dip(i),i=1,5)
     1   / 44.011 , 194.7, 304.2,  72.8,  94.0, 0.225 ,  0.0  ,
     4     18.015 , 373.2, 647.3, 217.6,  56.0, 0.344 ,  1.8  ,
     5     64.063 , 263.0, 430.8,  77.8, 122.0, 0.251 ,  1.6  ,
     2     28.013 ,  77.4, 126.2,  33.5,  89.5, 0.040 ,  0.0  ,
     3     31.999 ,  90.2, 154.6,  49.8,  73.4, 0.021 ,  0.0  /

      data ( acp(i) ,  bcp(i)  ,  ccp(i)  ,  dcp(i)  , i=1,nsp)
     1   / 1.980e+1 , 7.344e-2 ,-5.602e-5 , 1.715e-8 ,
     4     3.194e+1 , 1.436e-3 , 2.432e-5 ,-1.176e-8 ,
     5     2.385e+1 , 6.699e-2 ,-4.961e-5 , 1.328e-8 ,
     2     3.115e+1 ,-1.357e-2 , 2.680e-5 ,-1.168e-8 ,
     3     2.811e+1 ,-3.680e-6 , 1.746e-5 ,-1.065e-8 /

      data  order , aoxid , aprod ,  eoxid  , eprod , parmod , parswl
     1  /    0.6  , 590.  , 3.e+8 , 1.088e5 , 2.10e5,  0.3   ,  1.21 /

      end


      subroutine input
c-----------------------------------------------------------------------c
c     SUBROUTINE INPUT                                                  c
c-----------------------------------------------------------------------c

      implicit real*8 (a-h,o-z)
      include 'furn3d.h'
      character*80 card, title

c---- print card image of input data
   10 read(5,501,end=20) card
      write(6,501) card
      go to 10
   20 rewind 5

c---- problem title
      read(5,*) title
```

```
      write(6,502) title

c---- debug output index
      read(5,*) title, (iout(n), n = 1, 16)
      write(6,503) 'iout(1) - iout(16)'
      write(6,505) (iout(n), n = 1, 16)

c---- some parameters
      pi=2.*asin(1.0)

c---- selection of gray or spectral medium
      read(5,*) title, nfrq
      write(6,503) 'nfrq = 1 if gray medium and nfrq = 37 if spectral '
      write(6,506)  nfrq
      if (nfrq .gt. 1 .and. nfrq .ne. 37) then
         write(6,503) 'error in nfrq input : input 1 or 37'
         stop
      end if

c---- cut-off value of beta for P1 approximation and S4 and alpha
      read(5,*) title, betamx, betamn , alpha
      if(alpha .lt. 0.5 .or. alpha .ge. 1.) then
         write(6,503) 'error in alpha input: 0.5 <= alpha < 1.'
         stop
      end if
      if(betamn .lt. 0.005) then
         write(6,503) 'increase betamin to grater than 0.005'
         stop
      end if
      write(6,503) 'cut-off vales of beta for P1 & S4 and alpha'
      write(6,504) betamx,betamn,alpha

c---- maximum iterations in Gm solution, enclosure problem, energy equation
      read(5,*) title, nitergm, nitgmmn, niterj, maxcal
      write(6,503) 'nitergm, nitgmmn, niterj, maxcal'
      write(6,506) nitergm, nitgmmn, niterj, maxcal

c---- nonlinear solver parameters
      read(5,*) title, acc, deltg
      write(6,503) 'nonlinear solver parameters: acc, deltg'
      write(6,504) acc, deltg

c---- grid structure
      read(5,*) title,imax,jmax,kmax,nvol,(kvol(n), n = 1, nvol)
      if (nvol .gt. nv) then
          write(6,503) 'need to increase nv in common block'
          stop
       end if

      if (imax .gt. imx .or. jmax .gt. jmx .or. kmax .gt. kmx) then
         write(6,503) 'need to increase imx, jmx or kmx in common block'
         stop
      end if
      write(6,503) 'nodes : imax, jmax, kmax, nvol, kvol(n)'
      write(6,505) imax,jmax,kmax,nvol,(kvol(n), n = 1, nvol)

c---- convective heat transfer coefficients in W/m**2.K
      read(5,*) title,(hcoef(ivol),ivol = 1, nvol)
      write(6,503) 'convective heat transfer coefficients'
      write(6,504) (hcoef(ivol),ivol = 1, nvol)

c---- wall emissivity
      read(5,*) title, (ew(1,n), n = 1, nfrq)
      write(6,503) 'wall emissivity'
```

```
      write(6,504) (ew(1,n), n = 1, nfrq)
      do 40 k = 2, kmax
         do 30 ifrq = 1, nfrq
            ew(k,ifrq) = ew(1,ifrq)
   30    continue
   40 continue

c---- non-isotropicity factors
      read(5,*) title, (a1(1,n), n = 1, nfrq)
      write(6,503) 'non-isotropicity factors'
      write(6,504) (a1(1,n), n = 1, nfrq)
      do 60 k = 2, kmax
         do 50 ifrq = 1, nfrq
            a1(k,ifrq) = a1(1,ifrq)
   50    continue
   60 continue

c---- relaxation parameter(use 1.2)
      read(5,*) title, omegag
      write(6,503) 'relaxation parameter:  omegag'
      write(6,504) omegag

c---- furnace size
      read(5,*) title,xmax,ymax,zmax
      write(6,503) 'furnace size: xmax,   ymax,   zmax'
      write(6,504) xmax,ymax,zmax

c---- wall temperature
      read(5,*) title,txm,txp,tym,typ,tzm,tzp
      write(6,503) 'wall temperature: txm, txp, tym, typ, tzm, tzp'
      write(6,504) txm,txp,tym,typ,tzm,tzp

c---- fuel composition: ultimate analysis
      read(5,*) title, (fuel(n), n = 1,5)
      write(6,503) 'Ultimate: C  ,  H2  ,  S  ,  N2  ,  O2'
      write(6,504) (fuel(n), n = 1, 5)

c---- fuel composition: proximate analysis
      read(5,*) title, (fuel(n), n = 6,10)
      write(6,503) 'Proximate: H2O ,  ASH  ,  VM  ,  FC ,  SOOT'
      write(6,504) (fuel(n), n = 6,10)

c---- air composition
      read(5,*) title, (air(n), n = 1, 4)
      write(6,503) 'air: O2  ,  N2  ,  H2O , EXCESS AIR'
      write(6,504) (air(n), n = 1,4)

c---- gas recirculation
      read(5,*) title,fracr(1),fracr(2)
      write(6,503) 'flue gas recirc, combus gas recirc'
      write(6,504) fracr(1),fracr(2)

c---- combustion losses
      read(5,*) title,aloss(1),aloss(2),aloss(3)
      write(6,503) 'unburnt carb, unaccounted losses, rad loss'
      write(6,504) aloss(1),aloss(2),aloss(3)

c---- fuel/air/recirculated gas temperature
      read(5,*) title,temp(1),temp(2),temp(3)
      write(6,503) 'fuel, air preheat, recirc gas temperatures'
      write(6,504) temp(1),temp(2),temp(3)

c---- fuel high heating value and furnace rating
      read(5,*) title,hhv,qfurn
```

```
      write(6,503) 'hhv ','qfurn'
      write(6,504) hhv,qfurn

c---- ash composition
      read(5,*) title,(yash(n), n = 1,5)
      write(6,503) 'SiO2','Al2O3',' CaO','Fe2O3',' MGO'
      write(6,504) (yash(n), n = 1, 5)

c---- ash cumulative size distribution
      read(5,*) title,(ypt(1,n), n = 1, npt(1))
      write(6,503) 'ash cumulative mass fraction'
      write(6,504) (ypt(1,n), n = 1, npt(1))

c---- soot cumulative size distribution
      read(5,*) title,(ypt(2,n), n = 1, npt(2))
      write(6,503) 'soot cumulative mass fraction'
      write(6,504) (ypt(2,n), n = 1, npt(2))

c---- char cumulative size distribution
      read(5,*) title,(ypt(3,n), n = 1, npt(3))
      write(6,503) 'char cumulative mass fraction'
      write(6,504) (ypt(3,n), n = 1, npt(3))

c---- ash, soot, and char material densities
      read(5,*) title,rhopt(1),rhopt(2),rhopt(3)
      write(6,503) 'rash','rsot','rchr'
      write(6,504) rhopt(1),rhopt(2),rhopt(3)

c---  file names of extinction coefficients data
      read(5,*) title,qash,qsoot,qchar
      write(6,503) qash,qsoot,qchar

c---- include indices for efficiency factor calculation
      read(5,*) title,incl(1),incl(2),incl(3)
      write(6,503) 'iash','isot','ichr'
      write(6,506) incl(1),incl(2),incl(3)

c---- furnace pressure and temperature
      read(5,*) title,pgas,(trad(ivol), ivol = 1, nvol)
      write(6,503) 'pgas','trad'
      write(6,504) pgas,(trad(ivol), ivol = 1, nvol)

c---- read specific heat data
      open(unit=2,status='old',file='cp.d')
      do 70 is = 1, 8
         read(2,501)  title
         write(6,501) title
         read(2,507)  ((cp(is,n1,n2), n1=1,7), n2=1,2)
         write(6,507) ((cp(is,n1,n2), n1=1,7), n2=1,2)
   70 continue
      close(2)

c---- formats
  501 format(a80)
  502 format('1',5x,a50)
  503 format(/8 (3x,a,3x))
  504 format(8 (1pe10.3))
  505 format(20 (2x,i2))
  506 format(8 (3x,i4,3x))
  507 format(5 (e15.8))

      end
```

APPENDIX E: furn3d.h FILE

```
      parameter
     1 (  imx   =  16    , jmx    =  16    , kmx   = 60     , nf     =  37 ,
     2    imx2  = imx+2  , jmx2   = jmx+2  , kmx2  = kmx+2  , mumax  = 24  ,
     3    nv    = 10     , iwork  = 2*nv*nv+8*nv+6                        )

      character*15  qash, qsoot, qchar

      common /inpt1/
     1 ibeta(nf)      , ipl(nf)        , is4(nf)        , iout(20)       ,
     2 ixnu(mumax)    , iyxi(mumax)    , izet(mumax)    , imax           ,
     3 jmax           , kmax           , kvol(nv)       , maxcal         ,
     4 nitergm        , nitgmmn        , niterj         , nfrq           ,
     5 nvol


      common /inpt2/
     1 xmax           , ymax           , zmax

      common /inpt3/
     1 omegag

      common /inpt4/
     1 air(4)         , fracr(2)       , fuel(10)

      common /inpt5/
     1 aloss(3)       , cp(8,7,2)      , hhv            , qfurn          ,
     2 temp(3)

      common /inpt6/
     1 txm            ,  txp           , tym            , typ            ,
     2 tzm            ,  tzp

      common /inpt7/
     1 pgas           , rhopt(3)       , trad(nv)       , yash(5)        ,
     2 ypt(3,40)      , incl(3)        , npt(3)

      common /inpt8/
     1 acc            , deltg          , betamn         , betamx

      common /hbalc/
     1 amwg           , flow(4)        , divqv(nv)      , enth(nv)       ,
     2 gas(7)         , hfag(3)        , hres(nv)       , hv             ,
     3 tg(nv)

      common /radprop/
     1 al(kmx,nf)     , anum(3,40)     , beam           , beta(kmx,nf)   ,
     2 betal(kmx,nf)  , dfrq(37)       , ew(kmx,nf)     , frq(37)        ,
     2 omeg(kmx,nf)   , pco            , pco2           , ph2o           ,
     3 pdist(3,40,nv), qfrac(nv)       , rpt(3,40)

      common /files/
     1 qash           , qsoot          , qchar

      common /grids/
     1 delxm(imx)     , delxp(imx)     , delym(jmx)     , delyp(jmx)     ,
     2 delzm(kmx)     , delzp(kmx)     , dx(imx)        , dy(jmx)        ,
     3 dz(kmx)        , px(imx)        , py(jmx)        , pz(kmx)

      common /plnck/
     1 ebg(imx,jmx,kmx)    ,  ebwxm(jmx,kmx,nf) ,  ebwxp(jmx,kmx,nf)  ,
     2 ebwym(imx,kmx,nf)   ,  ebwyp(imx,kmx,nf) ,  ebwzm(imx,jmx,nf)  ,
     3 ebwzp(imx,jmx,nf)

      common /qflx/
```

```
     1 qxm(jmx,kmx,nf)     ,  qxp(jmx,kmx,nf)    ,  qym(imx,kmx,nf)     ,
     2 qyp(imx,kmx,nf)     ,  qzm(imx,jmx,nf)    ,  qzp(imx,jmx,nf)     ,
     3 qconv(nv)           ,  hcoef(nv)

      common /walls/
     1 xwall(nv)           ,  ywall(nv)          ,  zwall

      common /qflxt/
     1 qxmt(jmx,kmx) , qxpt(jmx,kmx) , qymt(imx,kmx) , qypt(imx,kmx) ,
     2 qzmt(imx,jmx) , qzpt(imx,jmx)

      common /dvrgq/
     1 divq(imx,jmx,kmx)   ,  gm(imx,jmx,kmx,nf),  gs(imx,jmx,kmx,nf)

      common /s4/
     1 ri(imx2,jmx2,kmx2,mumax)  ,
     2 wt(mumax)   , xnu(mumax)    , yxi(mumax)   , zet(mumax)     ,
     3 imax2       , jmax2         , kmax2

      common /field/
     1 t(imx,jmx,kmx)

      common /cons/
     1 pi

      common/coe/
     1 ae(imx,jmx,kmx)     ,  ah(imx,jmx,kmx)    ,  al(imx,jmx,kmx)    ,
     1 an(imx,jmx,kmx)     ,  ap(imx,jmx,kmx)    ,  as(imx,jmx,kmx)    ,
     2 aw(imx,jmx,kmx)     ,  s(imx,jmx,kmx)

      common /solve/
     1 tgl(nv)             ,  tgu(nv)            , rwork(iwork)

      common /tempr/
     1 alpha
```

APPENDIX F: cp.d FILE

```
CO2                 J 9/65C  1.O  2.00 0.00 0.G   300.000  5000.000
 0.44608041e+01 0.30981719e-02-0.12392571e-05 0.22741325e-09-0.15525954e-13
-0.48961442e+05-0.98635982e+00 0.24007797e+01 0.87350957e-02-0.66070878e-05
 0.20021861e-08 0.63274039e-15-0.48377527e+05 0.96951457e+01
H2O                 J 3/61H  2.O  1.00 0.00 0.G   300.000  5000.000
 0.27167633e+01 0.29451374e-02-0.80224374e-06 0.10226682e-09-0.48472145e-14
-0.29905826e+05 0.66305671e+01 0.40701275e+01-0.11084499e-02 0.41521180e-05
-0.29637404e-08 0.80702103e-12-0.30279722e+05-0.32270046e+00
SO2                 J 6/61S  1.O  2.00 0.00 0.G   300.000  5000.000
 0.52451364e+01 0.19704204e-02-0.80375769e-06 0.15149969e-09-0.10558004e-13
-0.37558227e+05-0.10873524e+01 0.32665338e+01 0.53237902e-02 0.68437552e-06
-0.52810047e-08 0.25590454e-11-0.36908148e+05 0.96513476e+01
N2                  J 9/65N  2.0  0.0  0.0  0.G   300.000  5000.000
 0.28963194e+01 0.15154866e-02-0.57235277e-06 0.99807393e-10-0.65223555e-14
-0.90586184e+03 0.61615148e+01 0.36748261e+01-0.12081500e-02 0.23240102e-05
-0.63217559e-09-0.22577253e-12-0.10611588e+04 0.23580424e+01
O2                  J 9/65O  2.0  0.0  0.0  0.G   300.000  5000.000
 0.36219535e+01 0.73618264e-03-0.19652228e-06 0.36201558e-10-0.28945627e-14
-0.12019825e+04 0.36150960e+01 0.36255985e+01-0.18782184e-02 0.70554544e-05
-0.67635137e-08 0.21555993e-11-0.10475226e+04 0.43052778e+01
C(S)                J 3/61C  1.0  0.0  0.0  0.S   300.000  5000.000
 0.13604942e+01 0.19182237e-02-0.84040389e-06 0.16448707e-09-0.11672670e-13
-0.65713870e+03-0.80070207e+01-0.44778053e+00 0.53691002e-02-0.39775571e-06
-0.40459298e-08 0.21134939e-11-0.94280688e+02 0.16840791e+01
ASH                 J 3/61C  1.0  0.0  0.0  0.S   300.000  5000.000
 0.00000000e+01 0.00000000e-02-0.00000000e-06 0.00000000e-09-0.00000000e-13
-0.00000000e+03-0.00000000e+01-0.00000000e+00 0.00000000e-02-0.00000000e-06
-0.00000000e-08 0.00000000e-11-0.00000000e+02 0.00000000e+01
COAL                J 3/61C  1.0  0.0  0.0  0.S   300.000  5000.000
 0.00000000e+01 0.00000000e-02-0.00000000e-06 0.00000000e-09-0.00000000e-13
-0.00000000e+03-0.00000000e+01-0.00000000e+00 0.00000000e-02-0.00000000e-06
-0.00000000e-08 0.00000000e-11-0.00000000e+02 0.00000000e+01
```

APPENDIX G: qchar FILE

4.8238332660962275E-05	1.3796158178635588E-04	5.1209270624316813E-04	1.7107550803998975E-03
4.7618735741401293E-03	1.1237481218442487E-02	2.3404269765925682E-02	4.4407671967047486E-02
7.8457208153175001E-02	2.0832518814530754E-01	4.6485223752027305E-01	8.7975638412533530E-01
1.4019251193606732E+00	1.9053337302594666E+00	2.2940450132632284E+00	2.6888026672657501E+00
2.7715755176627805E+00	2.7714719035643163E+00	2.7561322185786810E+00	2.7178327428447542E+00
2.6719443743076967E+00	2.6672363598959259E+00	2.6292957172890343E+00	2.5973376249018978E+00
2.5724890487789365E+00	2.5555394615493308E+00	2.5329033472984452E+00	2.5150598205835331E+00
2.4998463668806354E+00	2.4872983548409064E+00	2.4728959818013032E+00	2.4615983379501336E+00
2.4512303741991590E+00	2.4421591602692350E+00	2.4321446086880476E+00	2.4243806615006220E+00
2.4167086078808895E+00	2.4099681112597353E+00	2.4024648612175632E+00	2.3968698234307024E+00
3.8661359972040462E-07	1.5145793638915476E-05	2.4485518313541242E-04	1.2612562569362014E-03
4.0842033897608727E-03	1.0285134006320588E-02	2.2134494375895195E-02	4.2782175760861699E-02
7.6440278915930637E-02	2.0541721797948290E-01	4.6091796401987906E-01	8.7478414786152647E-01
1.3961935421735325E+00	1.8993308416259176E+00	2.2881724734535762E+00	2.6835461891408676E+00
2.7666349316415535E+00	2.7665250654443603E+00	2.7512663968288940E+00	2.7131700019469136E+00
2.6674375220739099E+00	2.6628858586574209E+00	2.6250504508475436E+00	2.5931920797127314E+00
2.5684106205828048E+00	2.5515286962833255E+00	2.5289432664781950E+00	2.5111481238764135E+00
2.4959718828821642E+00	2.4834605450108924E+00	2.4690882753570511E+00	2.4578185250105440E+00
2.4474746729932337E+00	2.4384256656448411E+00	2.4284317393222352E+00	2.4206851816846160E+00
2.4130307908854620E+00	2.4063042327448252E+00	2.3988169775864141E+00	2.3932326038102829E+00
2.2859171079535411E-02	5.9484330752945611E-02	1.4108949840758142E-01	2.9063289450788599E-01
5.9517835514003381E-01	1.1380484582980295E+00	1.8231453662379180E+00	2.4748070980143755E+00
3.0189474370486211E+00	3.7334691554104036E+00	4.0648392247057572E+00	4.2018308848212387E+00
4.1657802339543553E+00	4.0265036257684104E+00	3.8945726670618419E+00	3.7824398000595592E+00
3.7082469269698550E+00	3.6332455560143577E+00	3.5341819473765526E+00	3.4702051437391757E+00
3.3658053833580550E+00	3.2696605881472554E+00	3.1974943309461050E+00	3.1319442290162716E+00
3.0778861341432404E+00	3.0282478484898006E+00	2.9871740030854901E+00	2.9482007309629696E+00
2.9150020706339426E+00	2.8832256235497380E+00	2.8545861438977189E+00	2.8264814741681454E+00
2.8005020570526002E+00	2.7763186145568852E+00	2.7565865304982835E+00	2.7401856533141822E+00
2.7249002200785251E+00	2.7047221256392646E+00	2.6833575138150061E+00	2.6677425518235394E+00
1.3378207879993204E-05	5.3584260824222896E-04	9.3686802611315147E-03	5.4784724141092284E-02
2.0668494117893887E-01	5.7573377595098063E-01	1.1766462940166407E+00	1.8669349957338894E+00
2.5054599634396313E+00	3.3867986939192818E+00	3.7746537475766280E+00	3.9022942651524675E+00
3.8873238017178674E+00	3.7840642710010108E+00	3.6673903397024801E+00	3.5622296974008241E+00
3.5099069664701297E+00	3.4405178261426128E+00	3.3537401379242238E+00	3.2942032445714915E+00
3.2015429962390147E+00	3.1142618260382426E+00	3.0491165518477694E+00	2.9892790010716412E+00
2.9403111738871761E+00	2.8952092895479402E+00	2.8578206740380065E+00	2.8221997969252968E+00
2.7920103219153622E+00	2.7631444396988023E+00	2.7375700191886891E+00	2.7128236095770357E+00
2.6902389729715939E+00	2.6688683478380382E+00	2.6507527238450721E+00	2.6347697615111256E+00
2.6199860706358815E+00	2.6021967843608032E+00	2.5843649019488608E+00	2.5708456283746344E+00
1.9119797519594442E-01	4.7982904308392726E-01	9.6700245217583836E-01	1.4430629197039686E+00
1.8114643615453641E+00	1.9485102986398797E+00	1.9448914905687462E+00	1.9413827034206503E+00
1.9790763184594002E+00	2.1524991634480721E+00	2.3471236871008232E+00	2.4227552925350690E+00
2.4698103663847939E+00	2.5379847485719833E+00	2.5898192371307167E+00	2.6060331370113889E+00
2.6218656743966875E+00	2.5980936206394367E+00	2.5822095934624931E+00	2.5530459735142048E+00
2.5076855506573286E+00	2.4692062094708791E+00	2.4367216562715326E+00	2.4087026385824544E+00
2.3843480687572041E+00	2.3631262317573603E+00	2.3445310240052417E+00	2.3281069692294736E+00
2.3134874380692438E+00	2.3003875331668899E+00	2.2885796229904849E+00	2.2778773868522073E+00
2.2681275505161471E+00	2.2592030393869176E+00	2.2509991231962365E+00	2.2434284284343926E+00
2.2364161430310285E+00	2.2298999269746713E+00	2.2238259624621000E+00	2.2181478663591823E+00
3.5185951252136166E-05	1.3823404549701151E-03	2.2116543569172028E-02	1.0626159577457839E-01
2.7886698590948322E-01	4.6866154761393192E-01	6.0459735660500036E-01	6.9935937633889600E-01
7.7741484195889965E-01	9.2705655792734987E-01	1.0918381996665760E+00	1.2131011295659997E+00
1.2876016564480368E+00	1.3533936964623592E+00	1.4149834611647452E+00	1.4775355341772547E+00
1.5158879737551647E+00	1.5280657143526795E+00	1.5352868225060741E+00	1.5338415308607449E+00
1.5311000357763858E+00	1.5278946174091770E+00	1.5244986934946976E+00	1.5206430210734669E+00
1.5165518809391674E+00	1.5124998874784619E+00	1.5086065822784691E+00	1.5048958397135477E+00
1.5013698292324658E+00	1.4980291369087502E+00	1.4948702409853769E+00	1.4918841795161815E+00
1.4890595483860924E+00	1.4863847555550254E+00	1.4838489918968034E+00	1.4814420774745376E+00

.4791544697879397E+00	1.4769773826809172E+00	1.4749026701762122E+00	1.4729229946695483E+00
2.3700360551919038E-02	6.1913628838127330E-02	1.5000198482441482E-01	3.1824501961157198E-01
5.6732543286139323E-01	1.3459713232566601E+00	2.2533170817393691E+00	2.8129676622676527E+00
3.0472513438264111E+00	3.2172699285919952E+00	3.1392912486230431E+00	3.0457874587376850E+00
2.9660000316727824E+00	2.8981850663283817E+00	2.8345664959942387E+00	2.7225586706316292E+00
2.6465954290668945E+00	2.5891851057639812E+00	2.5454519777286939E+00	2.5108343311780925E+00
2.4563899129790761E+00	2.4144810369150314E+00	2.3810021768956489E+00	2.3537815272227243E+00
2.3311723955390979E+00	2.3119865735310876E+00	2.2954335745646435E+00	2.2809755200261890E+00
2.2682179889211782E+00	2.2568584801524305E+00	2.2466627868122164E+00	2.2374485044937900E+00
2.2290708812593101E+00	2.2214132193952008E+00	2.2143802943122823E+00	2.2078932930400357E+00
2.2018866743592889E+00	2.1963050418235426E+00	2.1911019982276110E+00	2.1862374815107648E+00
2.0373068270902135E-05	8.0792973959339497E-04	1.3600144728275991E-02	7.4076633776270967E-02
2.5116826600493858E-01	6.3051863003315189E-01	1.1868394062242182E+00	1.5921414453058884E+00
1.7311707071557958E+00	1.7461866834703184E+00	1.6266873302328533E+00	1.5272081274400846E+00
1.4688786481504663E+00	1.4304272507146749E+00	1.3958509206379177E+00	1.3425034835354377E+00
1.3182765791085640E+00	1.3057460249196866E+00	1.3003003811824387E+00	1.2979037467717114E+00
1.2949598825867961E+00	1.2918923883999280E+00	1.2887887552091364E+00	1.2860244962114631E+00
1.2835842397733692E+00	1.2813578091491051E+00	1.2792922815073042E+00	1.2773727595420314E+00
1.2755873932051938E+00	1.2739206517098771E+00	1.2723579976656556E+00	1.2708881545063482E+00
1.2695021729606626E+00	1.2681923123968628E+00	1.2669516385770683E+00	1.2657740396587851E+00
1.2646541869718859E+00	1.2635873876681183E+00	1.2625694748525857E+00	1.2615967278452254E+00
2.4541432555570498E-02	6.8523454751033205E-02	2.1599754184956671E-01	6.5592898998314930E-01
1.9337394460218338E+00	3.8807021781171729E+00	3.9957801980835792E+00	3.4982005418894624E+00
3.2574861384947105E+00	2.8324894454104901E+00	2.8194740580352575E+00	2.8334388273647715E+00
2.7691803320368096E+00	2.6896728374558818E+00	2.6409140571476528E+00	2.5855069762137859E+00
2.5302773752301899E+00	2.4896769004114638E+00	2.4560717396453517E+00	2.4276575274579759E+00
2.3830020761636104E+00	2.3488779234081663E+00	2.3217633270786617E+00	2.2995857002805238E+00
2.2810289052721786E+00	2.2652169728137066E+00	2.2515431187975099E+00	2.2395721954231047E+00
2.2289828101253866E+00	2.2195323136731258E+00	2.2110333813031215E+00	2.2033390378729409E+00
2.1963322113839485E+00	2.1899176240073102E+00	2.1840181844378113E+00	2.1785697409567719E+00
2.1735183712954922E+00	2.1688189801348576E+00	2.1644337886871159E+00	2.1603296845829894E+00
6.3388260143482883E-05	2.5410679219039405E-03	4.4421784180775671E-02	2.5616126439609860E-01
9.2365673789267111E-01	2.1158643638127037E+00	2.3921300499033342E+00	1.8437027491097864E+00
1.5370195289570832E+00	1.2587583526460056E+00	1.3526283234972838E+00	1.4557273712831023E+00
1.4455695237622070E+00	1.4046244975090323E+00	1.3936424261472478E+00	1.4008492417972367E+00
1.3929659492627993E+00	1.3890308465866437E+00	1.3852378399167085E+00	1.3815158493532060E+00
1.3753734423043202E+00	1.3701278113863011E+00	1.3655908287096861E+00	1.3616254059887947E+00
1.3581198765526348E+00	1.3549900093540870E+00	1.3521716018183518E+00	1.3496149026455109E+00
1.3472808276573456E+00	1.3451380381347662E+00	1.3431611367563920E+00	1.3413292572603348E+00
1.3396250690735987E+00	1.3380340385275971E+00	1.3365438983045508E+00	1.3351441656457546E+00
1.3338258565626908E+00	1.3325811980432121E+00	1.3314034184892745E+00	1.3302866361564250E+00
3.4866766570529811E-02	1.1906986297407181E-01	6.7042026779966624E-01	2.3215099084664153E+00
3.5149003247981070E+00	3.3182200845089911E+00	3.0215064058821675E+00	2.9405833188244994E+00
2.8789436636436978E+00	2.8028565697292280E+00	2.7352342078400098E+00	2.6677428721018330E+00
2.6187986587732746E+00	2.5798784502027137E+00	2.5461494052776867E+00	2.4911694339060761E+00
2.4493775953765251E+00	2.4159421903970104E+00	2.3885097344524349E+00	2.3654974820757930E+00
2.3288215680291913E+00	2.3006618848733531E+00	2.2781887572841111E+00	2.2597291012201421E+00
2.2442239141981202E+00	2.2309673521458362E+00	2.2194679425979822E+00	2.2093725443806358E+00
2.2004192155165794E+00	2.1924099830072530E+00	2.1851915736980585E+00	2.1786433549635640E+00
2.1726686703315239E+00	2.1671894589850220E+00	2.1621416760801866E+00	2.1574725084084969E+00
2.1531372523728356E+00	2.1490986947996378E+00	2.1453248258391620E+00	2.1417885119945685E+00
2.1663122662731309E-04	8.9553177456930966E-03	1.7697212425103034E-01	9.9125461341987720E-01
1.7883753035753163E+00	1.7421157050438618E+00	1.5125545329054895E+00	1.4866023351893787E+00
1.5004895390461424E+00	1.5340961454292292E+00	1.5364783885460978E+00	1.5212660689028950E+00
1.5140635527625881E+00	1.5108457809601559E+00	1.5059741992707274E+00	1.4964844803869870E+00
1.4889442543190841E+00	1.4823810537840194E+00	1.4766788445637837E+00	1.4716701063587523E+00
1.4632374998456414E+00	1.4563771844174933E+00	1.4506497763348347E+00	1.4457707696048474E+00
1.4415464440126440E+00	1.4378402880039867E+00	1.4345527496767920E+00	1.4316093646278842E+00
1.4289531092587329E+00	1.4265394818938304E+00	1.4243331510347041E+00	1.4223056521653517E+00

1.4204337378441076E+00	1.4186982307489382E+00	1.4170831173244052E+00	1.4155749383513736E+00
1.4141622618095933E+00	1.4128352989370336E+00	1.4115856344227276E+00	1.4104059588920466E+00
5.9118560031049323E-02	2.7955312695385770E-01	1.5916987765210497E+00	3.1128272535674268E+00
2.9940524675611928E+00	2.8660297272777386E+00	2.8951074970872357E+00	2.8125503382434855E+00
2.7596302630570677E+00	2.6882494668314334E+00	2.6323673626027775E+00	2.5822771435301024E+00
2.5429834859216758E+00	2.5109910634414079E+00	2.4834693512072361E+00	2.4391504816104681E+00
2.4049474589878792E+00	2.3773649068994502E+00	2.3546304109826757E+00	2.3354400731731220E+00
2.3046032101668059E+00	2.2806902066071904E+00	2.2614342694482308E+00	2.2454886258592222E+00
2.2319955562887857E+00	2.2203800844569082E+00	2.2102404137069547E+00	2.2012860151202300E+00
2.1933014218827753E+00	2.1861219676032411E+00	2.1796200252388274E+00	2.1736948659505360E+00
2.1682656840929000E+00	2.1632663095823856E+00	2.1586431023876966E+00	2.1543509117229940E+00
2.1503518998315063E+00	2.1466140430166707E+00	2.1431103893949683E+00	2.1398172198514125E+00
6.4723092048416669E-04	2.7889833539469853E-02	5.6214573704784399E-01	1.7267839568476502E+00
1.8151639812301521E+00	1.7586466806850227E+00	1.8206267246077343E+00	1.8068524148765359E+00
1.7871015186530661E+00	1.7767357006795848E+00	1.7608950865916597E+00	1.7442051533130352E+00
1.7313483206993592E+00	1.7202838955410996E+00	1.7102823356210677E+00	1.6937104591768248E+00
1.6805116594851761E+00	1.6695977582058186E+00	1.6604167090954220E+00	1.6525651734827880E+00
1.6397328707743555E+00	1.6296148371677055E+00	1.6213700886518632E+00	1.6144811721960277E+00
1.6086115387349449E+00	1.6035311760721203E+00	1.5990770710075639E+00	1.5951298942172287E+00
1.5915999636911520E+00	1.5884184449786669E+00	1.5855314536325340E+00	1.5828961313397449E+00
1.5804778978722569E+00	1.5782485095935654E+00	1.5761846141740907E+00	1.5742667195265256E+00
1.5724784404847461E+00	1.5708058228867241E+00	1.5692369640769916E+00	1.5677615824760456E+00
8.9845554938684569E-02	4.0140418163994285E-01	2.3360419831386317E+00	3.3808332435822916E+00
3.0236811600934352E+00	3.1125115135801642E+00	2.9886583256634438E+00	2.9456140573383349E+00
2.8979605657424083E+00	2.8146781561093648E+00	2.7497322311587538E+00	2.6994092657897908E+00
2.6581073078979109E+00	2.6231583177282332E+00	2.5936158440203845E+00	2.5462538470235865E+00
2.5089083581539873E+00	2.4783886717694905E+00	2.4528112748781217E+00	2.4310146317849828E+00
2.3953354982774742E+00	2.3670547397053130E+00	2.3438167473163278E+00	2.3242365602263857E+00
2.3073951572961473E+00	2.2926895260242013E+00	2.2796839300754121E+00	2.2680621418378597E+00
2.2575881958030521E+00	2.2480781110704280E+00	2.2393895744984138E+00	2.2314081098200482E+00
2.2240405923695841E+00	2.2172114184398306E+00	2.2108573152189703E+00	2.2049253864344172E+00
2.1993708022097636E+00	2.1941551145326175E+00	2.1892452384699257E+00	2.1846131069761978E+00
1.6695255161826711E-03	7.5723925004084452E-02	1.3759697690046042E+00	2.4542246542834172E+00
2.2184049168784790E+00	2.3148276237495531E+00	2.2561939188697875E+00	2.2306183033149178E+00
2.2121336195084074E+00	2.1646028851806811E+00	2.1269712610206915E+00	2.0971612584189749E+00
2.0720614681710825E+00	2.0506800444215401E+00	2.0325951024251734E+00	2.0031952649895892E+00
1.9797302326898842E+00	1.9604206995734883E+00	1.9442295989369058E+00	1.9303918448758655E+00
1.9077022388159766E+00	1.8897395293826542E+00	1.8750087872891774E+00	1.8626351545574040E+00
1.8520327407747466E+00	1.8428101839347424E+00	1.8346883912394532E+00	1.8274611052169694E+00
1.8209751167182651E+00	1.8151110862084940E+00	1.8097755963571700E+00	1.8048943230802375E+00
1.8004066103604681E+00	1.7962629433734647E+00	1.7924221815336916E+00	1.7888497151795681E+00
1.7855163934468399E+00	1.7823973016614743E+00	1.7794710021165150E+00	1.7767190248478417E+00
1.4794205728746174E-01	7.3037790176460704E-01	4.0830559578057688E+00	3.5476750460187323E+00
3.6549677150117486E+00	3.4188645287384984E+00	3.3913972390091991E+00	3.2701566205743142E+00
3.2260760435691989E+00	3.1116646627878195E+00	3.0263869215811665E+00	2.9592558006763685E+00
2.9041889704336645E+00	2.8575915327340278E+00	2.8172492447889326E+00	2.7501674730597703E+00
2.6962002271965817E+00	2.6514669458802707E+00	2.6133286173185244E+00	2.5801319925270478E+00
2.5248529560258257E+00	2.4801748935956760E+00	2.4430257340725294E+00	2.4114697305725898E+00
2.3842523589338254E+00	2.3604765712712066E+00	2.3394997111068090E+00	2.3208383225674036E+00
2.3041177875951857E+00	2.2890462796433311E+00	2.2753888017508155E+00	2.2629546688480624E+00
2.2515873522784222E+00	2.2411562355883223E+00	2.2315512983097365E+00	2.2226801597699373E+00
2.2144631059738140E+00	2.2068318083462222E+00	2.1997276440427580E+00	2.1930983835778690E+00
4.6025574634424825E-03	2.2913486417203074E-01	2.9851562948586343E+00	2.8337886411930184E+00
2.9138264151954862E+00	2.7832476439321638E+00	2.7588426920440989E+00	2.6838570823579433E+00
2.6489882853858098E+00	2.5691911069681770E+00	2.5080395409538654E+00	2.4589877577747243E+00
2.4182168318232922E+00	2.3834195105810929E+00	2.3531570785133580E+00	2.3027843497538267E+00
2.2623445655986782E+00	2.2288703889263668E+00	2.2003857571651482E+00	2.1757062834363849E+00
2.1349182875315615E+00	2.1022879951139850E+00	2.0754568429106715E+00	2.0529156420880564E+00
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1.9783547753662665E+00	1.9681880015021924E+00	1.9590444030355765E+00	1.9507774095256660E+00
1.9432676527928285E+00	1.9364162819165771E+00	1.9301408732085423E+00	1.9243723086047959E+00
1.9190518650136590E+00	1.9141295847416233E+00	1.9095625600990160E+00	1.9053137528745947E+00
2.2226136507605607E-01	1.2874881980318293E+00	4.9607202966640527E+00	3.8293074339864837E+00
3.9942947384429290E+00	3.7233693531705621E+00	3.6149213094195876E+00	3.5450840837390820E+00
3.4112887239604204E+00	3.2806177077545717E+00	3.1846028716353811E+00	3.1069229984109024E+00
3.0404093540483434E+00	2.9818595081922150E+00	2.9297135392690525E+00	2.8411456379826436E+00
2.7692541830609345E+00	2.7097095349049489E+00	2.6591402668564212E+00	2.6152532471031660E+00
2.5423359176711249E+00	2.4842562244841835E+00	2.4369413430110272E+00	2.3975903704852497E+00
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2.2717133246131112E+00	2.2552926471606569E+00	2.2407243790476650E+00	2.2277282201369029E+00
2.2160760509601505E+00	2.2055810593651684E+00	2.1960878064450422E+00	2.1874660403449209E+00
2.1796066156604557E+00	2.1724173546586276E+00	2.1658188941246119E+00	2.1597445541051536E+00
9.1354539720489465E-03	4.9432058338768514E-01	3.8760095293810508E+00	3.0605646782032085E+00
3.3005145057625467E+00	3.0586656612077725E+00	3.0241311451178476E+00	2.9480245634636768E+00
2.8671294960063030E+00	2.7641047410756410E+00	2.6881803899404977E+00	2.6271896246014430E+00
2.5754424445977229E+00	2.5302103459887206E+00	2.4900847692172006E+00	2.4220316205290837E+00
2.3667674571054369E+00	2.3210986550409838E+00	2.2826015136511297E+00	2.2495513076305333E+00
2.1955033578171781E+00	2.1532102592637319E+00	2.1193215846394278E+00	2.0916096131912543E+00
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2.0059618223662530E+00	1.9950979014824044E+00	1.9855022422348623E+00	1.9769684037099069E+00
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1.9454155771613106E+00	1.9406782019569364E+00	1.9363168739615790E+00	1.9322875599663720E+00
3.6061459561497233E-01	2.5871812921821080E+00	4.9392258731243013E+00	4.5785025495245675E+00
4.0483301346520468E+00	4.0463605742635256E+00	3.8115884964082891E+00	3.6828889424960560E+00
3.6025858037943017E+00	3.4195704844397481E+00	3.2871906804575399E+00	3.1827409362206494E+00
3.0905410360039807E+00	3.0120678313191132E+00	2.9469074246428315E+00	2.8380674487252762E+00
2.7506251953251049E+00	2.6788067365921218E+00	2.6185232886690040E+00	2.5675475888673880E+00
2.4860054247549592E+00	2.4239276517370403E+00	2.3753193673903699E+00	2.3364636819283255E+00
2.3048446662244011E+00	2.2787052587796923E+00	2.2568022341683616E+00	2.2382307456459376E+00
2.2223153115872170E+00	2.2085436686427968E+00	2.1965225491280123E+00	2.1859464228277710E+00
2.1765743003507128E+00	2.1682138936039781E+00	2.1607107744710001E+00	2.1539399809295841E+00
2.1477983320436778E+00	2.1422018238520328E+00	2.1370795725855922E+00	2.1323726154978728E+00
1.9552985579282048E-02	1.1812722645962903E+00	3.9775874556265962E+00	3.6521732252210062E+00
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3.0336175228420883E+00	2.8975319565359268E+00	2.7933273399366900E+00	2.7116536194444234E+00
2.6411232444460016E+00	2.5803652417069167E+00	2.5291741638285083E+00	2.4457000957683905E+00
2.3794210184947784E+00	2.3259893164581391E+00	2.2817635677166592E+00	2.2448477195970482E+00
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2.0628173415077597E+00	2.0452782053652410E+00	2.0305718890491344E+00	2.0180612855290243E+00
2.0072836196621036E+00	1.9978959070017650E+00	1.9896392481245804E+00	1.9823151111597908E+00
1.9757688485325853E+00	1.9698783033135114E+00	1.9645458655451020E+00	1.9596925281922244E+00
1.9552536863190291E+00	1.9511760726729905E+00	1.9474152749094753E+00	1.9439339997463965E+00
8.1098727877635846E-01	6.5132783959668794E+00	4.7718369667150027E+00	4.8704837362396702E+00
4.5625713089211057E+00	4.1351473889463772E+00	3.9446632115519602E+00	3.8158503967514026E+00
3.6578722337606151E+00	3.4343642837872492E+00	3.2699772293034512E+00	3.1258889664351717E+00
3.0181282043536819E+00	2.9264655356793043E+00	2.8472967812299479E+00	2.7218628425886862E+00
2.6270998352536297E+00	2.5530560404771236E+00	2.4941917695480735E+00	2.4463505237925833E+00
2.3741865992556663E+00	2.3228007679004103E+00	2.2846518489390060E+00	2.2553380094029931E+00
2.2321549499185456E+00	2.2133698214956823E+00	2.1978321496283613E+00	2.1847537136164239E+00
2.1735795061218450E+00	2.1639090403768133E+00	2.1554470450010283E+00	2.1479709535061056E+00
2.1413104131085374E+00	2.1353327451477364E+00	2.1299327752017527E+00	2.1250265939904613E+00
2.1205457687877263E+00	2.1164349939934533E+00	2.1126472575892712E+00	2.1091443306595083E+00
6.1553719531231739E-02	3.5293432476749280E+00	3.7676557050922947E+00	3.9949255896636418E+00
3.7192641041763683E+00	3.4288584063307970E+00	3.3157378344227473E+00	3.2055943429452398E+00
3.0841851443328099E+00	2.9184076309172382E+00	2.7920333962627213E+00	2.6864187298405677E+00
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2.3224140464434662E+00	2.2711961185906038E+00	2.2309988684719717E+00	2.1985667944889884E+00
2.1497501192927664E+00	2.1147427237581842E+00	2.0883613692501513E+00	2.0677033409402177E+00

2.0510342057322593E+00	2.0372593405119974E+00	2.0256552099114420E+00	2.0157243689294049E+00
2.0071131503456363E+00	1.9995629372978228E+00	1.9928799027697099E+00	1.9869157385859757E+00
1.9815548567872976E+00	1.9767057386986422E+00	1.9722948773420343E+00	1.9682625442382724E+00
1.9645596197946809E+00	1.9611453339065608E+00	1.9579855231445593E+00	1.9550513174787925E+00
1.9040423290724242E+00	9.1906039307646150E+00	5.6342487488239250E+00	4.6788712664588914E+00
4.3887800379951054E+00	4.2211359799792856E+00	3.9836348029144513E+00	3.7196030790161529E+00
3.5329376391076424E+00	3.3152787179308225E+00	3.1145527675636320E+00	2.9742169614350851E+00
2.8594893714749339E+00	2.7680347467432567E+00	2.6935670939033334E+00	2.5796457350643465E+00
2.4978645321314934E+00	2.4370203884122295E+00	2.3903564400775146E+00	2.3535968208358828E+00
2.2995626111676502E+00	2.2617793320579658E+00	2.2337959840715302E+00	2.2121436430397168E+00
2.1948179109069001E+00	2.1805855078409038E+00	2.1686483555657974E+00	2.1584662736673268E+00
2.1496601056724751E+00	2.1419550087368648E+00	2.1351466548018534E+00	2.1290793270485127E+00
2.1236323421484711E+00	2.1187108625622315E+00	2.1142385313309515E+00	2.1101534571381970E+00
2.1064052456333462E+00	2.1029515098130682E+00	2.0997576031502581E+00	2.0967935139296143E+00
1.8366369431778831E-01	5.5192711310068878E+00	4.1142627909956548E+00	3.7728344513686158E+00
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2.5072162304459731E+00	2.4443745274905750E+00	2.3941982115038312E+00	2.3178406123013033E+00
2.2632405909502844E+00	2.2223131930594842E+00	2.1904355436791199E+00	2.1648329181814385E+00
2.1260602591852269E+00	2.0978798332968940E+00	2.0763201673329252E+00	2.0592035314808115E+00
2.0452293066312159E+00	2.0335687773917490E+00	2.0236666820960028E+00	2.0151357319189214E+00
2.0076967998652790E+00	2.0011433114291028E+00	1.9953187174672171E+00	1.9901020971395045E+00
1.9853984577706871E+00	1.9811320174427014E+00	1.9772415619333976E+00	1.9736770205306926E+00
1.9703970623065110E+00	1.9673671978771898E+00	1.9645584155302027E+00	1.9619461385677321E+00
5.2008189986065414E+00	7.4454295304123139E+00	6.0754896377917404E+00	5.0491043398273945E+00
4.3882550616020479E+00	3.9731636320121346E+00	3.7052972400853221E+00	3.5170291398871827E+00
3.3633928162525448E+00	3.1066623378850253E+00	2.9307365186967722E+00	2.8018118308169693E+00
2.7013542694889532E+00	2.6254252820598110E+00	2.5639999426035320E+00	2.4738531042747378E+00
2.4108692572743871E+00	2.3645869246449522E+00	2.3291446401722551E+00	2.3010776530200729E+00
2.2592379336577384E+00	2.2292970301889330E+00	2.2066261419920714E+00	2.1887547252857713E+00
2.1742384532445502E+00	2.1621720804348992E+00	2.1519557027868190E+00	2.1431753966997484E+00
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2.1127130449019420E+00	2.1083602113819717E+00	2.1043952856361225E+00	2.1007653657436145E+00
2.0974282190476852E+00	2.0943477320086377E+00	2.0914945256483812E+00	2.0888422582494655E+00
6.2220111172030246E-01	4.7841578299896641E+00	4.4372611929435140E+00	3.8798785491380237E+00
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1.9882767625002506E+00	1.9843890969984312E+00	1.9808391460140413E+00	1.9775825134875566E+00
1.9745823978684622E+00	1.9718081034767103E+00	1.9692337380377765E+00	1.9668372777378083E+00
8.9417432545276956E+00	5.1157460105392181E+00	4.8857855845975173E+00	4.3536016284657935E+00
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3.0488024684257593E+00	2.8443226354557796E+00	2.7094366904957696E+00	2.6148251150035664E+00
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2.2610299082861243E+00	2.2437335774203886E+00	2.2290433660290381E+00	2.2053541526258860E+00
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2.0662156622283447E+00	2.0639341607339663E+00	2.0618405560810400E+00	2.0599113647109175E+00
2.0581267349900862E+00	2.0564701316606717E+00	2.0549272309468885E+00	2.0534863754883186E+00
1.4008201576048537E-01	1.2552166664645843E+00	2.2724568495819355E+00	2.4032178212030932E+00
2.3969177160865964E+00	2.3733504254760658E+00	2.3474425667376710E+00	2.3231400148269423E+00
2.3013318799671447E+00	2.2648328588070381E+00	2.2359383111915245E+00	2.2126097476633171E+00

2.1933813299820035E+00	2.1772384341873736E+00	2.1634705117613304E+00	2.1411634163899711E+00
2.1237894374926722E+00	2.1098098675400205E+00	2.0982745458570817E+00	2.0885637451533308E+00
2.0730489345111138E+00	2.0611307140775650E+00	2.0516344027086793E+00	2.0438557900769672E+00
2.0373448701994636E+00	2.0317994897236482E+00	2.0270085085909506E+00	2.0228195807853044E+00
2.0191197428946173E+00	2.0158232909881586E+00	2.0128639621732654E+00	2.0101895945714401E+00
2.0077585335312231E+00	2.0055370943593824E+00	2.0034976734128644E+00	2.0016174453027409E+00
1.9998773704178008E+00	1.9982613886606728E+00	1.9967558742602043E+00	1.9953491829635046E+00
2.6439856791962252E-01	1.3646543433372880E+00	2.3476574075073340E+00	2.4604683734988595E+00
2.4498742137746699E+00	2.4248764654327508E+00	2.3983311190219920E+00	2.3738013321373783E+00
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2.0142771282118539E+00	2.0131545840089471E+00	2.0121073677032797E+00	2.0111276422254769E+00
2.2981283116425777E-01	1.4621270721408886E+00	2.1900958922191225E+00	2.2456294811291486E+00
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2.2123562533782057E+00	2.1937769928328854E+00	2.1784769563412882E+00	2.1657932842506238E+00
2.1551337574543110E+00	2.1460481795405020E+00	2.1382037714781683E+00	2.1253112775190544E+00
2.1151156887420264E+00	2.1068146242399317E+00	2.0998994157464956E+00	2.0940319329766166E+00
2.0845691897074556E+00	2.0772254206826877E+00	2.0713264021019575E+00	2.0664624364990449E+00
2.0623688420742918E+00	2.0588657803966059E+00	2.0558268874005861E+00	2.0531600016438643E+00
2.0507972428198382E+00	2.0486858481559742E+00	2.0467855940978241E+00	2.0450641454262461E+00
2.0434958667215342E+00	2.0420600160363378E+00	2.0407393242507079E+00	2.0395194918494668E+00
2.0383889910137554E+00	2.0373375425535301E+00	2.0363564365098248E+00	2.0354386940842333E+00
2.0674256074322611E-01	1.4340460016403758E+00	2.1622695557677667E+00	2.2189317532224337E+00
2.2270907911645308E+00	2.2199292186247841E+00	2.2094071492061258E+00	2.1984958769117973E+00
2.1881459254978286E+00	2.1699494172574996E+00	2.1549145526067979E+00	2.1424254746854405E+00
2.1319146096375463E+00	2.1229462578671434E+00	2.1151966407433491E+00	2.1024481667242032E+00
2.0923566981792265E+00	2.0841343880454271E+00	2.0772809532008383E+00	2.0714630763843171E+00
2.0620752635017459E+00	2.0547852149183052E+00	2.0489268145222406E+00	2.0440945965257571E+00
2.0400262712705359E+00	2.0365439662353477E+00	2.0335223751590115E+00	2.0308704226317107E+00
2.0285201762464218E+00	2.0264198161854443E+00	2.0245290713037662E+00	2.0228161232998834E+00
2.0212554464823356E+00	2.0198263242724912E+00	2.0185117447757954E+00	2.0172975820316998E+00
2.0161720205157518E+00	2.0151250738001565E+00	2.0141482516859024E+00	2.0132342685496822E+00
2.5687689288813809E-01	1.5411874525519078E+00	2.1817269285381542E+00	2.2325750976155736E+00
2.2373049549213668E+00	2.2297057166532608E+00	2.2192568269709008E+00	2.2086714812761974E+00
2.1987265216878100E+00	2.1813637179275753E+00	2.1670861909257515E+00	2.1552556477457121E+00
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2.1079677672952397E+00	2.1002135436468539E+00	2.0937514466960248E+00	2.0882664680156240E+00
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2.0477831933204302E+00	2.0458027995188854E+00	2.0440199497547766E+00	2.0424045648049702E+00
2.0409328328698768E+00	2.0395850093873311E+00	2.0383452362533152E+00	2.0372001864835947E+00
2.0361385491003263E+00	2.0351513564382997E+00	2.0342298908444603E+00	2.0333677697849333E+00

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2.1787795069986124E+00	2.1616721470769584E+00	2.1475724431129675E+00	2.1358725500223451E+00
2.1260304686533416E+00	2.1176343967969400E+00	2.1103796527093577E+00	2.0984445659377102E+00
2.0889952508888596E+00	2.0812944067027361E+00	2.0748741050940560E+00	2.0694226905021602E+00
2.0606234494308513E+00	2.0537878394022235E+00	2.0482928398402556E+00	2.0437590387890952E+00
2.0399409759278417E+00	2.0366721399049696E+00	2.0338351961642722E+00	2.0313448452313927E+00
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2.0223119382724049E+00	2.0209687899282169E+00	2.0197331609743574E+00	2.0185918084008034E+00
2.0175336400864641E+00	2.0165493001977368E+00	2.0156308093445188E+00	2.0147713420439688E+00
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2.2254023950540787E+00	2.2176026740231558E+00	2.2074294206827170E+00	2.1972684461130196E+00
2.1877879472083284E+00	2.1713130214753957E+00	2.1578070045849209E+00	2.1466319493549744E+00
2.1372479143643015E+00	2.1292517623673439E+00	2.1223484207148511E+00	2.1110007175926362E+00
2.1020231016019606E+00	2.0947101688018024E+00	2.0886151826086050E+00	2.0834413344374032E+00
2.0750916096113965E+00	2.0686067571113811E+00	2.0633943609103742E+00	2.0590939443074703E+00
2.0554726083123511E+00	2.0523722257899286E+00	2.0496814856241912E+00	2.0473197599715540E+00
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2.1711366037669451E+00	2.1548359369532268E+00	2.1414517579891612E+00	2.1303663653022302E+00
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2.0860404110438107E+00	2.0787642961489627E+00	2.0726982283004274E+00	2.0675474873874613E+00
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2.0230134529423758E+00	2.0217427650590731E+00	2.0205737246454274E+00	2.0194938272958387E+00
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2.1787665856727148E+00	2.1629647972941219E+00	2.1500617777695141E+00	2.1394072505142430E+00
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2.1647069761075257E+00	2.1490261617240005E+00	2.1362079258211111E+00	2.1256160226370930E+00
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2.2084297238854180E+00	2.1997443923330913E+00	2.1897293854959892E+00	2.1800485331438137E+00
2.1711554674389166E+00	2.1558822000349349E+00	2.1434650093081511E+00	2.1332360116745073E+00
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2.2019596500511383E+00	2.1928833451438838E+00	2.1828497468233863E+00	2.1733074782421662E+00
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4.0421356548583653E-01	1.8242106704468299E+00	2.1576465053624538E+00	2.1935165684866895E+00
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2.0787280089224054E+00	2.0723677982775066E+00	2.0670699288892340E+00	2.0625742535651663E+00
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2.0276245276553828E+00	2.0268718115672999E+00	2.0261695621701503E+00	2.0255123580070600E+00
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2.1459961431683245E+00	2.1318446404706131E+00	2.1204894844991826E+00	2.1112039677808911E+00
2.1034634911020031E+00	2.0969003936111927E+00	2.0912539838401769E+00	2.0820052398498192E+00
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APPENDIX H: qsoot FILE

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2.1988604548721830E-02	2.5884549906517822E-02	3.0295037823658694E-02	3.5267186053515164E-02
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1.1814930581714238E+00	1.2860969491836298E+00	1.3953896537681019E+00	1.5086431276924901E+00
1.6249220440311911E+00	1.7430945210497897E+00	1.8618576444313240E+00	1.9797790157856328E+00
2.0953511771958278E+00	2.2070576107271593E+00	2.4131823907544496E+00	2.5884626581866166E+00
2.7270415102103351E+00	2.8277279041342704E+00	2.8937138196746215E+00	2.9314198031002903E+00
2.9489302027645024E+00	2.9544687792600444E+00	2.9552053451765237E+00	2.9564877046507791E+00
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5.9120191581586311E-04	1.2318976670009799E-03	2.2948417129927804E-03	3.9386445608870779E-03
6.3499709263436007E-03	9.7443471231973351E-03	1.4366530325998886E-02	2.0490186404584533E-02
2.8416559569195480E-02	3.8471764331393460E-02	5.1002292141974506E-02	6.6368261121897518E-02
8.4933992645978271E-02	1.0705559612844495E-01	1.3306529122539132E-01	1.6325258135107645E-01

1.9784285272985955E-01	2.3697422532213377E-01	2.8067424066468677E-01	3.2883879298971436E-01
3.8121533780578359E-01	4.3739378903152376E-01	4.9680678920940513E-01	5.5874177746734155E-01
6.2236483719223124E-01	6.8675544440436276E-01	8.1398475875511533E-01	9.3302964669724175E-01
1.0378963875166443E+00	1.1248797000871875E+00	1.1927825698862160E+00	1.2425917753102815E+00
1.2768655641710545E+00	1.2990632993835507E+00	1.3129467508494599E+00	1.3220907367625396E+00
3.6176586503116538E-02	7.2645777474522416E-02	1.0971872155690907E-01	1.4772779145562415E-01
1.8702748177242148E-01	2.2799490523638599E-01	2.7102966981893406E-01	3.1655284957990920E-01
3.6500464757501594E-01	4.1684053106603858E-01	4.7252508624090378E-01	5.3252331502874528E-01
5.9728860792445881E-01	6.6724716178969989E-01	7.4277810234518693E-01	8.2418960721135115E-01
9.1169068574112777E-01	1.0053604594717527E+00	1.1051153047142916E+00	1.2106775482167718E+00
1.3215478464768935E+00	1.4369867467124009E+00	1.5560079618536873E+00	1.6773884861547816E+00
1.7996976590287457E+00	1.9213461829901546E+00	2.0406522039205672E+00	2.1559210909573223E+00
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2.7868132280540685E+00	2.8512701107658560E+00	2.8879981980182898E+00	2.9063103705003877E+00
2.9151847277763219E+00	2.9218616029051283E+00	2.9310182910795199E+00	2.9445106694500263E+00
1.2186389324083231E-06	1.9530883119372238E-05	9.9141782624034770E-05	3.1447584664938785E-04
7.7120202646438116E-04	1.6075118218499924E-03	2.9955219825677126E-03	5.1426337630455302E-03
8.2926224356429934E-03	1.2726172679507763E-02	1.8760482941510077E-02	2.6747479023248085E-02
3.7070090102621647E-02	5.0135972644617922E-02	6.6367999190342530E-02	8.6190952633371370E-02
1.1001390811284865E-01	1.3820821791406401E-01	1.7108134932058483E-01	2.0884778647079669E-01
2.5159869223638703E-01	2.9927327923562380E-01	3.5163535536321122E-01	4.0825907818064966E-01
4.6852728851159775E-01	5.3164551460046450E-01	5.9667190064274056E-01	6.6256184905192672E-01
7.2822319173169092E-01	7.9257622452209020E-01	9.1344169579610712E-01	1.0187466670534022E+00
1.1048682688976750E+00	1.1710692023796279E+00	1.2189783536753576E+00	1.2518127866563373E+00
1.2735906235933554E+00	1.2884410711962597E+00	1.3000325989862547E+00	1.3111277894663460E+00
3.8492226250332016E-02	7.7332566075679288E-02	1.1689242850437004E-01	1.5756980013309374E-01
1.9979009863089328E-01	2.4400635398721551E-01	2.9069833354190733E-01	3.4037011200914086E-01
3.9354563896530859E-01	4.5076155416888575E-01	5.1255635279868494E-01	5.7945569759439441E-01
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1.9569333169821810E+00	2.0772021391910824E+00	2.1919422493548044E+00	2.2994859690356808E+00
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2.8074942278407002E+00	2.8471648782809447E+00	2.8691587192271961E+00	2.8832520629608926E+00
2.8967498933087262E+00	2.9135665235822765E+00	2.9341490973445672E+00	2.9561811506027538E+00
1.5651762334488565E-06	2.5088621411741960E-05	1.2738317836569511E-04	4.0417241568511909E-04
9.9147920569169347E-04	2.0673049805549713E-03	3.8533755445632296E-03	6.6166573703868763E-03
1.0670246545783092E-02	1.6373126275831727E-02	2.4128132489605922E-02	3.4377357408119424E-02
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1.1020700565239525E+00	1.2178092664039926E+00	1.3392364699916832E+00	1.4651701330274463E+00
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2.1013450805837728E+00	2.2158098690300068E+00	2.3216517387893778E+00	2.4175419394619033E+00
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2.9022362701379594E+00	2.9287110587952845E+00	2.9535285847713970E+00	2.9720820511554384E+00
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1.7661816074933265E-01	2.1961237747904977E-01	2.6850082684728782E-01	3.2301714076008264E-01
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9.0968539650680036E-01	9.6382281048953466E-01	1.0558942968934388E+00	1.1262159157023734E+00
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2.1995015742443344E-01	2.6971939541080314E-01	3.2286281174635240E-01	3.8006718908939446E-01
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1.6511505523672435E-02	2.5319759919288726E-02	3.7264257034654642E-02	5.2982398409835235E-02
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9.6802909822308991E-01	1.0163511950132926E+00	1.0957808365627566E+00	1.1540653762288771E+00
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1.2911189052400649E+00	1.3120927387777024E+00	1.3311261480673515E+00	1.3460589520189470E+00
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4.6022720702635517E-01	5.3197073345459711E-01	6.1058011259703548E-01	6.9668939739515057E-01
7.9078060006124529E-01	8.9311599955465037E-01	1.0036655998243349E+00	1.1220368505465297E+00
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9.0086352076666532E-01	9.5947084681207206E-01	1.0116005753605828E+00	1.0572009103580675E+00
1.0965045771867883E+00	1.1299836482388030E+00	1.1822650901470257E+00	1.2206432050229923E+00
1.2517687509359143E+00	1.2801995955124457E+00	1.3071480285059578E+00	1.3308603984204654E+00
1.3484401329313314E+00	1.3579434392113188E+00	1.3595224863001920E+00	1.3552610916479333E+00
4.5963089938268517E-02	9.2644703682952328E-02	1.4083381582590179E-01	1.9139812462068845E-01
2.4528306376722722E-01	3.0350543816857667E-01	3.6713873132213787E-01	4.3728624329818133E-01
5.1503863717911613E-01	6.0141131460947428E-01	6.9726002088980843E-01	8.0317487153685674E-01
9.1935970572643777E-01	1.0455097684656522E+00	1.1807094932484046E+00	1.3233773455022226E+00
1.4712829590993599E+00	1.6216496374541562E+00	1.7713376033146304E+00	1.9170766650656672E+00
2.0557108838003746E+00	2.1844176383353955E+00	2.3008867961740003E+00	2.4034671840395183E+00
2.4912859628629969E+00	2.5643348972498159E+00	2.6234894167984533E+00	2.6704289525735625E+00
2.7074409461181324E+00	2.7371378395237254E+00	2.7847455148773714E+00	2.8292081271723850E+00
2.8762404970004734E+00	2.9213384055883291E+00	2.9550868098840022E+00	2.9703274750937259E+00
2.9666288730331218E+00	2.9498488125428373E+00	2.9283603532143259E+00	2.9089611840881142E+00
4.6644733961185334E-06	7.4835881557884794E-05	3.8047177233052463E-04	1.2090954500220635E-03
2.9708121536404955E-03	6.2029415376253722E-03	1.1571980939390877E-02	1.9869739127461428E-02
3.1999490706092752E-02	4.8947102769028777E-02	7.1731875833584299E-02	1.0133265749304743E-01
1.3858817705104715E-01	1.8407617855239464E-01	2.3798502248328302E-01	3.0000060462965178E-01
3.6923913754384347E-01	4.4425435153574988E-01	5.2313629180903498E-01	6.0369317967002811E-01
6.8368234367378575E-01	7.6103805249813283E-01	8.3404288759091993E-01	9.0142008984467414E-01
9.6234467632729814E-01	1.0164067605271432E+00	1.0635574958943705E+00	1.1040600451669773E+00
1.1384459991528435E+00	1.1674682677628223E+00	1.2131473580715297E+00	1.2487639561194896E+00
1.2802870554760104E+00	1.3098825945815307E+00	1.3358755795909754E+00	1.3548666682409727E+00
1.3645034027993601E+00	1.3650614851421563E+00	1.3592210727950334E+00	1.3506857310677483E+00
4.6638937326495343E-02	9.4063607655276188E-02	1.4314164035712956E-01	1.9483209967020373E-01
2.5018387739338216E-01	3.1032733187431433E-01	3.7645513267300540E-01	4.4978784021149504E-01
5.3151878447293166E-01	6.2273450808193254E-01	7.2430755448117023E-01	8.3676579451155286E-01
9.6014795090289595E-01	1.0938670009679139E+00	1.2366118911695212E+00	1.3863206265343149E+00
1.5402503541170940E+00	1.6951491701247783E+00	1.8475028773384414E+00	1.9938103228749606E+00
2.1308388559496247E+00	2.2558364150441927E+00	2.3667076035772285E+00	2.4621713703290409E+00
2.5418976902573003E+00	2.6065797975345726E+00	2.6578864087432268E+00	2.6982594978075758E+00
2.7305818399131363E+00	2.7577799901387934E+00	2.8065242338478003E+00	2.8565988401602374E+00
2.9072420801458101E+00	2.9488926256581545E+00	2.9717768465814762E+00	2.9730367518702696E+00
2.9579488129811438E+00	2.9359449618422984E+00	2.9153443565733470E+00	2.8999430166719149E+00
5.3533321774622261E-06	8.5901469567143323E-05	4.3683111784093015E-04	1.3885716765368410E-03
3.4126912325349590E-03	7.1270168501588746E-03	1.3296939225512987E-02	2.2828676242088605E-02

3.6748979926657176E-02	5.6164746299688345E-02	8.2195997202438018E-02	1.1587775297291378E-01
1.5803161900796681E-01	2.0911714430526768E-01	2.6908555741220680E-01	3.3726968308437638E-01
4.1234924970744341E-01	4.9242130710420556E-01	5.7517960239416999E-01	6.5817165988926207E-01
7.3907196334498260E-01	8.1590345599764103E-01	8.8716235042818181E-01	9.5184387314809649E-01
1.0094024439953064E+00	1.0596922838685863E+00	1.1029174074527779E+00	1.1395924969101650E+00
1.1704977647189367E+00	1.1966112553371546E+00	1.2387705575431964E+00	1.2738498973398296E+00
1.3061344587184742E+00	1.3351662678576481E+00	1.3574350028146545E+00	1.3697305797183073E+00
1.3716441477188064E+00	1.3658153279789831E+00	1.3564348229571423E+00	1.3472764531027157E+00
4.7321064295041654E-02	9.5505111585970748E-02	1.4551117912047082E-01	1.9840532487128293E-01
2.5535841611399163E-01	3.1763503626162004E-01	3.8656846886233354E-01	4.6351584050490702E-01
5.4978675186291759E-01	6.4654033377737818E-01	7.5464932680944630E-01	8.7453790980017987E-01
1.0060111182798137E+00	1.1481077016675751E+00	1.2990185724197230E+00	1.4561082023610390E+00
1.6160613120294454E+00	1.7751355449487993E+00	1.9294697629091924E+00	2.0753828601763722E+00
2.2096246306927805E+00	2.3295834457025495E+00	2.4334849865327643E+00	2.5205893389195371E+00
2.5913382770357032E+00	2.6473608943333162E+00	2.6912731091061746E+00	2.7262861574037718E+00
2.7557119076819281E+00	2.7824780631156711E+00	2.8356990348539770E+00	2.8912891196686763E+00
2.9411426699334067E+00	2.9729230250114949E+00	2.9804565788809088E+00	2.9677405489114554E+00
2.9452431916522293E+00	2.9231900567054092E+00	2.9066825918190640E+00	2.8946763512993936E+00
6.1838144066369933E-06	9.9245633324152347E-05	5.0482222889049958E-04	1.6051854144945507E-03
3.9462246318727797E-03	8.2430699113513143E-03	1.5380254609006817E-02	2.6400710226914550E-02
4.2476198493360394E-02	6.4850649581383465E-02	9.4748532109752204E-02	1.3324431489970023E-01
1.8109786475562570E-01	2.3857506311889520E-01	3.0528931755838762E-01	3.8011229487527332E-01
4.6120006468217661E-01	5.4615633975504863E-01	6.3231088771540100E-01	7.1704525750924664E-01
7.9807679211763016E-01	8.7363100825163975E-01	9.4248710625333121E-01	1.0039350405646892E+00
1.0577077682498424E+00	1.1039306209913156E+00	1.1430905437848797E+00	1.1759971449976832E+00
1.2037100962199323E+00	1.2274234650308051E+00	1.2674192624586791E+00	1.3027969649881599E+00
1.3350347533916582E+00	1.3609451752213695E+00	1.3764035622802926E+00	1.3800413795958302E+00
1.3743030021674973E+00	1.3639201457538215E+00	1.3534321424750477E+00	1.3452535757041488E+00
4.8110074493622895E-02	9.7184807193650427E-02	1.4830495096729013E-01	2.0268058310401307E-01
2.6164777867911765E-01	3.2665341014181137E-01	3.9922088651739857E-01	4.8088908638290284E-01
5.7311502456425456E-01	6.7713527814320307E-01	7.9378657459211210E-01	9.2329972719059183E-01
1.0650987427350873E+00	1.2176545744417122E+00	1.3784481075419102E+00	1.5440838867623525E+00
1.7105488132553321E+00	1.8735601065024845E+00	2.0289184485276186E+00	2.1728039531251460E+00
2.3020216254150543E+00	2.4142516120422881E+00	2.5083330356105176E+00	2.5845108695956642E+00
2.6445042438364195E+00	2.6912799510694030E+00	2.7285516558580736E+00	2.7601272190458048E+00
2.7892839244135339E+00	2.8182962155442275E+00	2.8787367173773561E+00	2.9361704136900388E+00
2.9761767526873815E+00	2.9892275515951590E+00	2.9781701602378061E+00	2.9548621497004581E+00
2.9315593075584019E+00	2.9142912411245647E+00	2.9015145989751092E+00	2.8876189100614580E+00
7.3363567497084205E-06	1.1777108879201605E-04	5.9926016556668287E-04	1.9062264003418935E-03
4.6880924907879706E-03	9.7954215672156047E-03	1.8277823349255602E-02	3.1365461994857166E-02
5.0423740979102252E-02	7.6869678831594693E-02	1.1204067117488015E-01	1.5701417278786539E-01
2.1239276814525115E-01	2.7809097596366322E-01	3.5318214443547730E-01	4.3587173081210090E-01
5.2364125269473938E-01	6.1355431124899051E-01	7.0264925656275001E-01	7.8829961529615789E-01
8.6844019043241039E-01	9.4162736817272996E-01	1.0069855202193363E+00	1.0641286784641519E+00
1.1131173785802013E+00	1.1544442661072543E+00	1.1890036195225544E+00	1.2180014049795325E+00
1.2428000097989444E+00	1.2647234687670421E+00	1.3039279694629947E+00	1.3393957694455048E+00
1.3685823286083869E+00	1.3865724229550358E+00	1.3911344381364321E+00	1.3847312843854038E+00
1.3728658141114130E+00	1.3608340717900406E+00	1.3514620763770495E+00	1.3440968848496326E+00
4.9481162116690576E-02	1.0013092724582320E-01	1.5327872505593199E-01	2.1043310440079999E-01
2.7327572236203490E-01	3.4363538402038840E-01	4.2342991516371992E-01	5.1456157594565888E-01
6.1875267157115332E-01	7.3731617698044449E-01	8.7087401367413175E-01	1.0190643504871217E+00
1.1803121489991766E+00	1.3517520389533304E+00	1.5293694012959429E+00	1.7083487878378281E+00
1.8835297704235783E+00	2.0498356281102907E+00	2.2026157936019244E+00	2.3379776674978587E+00
2.4532265039393542E+00	2.5473858350795431E+00	2.6215593575346716E+00	2.6788443672678066E+00
2.7237109478960360E+00	2.7610363919261016E+00	2.7951048278714232E+00	2.8288428150040454E+00
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3.0036836485130469E+00	2.9848720888891660E+00	2.9586659892741016E+00	2.9367757614515115E+00
2.9205602428209794E+00	2.9041416844497521E+00	2.8818550632040694E+00	2.8532958777392667E+00
9.8277103749080088E-06	1.5784002343111539E-04	8.0369675534192715E-04	2.5585375221983736E-03

6.2969753200189027E-03	1.3163533866788047E-02	2.4562756640810680E-02	4.2117935587543294E-02
6.7579943848623786E-02	1.0266816952210930E-01	1.4883491944273125E-01	2.0696784660061823E-01
2.7708221406996636E-01	3.5809480170426561E-01	4.4778764182238795E-01	5.4303229539361875E-01
6.4024689833392001E-01	7.3594269203441565E-01	8.2716255928452065E-01	9.1168046014834492E-01
9.8798243922431339E-01	1.0551697447521575E+00	1.1129173025759460E+00	1.1614999010802953E+00
1.2018018814334601E+00	1.2352185598656074E+00	1.2634295895622070E+00	1.2880949553430925E+00
1.3105536752519857E+00	1.3316021822846809E+00	1.3695794046405700E+00	1.3979375268700260E+00
1.4112077634770905E+00	1.4089662207332430E+00	1.3966079402931979E+00	1.3814417912130745E+00
1.3682268562123090E+00	1.3573913307753052E+00	1.3466897679781076E+00	1.3342619821710338E+00
5.1416135723773418E-02	1.0432511452180755E-01	1.6046055191730274E-01	2.2182458578139738E-01
2.9067592228387990E-01	3.6947988357625305E-01	4.6079630686764805E-01	5.6707746126076719E-01
6.9035592208534269E-01	8.3182901592968161E-01	9.9139686111590775E-01	1.1672790126087429E+00
1.3558730111353923E+00	1.5519759271911073E+00	1.7493282581562231E+00	1.9412608984126496E+00
2.1212130487006093E+00	2.2831434135654227E+00	2.4221406262907723E+00	2.5354134107455049E+00
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2.8209634959759478E+00	2.8607300207320883E+00	2.9018593987395057E+00	2.9424486431915575E+00
2.9790024326751694E+00	3.0077890777351493E+00	3.0331993594601165E+00	3.0195498420502913E+00
2.9887674039328278E+00	2.9614896954032446E+00	2.9423054758406200E+00	2.9226812386855925E+00
2.8942996006852089E+00	2.8580027485723787E+00	2.8213651220857523E+00	2.7908441022735877E+00
1.4144694210370237E-05	2.2733293617385614E-04	1.1587064941437281E-03	3.6928558736686176E-03
9.0978868890150919E-03	1.9029600529263061E-02	3.5498966859319130E-02	6.0771411986124756E-02
9.7162213794445257E-02	1.4670241962186112E-01	2.1068709885885351E-01	2.8918844325662324E-01
3.8069989661530945E-01	4.8211451226731078E-01	5.8915703311242829E-01	6.9716999749931796E-01
8.0192565703761554E-01	9.0010324049892831E-01	9.8932379359952427E-01	1.0679801263601489E+00
1.1351902807001264E+00	1.1909504483905502E+00	1.2362695585174626E+00	1.2730467199593256E+00
1.3036519650684288E+00	1.3303556611969829E+00	1.3548003536303825E+00	1.3776771247440287E+00
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1.4268549033049147E+00	1.4064657939224527E+00	1.3883544974211162E+00	1.3734479660578305E+00
1.3582296047109574E+00	1.3403492247027784E+00	1.3211396233784760E+00	1.3038323038587867E+00
5.3625081968346124E-02	1.0914334165322095E-01	1.6879903273850128E-01	2.3522852172979708E-01
3.1143730463786812E-01	4.0070639879038923E-01	5.0638161218585687E-01	6.3149621263550104E-01
7.7820689599880710E-01	9.4709745374044840E-01	1.1365297632010722E+00	1.3423257971317535E+00
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2.3544711080815079E+00	2.4971213718101275E+00	2.6077212362009745E+00	2.6890912847791695E+00
2.7487197995603809E+00	2.7961903033528035E+00	2.8400185941224474E+00	2.8852641327183810E+00
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2.9681799051597437E+00	2.9467575509597905E+00	2.9154406674018509E+00	2.8726326036407208E+00
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1.9941200206193184E-05	3.2075193396124816E-04	1.6367240726384655E-03	5.2228192847399626E-03
1.2880475277614234E-02	2.6952094923927160E-02	5.0237912878516332E-02	8.5773340218081209E-02
1.3640629166919155E-01	2.0415961523419815E-01	2.8947901582756458E-01	3.9063207229339109E-01
5.0362765571685320E-01	6.2288909910506518E-01	7.4248545933610977E-01	8.5728163265191937E-01
9.6339858189096228E-01	1.0580169230780807E+00	1.1391746981823552E+00	1.2060290944612595E+00
1.2593006780408544E+00	1.3012893154927518E+00	1.3352484761456151E+00	1.3643928444706337E+00
1.3909678906000973E+00	1.4157097110292973E+00	1.4378684632615646E+00	1.4557702681617113E+00
1.4676758944101742E+00	1.4725660675557630E+00	1.4628447562361777E+00	1.4381717918419084E+00
1.4130961716483972E+00	1.3929371157280306E+00	1.3736027046188402E+00	1.3508567583300444E+00
1.3262799550698721E+00	1.3047022087235995E+00	1.2889512106800114E+00	1.2780782633183534E+00
5.6216966873181666E-02	1.1482108486691772E-01	1.7869898245971130E-01	2.5129571097694586E-01
3.3657062493148743E-01	4.3882525032602809E-01	5.6231570039628853E-01	7.1057294012289274E-01
8.8543857895013511E-01	1.0860153502394077E+00	1.3079691589966131E+00	1.5436587097234049E+00
1.7831355409498659E+00	2.0153600037230941E+00	2.2289637891415737E+00	2.4131191411220927E+00
2.5599265502447706E+00	2.6679273285061371E+00	2.7436918758874533E+00	2.7993614259201185E+00
2.8476100899750767E+00	2.8970354161230749E+00	2.9497984625849187E+00	3.0019418153112252E+00
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3.0622440473495467E+00	3.0397081451923422E+00	2.9999388724269727E+00	2.9742914551823310E+00
2.9451728907128598E+00	2.8997880858519625E+00	2.8477030776150429E+00	2.8045215880125145E+00
2.7735673144242061E+00	2.7472381786653650E+00	2.7198294188761891E+00	2.6932774938228921E+00

2.7593261908479176E-05	4.4423833970582441E-04	2.2697257079258579E-03	7.2524098787833998E-03
1.7903451300094131E-02	3.7465005565590140E-02	6.9722176235953420E-02	1.1854546011063434E-01
1.8708144614040331E-01	2.7665892570198075E-01	3.8576454897290008E-01	5.0970826298037630E-01
6.4147908408745369E-01	7.7355320029961205E-01	8.9954379922002792E-01	1.0146621256750097E+00
1.1152814054483244E+00	1.1989057371055329E+00	1.2649873668442830E+00	1.3155549825247086E+00
1.3546778330148341E+00	1.3869568692651808E+00	1.4158760666421502E+00	1.4427332015305747E+00
1.4665396313184642E+00	1.4849027673507584E+00	1.4954503920395030E+00	1.4970741822865115E+00
1.4904431825528948E+00	1.4777218590114996E+00	1.4453658058840160E+00	1.4170472597136980E+00
1.3936628025419486E+00	1.3677075623466222E+00	1.3379706480361138E+00	1.3106559422612012E+00
1.2908016891618428E+00	1.2776132968646616E+00	1.2676002704750906E+00	1.2591998779476421E+00
5.9265182891651634E-02	1.2152566819129787E-01	1.9047177094332984E-01	2.7057024398988649E-01
3.6698070375225689E-01	4.8524286732526822E-01	6.3058211131418678E-01	8.0673141759342704E-01
1.0143947801568831E+00	1.2498926129008989E+00	1.5048286724023561E+00	1.7671796160864881E+00
2.0229821778543813E+00	2.2573957931302742E+00	2.4559758425810396E+00	2.6086596465029088E+00
2.7153492444901448E+00	2.7872988780453958E+00	2.8417044955951956E+00	2.8935847128273919E+00
2.9499716996647196E+00	3.0084313003147987E+00	3.0598858700425331E+00	3.0943366525525695E+00
3.1064546440823397E+00	3.0979292116836818E+00	3.0758836066748403E+00	3.0491685062105640E+00
3.0248031764931600E+00	3.0059017170180118E+00	2.9778887876642299E+00	2.9390644584792005E+00
2.8820411300961668E+00	2.8264650712186628E+00	2.7866450112259451E+00	2.7569413508354330E+00
2.7270691135087555E+00	2.6971328305195246E+00	2.6729853572091717E+00	2.6558834087560963E+00
3.7539441766091896E-05	6.0498095525452931E-04	3.0952939039476986E-03	9.9040431939805291E-03
2.4469907962376435E-02	5.1182724674003435E-02	9.4990881309139324E-02	1.6051882495604716E-01
2.5063576015646427E-01	3.6481757121323732E-01	4.9820334908384145E-01	6.4236318389370439E-01
7.8775996417454068E-01	9.2621826446393674E-01	1.0515685269272108E+00	1.1589968240973698E+00
1.2453588322976041E+00	1.3107213791984562E+00	1.3589362370711069E+00	1.3960790131383478E+00
1.4277859861850644E+00	1.4570358796661864E+00	1.4833572835879465E+00	1.5037701116744657E+00
1.5149251177213505E+00	1.5151759671889982E+00	1.5054717099621635E+00	1.4888810269761321E+00
1.4693184244625661E+00	1.4501612846458511E+00	1.4186659473603831E+00	1.3910431004775692E+00
1.3584976915545031E+00	1.3244165112694946E+00	1.2977082629508854E+00	1.2805750355154479E+00
1.2686847821182863E+00	1.2589365296517234E+00	1.2520090183663590E+00	1.2489935332440758E+00
6.2826328545589907E-02	1.2939438996377256E-01	2.0439381122628010E-01	2.9356974450235213E-01
4.0356603533581548E-01	5.4136686997067784E-01	7.1308562737725079E-01	9.2201575387758039E-01
1.1663964490332484E+00	1.4380814642032491E+00	1.7232648081132018E+00	2.0047076027299564E+00
2.2634226760500096E+00	2.4803869948704738E+00	2.6423610582238468E+00	2.7502951054726616E+00
2.8205591948314441E+00	2.8756606191687091E+00	2.9324022485567247E+00	2.9950758855554120E+00
3.0558043666347325E+00	3.1011301168013010E+00	3.1211077432346928E+00	3.1150837620584704E+00
3.0910089400975989E+00	3.0603153985883327E+00	3.0323958039041665E+00	3.0112976729803536E+00
2.9954104841701135E+00	2.9797517263413913E+00	2.9325421721347200E+00	2.8672885499934502E+00
2.8109925175167527E+00	2.7735968281147394E+00	2.7423033696231749E+00	2.7092453685594871E+00
2.6803198392781900E+00	2.6602148634295406E+00	2.6452593042650041E+00	2.6307852683104249E+00
5.0290070421581165E-05	8.1137715790566690E-04	4.1574920372834910E-03	1.3321253727046057E-02
3.2931929613651809E-02	6.8798910674955444E-02	1.2714145310795816E-01	2.1298782195503288E-01
3.2786587296886055E-01	4.6780321951365045E-01	6.2338688978422452E-01	7.8268212365475853E-01
9.3498114170982582E-01	1.0721329153207617E+00	1.1877333604666447E+00	1.2778010917117399E+00
1.3431682252128054E+00	1.3898193244369876E+00	1.4259088540527263E+00	1.4577407094527965E+00
1.4871378993554880E+00	1.5114496577977463E+00	1.5261078131230539E+00	1.5280327737715624E+00
1.5176423445249725E+00	1.4985742258805084E+00	1.4758865340787666E+00	1.4539661210563808E+00
1.4350433089474470E+00	1.4188522366412151E+00	1.3871240344204234E+00	1.3494269792682720E+00
1.3133268183074922E+00	1.2884805397127401E+00	1.2733763645093523E+00	1.2620810263016213E+00
1.2534959445253628E+00	1.2493427618342527E+00	1.2492517760947353E+00	1.2509783128857786E+00
6.6950739882685184E-02	1.3855612721367261E-01	2.2074047026110047E-01	3.2083181997929949E-01
4.4727303910052874E-01	6.0864373377263192E-01	8.1161247780264356E-01	1.0578864400406696E+00
1.3413488675703871E+00	1.6474976963891907E+00	1.9558530414202808E+00	2.2427448498963116E+00
2.4835788635841531E+00	2.6602483437507360E+00	2.7733031634831438E+00	2.8440281764536515E+00
2.9007146139664033E+00	2.9621051388885524E+00	3.0294198519818303E+00	3.0893404694441586E+00
3.1253884748060585E+00	3.1300188298418385E+00	3.1087202430266134E+00	3.0749842230680025E+00
3.0420383785358562E+00	3.0168669538804305E+00	2.9986623411846685E+00	2.9814760172990411E+00
2.9591033376549181E+00	2.9291179400514076E+00	2.8580008304136473E+00	2.8009463814580258E+00
2.7642255936785944E+00	2.7305789797904336E+00	2.6961708245054679E+00	2.6698280041336164E+00

2.6524016008723534E+00	2.6373292929922001E+00	2.6220953042537500E+00	2.6085300763452515E+00
6.6438017020142365E-05	1.0732206705104440E-03	5.5078754647495008E-03	1.7671613854481669E-02
4.3694274231213456E-02	9.1077169996719401E-02	1.6726117263700863E-01	2.7690355188873456E-01
4.1855888655562057E-01	5.8308539543017179E-01	7.5617415534085131E-01	9.2368128407747396E-01
1.0746389551790105E+00	1.2005586467707152E+00	1.2962115331748130E+00	1.3629899354023614E+00
1.4090933483864982E+00	1.4448480485888657E+00	1.4770702638982447E+00	1.5061216903575478E+00
1.5272080090469917E+00	1.5349260561733480E+00	1.5275816690642627E+00	1.5083259008738017E+00
1.4832298293507764E+00	1.4582477649220191E+00	1.4367723871823661E+00	1.4188026859586433E+00
1.4020300065631373E+00	1.3840236662686518E+00	1.3428850881604681E+00	1.3058218399390624E+00
1.2826705559216909E+00	1.2688847941214987E+00	1.2583503222674426E+00	1.2517299681961394E+00
1.2503212321173736E+00	1.2520795160068134E+00	1.2545324007472589E+00	1.2570261866382841E+00
7.1688433860949585E-02	1.4914377280409508E-01	2.3980577997213987E-01	3.5294093783701386E-01
4.9912028365494632E-01	6.8854325977815101E-01	9.2769490907805574E-01	1.2148868168134599E+00
1.5372468295139337E+00	1.8720013270561473E+00	2.1905549309056775E+00	2.4618953754307684E+00
2.6608298561261754E+00	2.7845699805573236E+00	2.8581246029149865E+00	2.9163924758792801E+00
2.9812954485192837E+00	3.0516896392287838E+00	3.1093406020116321E+00	3.1358107047236010E+00
3.1271059283577203E+00	3.0948169304630415E+00	3.0564015961129893E+00	3.0246156009691902E+00
3.0023418566207689E+00	2.9839959483490093E+00	2.9615264100119587E+00	2.9306748412791670E+00
2.8933114535417435E+00	2.8551859266765049E+00	2.7957294951682039E+00	2.7584289985701647E+00
2.7229434591029240E+00	2.6882852219989393E+00	2.6640769710259051E+00	2.6475418291339365E+00
2.6315754425549645E+00	2.6160726171524127E+00	2.6029222710533659E+00	2.5910416783734629E+00
8.6671125400587535E-05	1.4019189639847324E-03	7.2066366895460901E-03	2.3149753098320233E-02
5.7216025680144625E-02	1.1882908406172386E-01	2.1632051837168298E-01	3.5261826667622131E-01
5.2120180564017160E-01	7.0651795978848664E-01	8.9024979975395531E-01	1.0573727937169763E+00
1.1965887938444724E+00	1.3007284826923426E+00	1.3710512565829140E+00	1.4177922820487847E+00
1.4537015158543778E+00	1.4863605886246518E+00	1.5147851193584434E+00	1.5323163989422386E+00
1.5333534289191217E+00	1.5181809749183095E+00	1.4926869418529429E+00	1.4646650489143085E+00
1.4398229032996355E+00	1.4195918392359546E+00	1.4017230219436396E+00	1.3830445418115780E+00
1.3621382520443126E+00	1.3400726355167318E+00	1.3020251943652437E+00	1.2798233149732452E+00
1.2670356915077785E+00	1.2575378414744087E+00	1.2529096385533016E+00	1.2534870053878981E+00
1.2561808282035913E+00	1.2589446203741372E+00	1.2616732090582252E+00	1.2643008364397434E+00
7.7092547371240341E-02	1.6130173183277088E-01	2.6191492970016333E-01	3.9054367615077273E-01
5.6019974753743829E-01	7.8249161344382434E-01	1.0623809003885112E+00	1.3922037260197135E+00
1.7495917916298440E+00	2.1015817594675585E+00	2.4102117334258857E+00	2.6410275686889650E+00
2.7834316366028791E+00	2.8632090851417615E+00	2.9226896774887066E+00	2.9894744365199926E+00
3.0619704038570337E+00	3.1177796441102261E+00	3.1366449545560293E+00	3.1179100356129337E+00
3.0784317850884988E+00	3.0382720683710991E+00	3.0084602187733220E+00	2.9874961291574436E+00
2.9663495747417477E+00	2.9373021756350228E+00	2.8997747539068905E+00	2.8594816124405025E+00
2.8233810800793164E+00	2.7951922431731289E+00	2.7563404658520634E+00	2.7198256558761171E+00
2.6849199683219411E+00	2.6616017110118464E+00	2.6448659807509207E+00	2.6279680848319829E+00
2.6122469490309062E+00	2.5988675380024273E+00	2.5860215417661512E+00	2.5728250863254605E+00
1.1178661184466120E-04	1.8107440009366802E-03	9.3238949704978896E-03	2.9980302327812441E-02
7.4008766091748168E-02	1.5287433597724631E-01	2.7502443969774243E-01	4.3961886961436880E-01
6.3286590365806927E-01	8.3267717486457049E-01	1.0183490955334655E+00	1.1745213841180129E+00
1.2911249070443296E+00	1.3680378890217140E+00	1.4169350336983026E+00	1.4533919617678135E+00
1.4865220553646068E+00	1.5145391887184485E+00	1.5292084809035345E+00	1.5249425362565090E+00
1.5040335835730441E+00	1.4747579257024532E+00	1.4459330548412814E+00	1.4222687412990485E+00
1.4030180948344850E+00	1.3844442863338662E+00	1.3637973865713213E+00	1.3413996650421534E+00
1.3198388924139315E+00	1.3018436691391440E+00	1.2795594369254937E+00	1.2676204389433333E+00
1.2591616291348540E+00	1.2560125704062903E+00	1.2577768118739172E+00	1.2608804316752529E+00
1.2637305225954536E+00	1.2664355207054674E+00	1.2687567407786433E+00	1.2702645916101947E+00
8.3221475356283950E-02	1.7519076940839409E-01	2.8743221604860208E-01	4.3435503849020868E-01
6.3165554232008347E-01	8.9174684706036933E-01	1.2159080184108204E+00	1.5871458602675084E+00
1.9707385096635126E+00	2.3218649577123194E+00	2.5953779326596060E+00	2.7676070229215868E+00
2.8594131436936183E+00	2.9202489027936753E+00	2.9870021197504628E+00	3.0610512805814403E+00
3.1169165633438691E+00	3.1316003374327108E+00	3.1063858887057569E+00	3.0623556053703602E+00
3.0215669899955238E+00	2.9931979936153921E+00	2.9720239475444474E+00	2.9470815252990032E+00
2.9124665853116447E+00	2.8713598010807040E+00	2.8317575138503224E+00	2.7998221108208137E+00
2.7763791574730083E+00	2.7578723449847877E+00	2.7210841896037983E+00	2.6853563360396455E+00

2.6615962151882444E+00	2.6441567682161460E+00	2.6263527533473687E+00	2.6100983459845621E+00
2.5959817378528909E+00	2.5820500287442583E+00	2.5679493095183314E+00	2.5543535095198875E+00
1.4270766975781174E-04	2.3151220146505843E-03	1.1941119693747042E-02	3.8420461436446757E-02
9.4629176897363221E-02	1.9397732324104611E-01	3.4362682346147672E-01	5.3631128597577904E-01
7.4930951286193292E-01	9.5517670272842670E-01	1.1322864542603428E+00	1.2663444325527407E+00
1.3541141716888709E+00	1.4074033854915897E+00	1.4449304096648892E+00	1.4786253212277720E+00
1.5069330428940158E+00	1.5202615804467783E+00	1.5127338952820031E+00	1.4882352449189713E+00
1.4570195701715118E+00	1.4285318230030992E+00	1.4062722277769633E+00	1.3876489543270907E+00
1.3683151879654631E+00	1.3466425373958248E+00	1.3245549287574274E+00	1.3053247055866675E+00
1.2910470013145037E+00	1.2815724118220646E+00	1.2702425712002641E+00	1.2626206601739782E+00
1.2602548803839173E+00	1.2625913152369015E+00	1.2658255466996118E+00	1.2685884975087709E+00
1.2710673001048449E+00	1.2729692737159242E+00	1.2739867615342269E+00	1.2742726187274087E+00
9.0140364499258580E-02	1.9099149041613345E-01	3.1676634694849987E-01	4.8515727206873321E-01
7.1463538041601693E-01	1.0172079127546751E+00	1.3872883419472803E+00	1.7945818202908248E+00
2.1894216629702630E+00	2.5156246958800961E+00	2.7320730400963993E+00	2.8459291262559687E+00
2.9102302428177360E+00	2.9749808724921190E+00	3.0498419010380147E+00	3.1083551218887426E+00
1.1231426134200273E+00	3.0949536472156844E+00	3.0479989827246312E+00	3.0065478123540257E+00
2.9787398268270877E+00	2.9566569596761552E+00	2.9283860368990240E+00	2.8901541859732003E+00
2.8480710182397222E+00	2.8109578387759804E+00	2.7831777344334934E+00	2.7628311242790673E+00
2.7449837532733414E+00	2.7262914326643868E+00	2.6892573428931712E+00	2.6637489621628112E+00
2.6453314479442329E+00	2.6265753108746801E+00	2.6094010571341419E+00	2.5942923101191275E+00
2.5793384397163650E+00	2.5644345816120677E+00	2.5502485016811813E+00	2.5368386339158229E+00
1.8050271064962349E-04	2.9329645018080683E-03	1.5152685768517889E-02	4.8761763296075671E-02
1.1966333178224589E-01	2.4275582143257982E-01	4.2172814607404818E-01	6.3992216542471059E-01
8.6522776923066480E-01	1.0668977538653268E+00	1.2241157574083679E+00	1.3285054614022356E+00
1.3897260461153866E+00	1.4293373059423824E+00	1.4637208770705386E+00	1.4932384545269728E+00
1.5072612723491148E+00	1.4988675181756947E+00	1.4727588284692148E+00	1.4408225521505913E+00
1.4131332959306984E+00	1.3922382148383770E+00	1.3742241016721011E+00	1.3546795396359319E+00
1.3331656784428290E+00	1.3126933520757942E+00	1.2965277045416284E+00	1.2857505893020247E+00
1.2790744818776605E+00	1.2744272897355768E+00	1.2674473202249925E+00	1.2651923910522915E+00
1.2676335464900426E+00	1.2708529192945734E+00	1.2734139754605391E+00	1.2755733936235500E+00
1.2770856883016111E+00	1.2777367859388771E+00	1.2777553568280726E+00	1.2774563381840867E+00

APPENDIX I: qash FILE

NOTE: Efficiency data in this file are only appropriate for ash composition listed in Table 4.1. For ash of different composition the data must be regenerated using procedure explained in Chapters 3, 4 and 5.

1.3274665889109305E-02	3.3229776001236527E-02	6.6749819774507321E-02	1.0078515384719698E-01
1.3545848083108530E-01	1.7074963122248538E-01	2.0645578509986220E-01	2.4216636167907196E-01
2.7727168022874249E-01	3.4262659836502019E-01	3.9693842594431250E-01	4.3802226156826030E-01
4.6826397041845769E-01	4.9240215328598891E-01	5.1472972690491448E-01	5.6206556629183602E-01
6.1220161992778999E-01	6.6067089916887900E-01	7.0927482854709856E-01	7.6051853218823195E-01
8.6712745520425916E-01	9.7824620710925603E-01	1.0928158855230126E+00	1.2087342815237734E+00
1.3237791996296491E+00	1.4358858012846620E+00	1.5429748852090430E+00	1.6433232123794468E+00
1.7353735191194783E+00	1.8179614684159895E+00	1.8901908679013939E+00	1.9515580485093000E+00
2.0018727225061737E+00	2.0412804539353799E+00	2.0701923185569253E+00	2.0892777002857152E+00
2.0994088243344038E+00	2.1016445432625939E+00	2.0971709086886232E+00	2.0872533013455747E+00
9.4026717903909070E-08	3.6748526703401987E-06	5.8860896374788782E-05	2.9799542356285792E-04
9.3930298551732154E-04	2.2766228902863111E-03	4.6555776687434627E-03	8.4315478377988678E-03
1.3909931624577522E-02	3.0545995736044697E-02	5.3835502952806619E-02	8.0494822973228158E-02
1.0679594947329842E-01	1.3059363723523140E-01	1.5169312835118134E-01	1.9002751848326344E-01
2.2964891879007227E-01	2.7174645393065577E-01	3.1470625285105247E-01	3.5891885218672903E-01
4.5351201543610409E-01	5.5390755379580803E-01	6.5884166787355991E-01	7.6587731620191080E-01
8.7296337814318836E-01	9.7773619031049419E-01	1.0781615350657585E+00	1.1723393521272021E+00
1.2587227237764349E+00	1.3360201693543794E+00	1.4033262600720613E+00	1.4600686439115005E+00
1.5060137545115395E+00	1.5412360167858099E+00	1.5661299254684868E+00	1.5813589294127910E+00
1.5877979564247198E+00	1.5864939390341504E+00	1.5786497188914415E+00	1.5655424355013325E+00
4.6617861183879333E-01	9.3315666062553726E-01	9.7372745505057912E-01	9.0857964604775210E-01
1.0007727538036990E+00	1.2356604769208812E+00	1.6746781734816731E+00	2.2892068400687622E+00
2.7158396546609902E+00	3.3658980079725138E+00	3.4476969283742096E+00	3.3031394733269295E+00
3.3274041681336297E+00	3.4769422036552475E+00	3.4002764770419853E+00	3.2162003883038830E+00
3.2517320365920899E+00	3.1379401159120333E+00	3.1537266776151407E+00	3.0372411408734310E+00
2.9740687772320840E+00	2.9172450823213687E+00	2.8677557891491912E+00	2.7992802668466958E+00
2.7441493185846602E+00	2.7059519824080400E+00	2.6888619308633404E+00	2.6745293116255615E+00
2.6384270648055432E+00	2.5950089738124786E+00	2.5782586257895801E+00	2.5673852252385680E+00
2.5478969018877717E+00	2.5341263604074449E+00	2.5164224915295832E+00	2.4977063683828895E+00
2.4770672463940326E+00	2.4710014140264747E+00	2.4706390739781963E+00	2.4527816113832466E+00
6.3865218902737976E-04	1.8989912650998010E-02	1.1839087796511744E-01	2.1837371178225320E-01
3.2840811071135384E-01	5.2584023024584914E-01	9.2844842648472081E-01	1.5348727216213465E+00
1.9896236662348974E+00	2.6123755199479524E+00	2.8518850830891207E+00	2.8077721728327298E+00
2.8557243976801638E+00	2.9579148986852850E+00	2.9239266021141628E+00	2.8057466915040665E+00
2.8497920980744702E+00	2.7639393802143113E+00	2.7847085366730875E+00	2.6959634871787661E+00
2.6498670255333199E+00	2.6085946181043531E+00	2.5720091372974778E+00	2.5153490582878648E+00
2.4714437697128586E+00	2.4416752424456067E+00	2.4303443237321809E+00	2.4201021191257315E+00
2.3889883763224837E+00	2.3527688110500762E+00	2.3408414612047741E+00	2.3328996684832100E+00
2.3155416105381930E+00	2.3029878693498151E+00	2.2899276134547120E+00	2.2748596417743303E+00
2.2569276972912586E+00	2.2521180837862769E+00	2.2508649454780567E+00	2.2356949235551924E+00
2.7980043922397873E-02	7.1325535780218066E-02	1.7478462828651464E-01	4.4907549078464137E-01
1.3154173836864180E+00	2.1708777377730340E+00	1.9612141811468098E+00	1.9719788118126049E+00
2.1332113804245800E+00	2.5318409022198129E+00	3.0682330406581269E+00	3.1431722457102187E+00
3.2978794350369189E+00	3.3384725507174489E+00	3.3504101937121757E+00	3.1033299383090807E+00
2.9978107474774958E+00	2.8070632098491410E+00	2.8010339019964761E+00	2.7462711005397180E+00
2.7029405903949120E+00	2.6429696832142313E+00	2.5943497137313272E+00	2.5546129909284980E+00
2.5172226893614575E+00	2.4825994075627356E+00	2.4530709926107437E+00	2.4286510452453207E+00
2.4076540535159392E+00	2.3887150386049743E+00	2.3712583519746131E+00	2.3550654763988548E+00
2.3402277779001150E+00	2.3269083774785915E+00	2.3151778741820221E+00	2.3049842406088681E+00
2.2961405698619606E+00	2.2883087268622351E+00	2.2810985105238810E+00	2.2741744835479643E+00
5.4256027850342086E-05	2.0576069386156119E-03	3.1549273372592480E-02	1.7882638635925260E-01
7.7988169698224064E-01	1.5938967324707973E+00	1.5428304064095408E+00	1.5966569741796908E+00
1.7447377227696623E+00	1.9950415631583789E+00	2.4434949749002395E+00	2.5506377604015138E+00
2.6248208471270438E+00	2.6518021140228489E+00	2.6509523998325486E+00	2.3930806895399925E+00
2.2723047251308022E+00	2.1117602465945438E+00	2.1176411996121485E+00	2.0796648087578888E+00
2.0653764259654737E+00	2.0249238837415122E+00	1.9923628983607427E+00	1.9675609838982417E+00
1.9447432557462916E+00	1.9233448249213636E+00	1.9051778484510216E+00	1.8903257951977306E+00
1.8773541398445106E+00	1.8653269614885422E+00	1.8539726495396309E+00	1.8433148787516664E+00
1.8335489594225276E+00	1.8248427551328839E+00	1.8172370646538183E+00	1.8106691027839541E+00

1.8049784794154025E+00	1.7998855535460008E+00	1.7950873612386857E+00	1.7903692416909438E+00
8.6312413798992502E-02	2.1812731620148798E-01	4.5203361000264602E-01	7.1249594268572336E-01
1.0001374428943204E+00	1.3023944664661102E+00	1.5966805027346525E+00	1.8591510668419369E+00
2.0717899342192401E+00	2.3057992463020676E+00	2.3934488663792184E+00	2.4548925575130527E+00
2.4345305729062048E+00	2.4184303273601464E+00	2.4047718205125386E+00	2.3830671847592710E+00
2.3802515218162199E+00	2.3785574168440777E+00	2.3691956712502242E+00	2.3560987160786944E+00
2.3344671184633166E+00	2.3170376583100452E+00	2.2999300144835138E+00	2.2850996012119427E+00
2.2718007941006393E+00	2.2597536322772513E+00	2.2489763323059138E+00	2.2391848948587278E+00
2.2302881500134419E+00	2.2221698313725566E+00	2.2147211427880507E+00	2.2078684010002432E+00
2.2015373550943123E+00	2.1956692980893120E+00	2.1902132451773118E+00	2.1851250655125019E+00
2.1803672778686480E+00	2.1759067389356024E+00	2.1717150637661220E+00	2.1677673739534478E+00
1.2683719331362395E-05	4.9600155791539502E-04	7.8900788604811256E-03	3.8717756728000235E-02
1.1345170634268890E-01	2.4174379901309018E-01	4.0904966361922823E-01	5.8238880099540913E-01
7.3362203603312659E-01	9.2700442629735880E-01	1.0032139212305009E+00	1.0574272940336156E+00
1.0657488372768453E+00	1.0634179596666256E+00	1.0722723073024885E+00	1.0951616638533892E+00
1.1330296006290903E+00	1.1643673494315179E+00	1.1828234217991431E+00	1.1935566492713581E+00
1.2105350172477214E+00	1.2235516902802543E+00	1.2310237144067870E+00	1.2364222196451360E+00
1.2400668314868242E+00	1.2424547125367233E+00	1.2441382544255866E+00	1.2452199922571072E+00
1.2459018850900501E+00	1.2462932969879534E+00	1.2464600614222197E+00	1.2464663845033086E+00
1.2463486028283068E+00	1.2461375910530137E+00	1.2458564183958223E+00	1.2455215848445438E+00
1.2451465624504858E+00	1.2447414104362680E+00	1.2443140649749247E+00	1.2438707467386723E+00
1.9328597052888565E-02	4.8604465147389919E-02	9.9383815552003860E-02	1.5458629674530172E-01
2.1568841104573536E-01	2.8263436835415279E-01	3.5379298744890458E-01	4.2735481646267481E-01
5.0365158104058827E-01	6.7382743820429325E-01	8.5429258121398943E-01	1.0301886960434690E+00
1.2119880961922624E+00	1.3868004721536928E+00	1.5578619111708623E+00	1.8706681188522254E+00
2.1332334243450486E+00	2.3358050906660965E+00	2.4752900460589888E+00	2.5539890446019959E+00
2.5608075621860840E+00	2.4474935043072081E+00	2.3117038371137824E+00	2.2185922562536491E+00
2.1866406339124760E+00	2.1976476983412367E+00	2.2198659947505743E+00	2.2289914791454488E+00
2.2181889564040542E+00	2.1952502394774926E+00	2.1730812740676297E+00	2.1603796638561552E+00
2.1579052115738593E+00	2.1604092073183896E+00	2.1615877324048873E+00	2.1581088116939160E+00
2.1507249824891157E+00	2.1425672941700862E+00	2.1365162117593064E+00	2.1334671053784753E+00
2.4163759411982482E-06	9.3610259723552161E-05	1.4490463018479837E-03	6.8866367865818168E-03
1.9680410315983766E-02	4.1619079137950682E-02	7.1669996489356555E-02	1.0702829354680927E-01
1.4643712940607587E-01	2.4630374555029105E-01	3.6929664743642676E-01	4.9590311776148066E-01
6.3274233721659168E-01	7.6820418879849373E-01	9.0412823296819078E-01	1.1557815734497836E+00
1.3678692153459775E+00	1.5281305424537936E+00	1.6313262925042495E+00	1.6788430553153679E+00
1.6355002190621122E+00	1.4841044335382652E+00	1.3193888491839989E+00	1.2044474299702150E+00
1.1561324339469248E+00	1.1551800646615678E+00	1.1688950465847374E+00	1.1722799743782959E+00
1.1579621174422190E+00	1.1332262093617049E+00	1.1105733950829868E+00	1.0983065149727347E+00
1.0968798249246672E+00	1.1008291126806189E+00	1.1036608835704200E+00	1.1019618765552E+00
1.0964434617524856E+00	1.0901821734515036E+00	1.0860355224509166E+00	1.0848793659944178E+00
2.3663026913755742E-03	6.7202707199551445E-03	2.4271692552465293E-02	7.6411906652073619E-02
1.8606304220646547E-01	3.5010202731776247E-01	5.6877235331104314E-01	8.6982985139363844E-01
1.1833660657727658E+00	1.8246797908611143E+00	2.4155577067045559E+00	2.9277329885325249E+00
3.3034206350160735E+00	3.5049148006585518E+00	3.5421463459830838E+00	3.3162278431739667E+00
2.8771310231653016E+00	2.5574131820832231E+00	2.4227364294340408E+00	2.4338558551563194E+00
2.4214793960076437E+00	2.2880745113636771E+00	2.3075971721964690E+00	2.3251847865718278E+00
2.2701347776393983E+00	2.2639236513577905E+00	2.2533297232594376E+00	2.2140527490231774E+00
2.2116567200230328E+00	2.2100852140939735E+00	2.1921712152766015E+00	2.1914125258072779E+00
2.1900624026072011E+00	2.1656285601345711E+00	2.1673072010557308E+00	2.1638441211168198E+00
2.1544142273864728E+00	2.1548116057368270E+00	2.1511341084292206E+00	2.1437649503310294E+00
1.8376813265480236E-05	7.1746711075208627E-04	1.1375655620948151E-02	5.5183411249676462E-02
1.5519179688256327E-01	3.0854380767298578E-01	5.1440721849297788E-01	8.0108874333007574E-01
1.1023804343489303E+00	1.7183275535817595E+00	2.2852911383766297E+00	2.7738257802153448E+00
3.1253911821371205E+00	3.3031230553744106E+00	3.3195448676115653E+00	3.0493474019876805E+00
2.5710719570091216E+00	2.2114647066299549E+00	2.0425754607778170E+00	2.0199994371318306E+00
1.9517548906562141E+00	1.7743321940689674E+00	1.7571970767794147E+00	1.7441409306724771E+00
1.6573721998465691E+00	1.6232234809699124E+00	1.5870726835289581E+00	1.5246556762433561E+00
1.5012295261434050E+00	1.4801662420809569E+00	1.4442872129132684E+00	1.4257771475382917E+00

1.4074499173626256E+00	1.3719083320358145E+00	1.3592974095102526E+00	1.3422641670452544E+00
1.3223985325753056E+00	1.3121226324221600E+00	1.2986907842247912E+00	1.2823995697705262E+00
1.0510256982436037E-03	4.7339609779861831E-03	3.9957754161990731E-02	1.7112825169962223E-01
4.2962027169733091E-01	8.0504128141889042E-01	1.4000195915814215E+00	1.8992512866658944E+00
2.3881273071647322E+00	3.2996107940678265E+00	3.9252271046038492E+00	4.1069253723936381E+00
3.8832389884317107E+00	3.4080188910333531E+00	2.8405885082576514E+00	1.9544241997442495E+00
2.0336820209680213E+00	2.5402815224438342E+00	2.7920751739409653E+00	2.5519426359714927E+00
2.0968047518923099E+00	2.4497687359599447E+00	2.2299264545739370E+00	2.2192852298764310E+00
2.2768700958295658E+00	2.1850125110317964E+00	2.2232032572894713E+00	2.1798582967634470E+00
2.1966094696388687E+00	2.1577882753342643E+00	2.1720598834892422E+00	2.1746251348873318E+00
2.1314171818838252E+00	2.1721508779886443E+00	2.1336125706125508E+00	2.1379802882499108E+00
2.1451263448630571E+00	2.1184405560147948E+00	2.1391023113005039E+00	2.1146444134700464E+00
5.4661515033990551E-05	2.1415436207105774E-03	3.4099506035876123E-02	1.6099278025437919E-01
4.1437075161055709E-01	7.8298040703111793E-01	1.3690217867638701E+00	1.8636064246598334E+00
2.3463625092017564E+00	3.2448558934746461E+00	3.8560667818995054E+00	4.0232947165826385E+00
3.7895485332758465E+00	3.3045576875021405E+00	2.7218833182947928E+00	1.8140783692181957E+00
1.8701989995446444E+00	2.3595855505024397E+00	2.5923284700331042E+00	2.3385178688445269E+00
1.8614989290624908E+00	2.1960474125832539E+00	1.9553896432279712E+00	1.9249143317990354E+00
1.9603941884391420E+00	1.8509557256679752E+00	1.8714691302462325E+00	1.8137512034794017E+00
1.8147986598865813E+00	1.7607502349035227E+00	1.7605617190627330E+00	1.7502107113410368E+00
1.6956561112025574E+00	1.7234449282031314E+00	1.6737271443628967E+00	1.6674206726150418E+00
1.6635040725449781E+00	1.6278418302005844E+00	1.6380726771241012E+00	1.6048915382415057E+00
7.4203516332254878E-04	6.1502664293266208E-03	7.4870253252157626E-02	3.1863955913859743E-01
7.4473974759955663E-01	1.4751008124940914E+00	2.0971125323644992E+00	2.7735699409081982E+00
3.3364986652584370E+00	4.0421697775255270E+00	4.0844421107217475E+00	3.5939798002514136E+00
2.8668626212654855E+00	2.2306875984046339E+00	1.9113826218073835E+00	2.2377624474706970E+00
2.7785032200830395E+00	2.6221038672861168E+00	2.1880830749281883E+00	2.1483697308312504E+00
2.4289223537753770E+00	2.1818318754529029E+00	2.2814141712397813E+00	2.2137483460616934E+00
2.1913522300438379E+00	2.2187367653057590E+00	2.1514385651360803E+00	2.2081633803071594E+00
2.1431438508768248E+00	2.1697134704449712E+00	2.1486361080937235E+00	2.1440457594147211E+00
2.1367060736185048E+00	2.1327691085481626E+00	2.1306499229468390E+00	2.1280376901764662E+00
2.1141955988827426E+00	2.1270045883984090E+00	2.1029587404830687E+00	2.1153059822838007E+00
1.1389679243722721E-04	4.4760566022889183E-03	7.0857532616799696E-02	3.1143889326875551E-01
7.3296886635565273E-01	1.4573591905663197E+00	2.0768602923918880E+00	2.7464489931709579E+00
3.3069719036642451E+00	4.0039107600388313E+00	4.0379203250179465E+00	3.5386469358379058E+00
2.8023680912250115E+00	2.1572610366386140E+00	1.8289764992800090E+00	2.1384673257744344E+00
2.6665817167647692E+00	2.4987100585215214E+00	2.0549264759653436E+00	2.0095348771130892E+00
2.2761042002825795E+00	2.0109717886564451E+00	2.0928397653842503E+00	2.0095021057148998E+00
1.9744205139767808E+00	1.9878563479028646E+00	1.9068259129390768E+00	1.9481711329617346E+00
1.8737341376561245E+00	1.8876322158270940E+00	1.8536880569640184E+00	1.8397879358281595E+00
1.8223463174439876E+00	1.8064183620896437E+00	1.7945873014903815E+00	1.7822285704633805E+00
1.7595968331433300E+00	1.7627608579796723E+00	1.7303172498057509E+00	1.7346333367498947E+00
8.8731945834742796E-04	1.0574849752440047E-02	1.4054480110761119E-01	5.4239377089589569E-01
1.2971088175450187E+00	2.1352291569857771E+00	2.9499218165130365E+00	3.5270166808326917E+00
4.0567053574884566E+00	4.1707177933371788E+00	3.4867509497614813E+00	2.5890952115342536E+00
1.9985616377709643E+00	1.9253081487834889E+00	2.2705670284383306E+00	2.8827482649059673E+00
2.4021801337972635E+00	2.0436543201010644E+00	2.4197246583722487E+00	2.4726932022135863E+00
2.1885368653723138E+00	2.2538250399210833E+00	2.2285719120082659E+00	2.1825549984980093E+00
2.1959804702922034E+00	2.1758356424393992E+00	2.1559489535935130E+00	2.1644886883822099E+00
2.1482863228537767E+00	2.1371939493494962E+00	2.1456054999846268E+00	2.1176218560205959E+00
2.1376841569043670E+00	2.1119392278307623E+00	2.1207377910333691E+00	2.1116257123657443E+00
2.1107771578031405E+00	2.1045402167409941E+00	2.1078477341502442E+00	2.0955781319667950E+00
2.2241974920127154E-04	8.7672831023799438E-03	1.3603802251487024E-01	5.3407331275259562E-01
1.2823131917819186E+00	2.1169595303955919E+00	2.9249005872490819E+00	3.4987742470981975E+00
4.0218198376723091E+00	4.1265249579210872E+00	3.4333284953347318E+00	2.5250748830948200E+00
1.9236976127235139E+00	1.8418869506961604E+00	2.1799039694295379E+00	2.7753406075463505E+00
2.2810037980684768E+00	1.9142720301677141E+00	2.2773042374022148E+00	2.3256345602760962E+00
2.0183868885380547E+00	2.0626951996378162E+00	2.0207143189965375E+00	1.9564669259106746E+00
1.9525338839767641E+00	1.9151701230517755E+00	1.8791247150519490E+00	1.8715113745655749E+00

1.8388892806077735E+00	1.8130426973748297E+00	1.8066940678371379E+00	1.7639556357462862E+00
1.7700740806630306E+00	1.7313134536235817E+00	1.7266294030422651E+00	1.7045826868645955E+00
1.6909260110710875E+00	1.6723684626454640E+00	1.6638481283307394E+00	1.6396813788705744E+00
1.0475762662016999E-03	1.5037375777970000E-02	2.0290627672868242E-01	7.2888224115841116E-01
1.7773900683468937E+00	2.4917556071453855E+00	3.5003810688552539E+00	3.9494230193946445E+00
4.1234470465058912E+00	3.7302822751006901E+00	2.9391742873361517E+00	2.0942830816178963E+00
1.8070956179190290E+00	2.2568288110431443E+00	2.7663418301411640E+00	2.6512942582276033E+00
1.9727147928943252E+00	2.4190742587958511E+00	2.5295913892104140E+00	2.0537834781343318E+00
2.4276505923545195E+00	2.1730812661431020E+00	2.1366564596022117E+00	2.3094382469872814E+00
2.0979458769967572E+00	2.1723275583828809E+00	2.1992367387583887E+00	2.0899792913962028E+00
2.1728688350307035E+00	2.1389484206362761E+00	2.1005642845137280E+00	2.1473344363115006E+00
2.1101848885950094E+00	2.1081580687302397E+00	2.1218572048891216E+00	2.0981568990558217E+00
2.1040206272077371E+00	2.1014126836062208E+00	2.0945214542701067E+00	2.0945294259977252E+00
3.3062569916998973E-04	1.3055216312461062E-02	1.9782390893211657E-01	7.1913506272724348E-01
1.7604889217834245E+00	2.4712099608723963E+00	3.4733919040574999E+00	3.9158769579183379E+00
4.0878486927855313E+00	3.6823489125084352E+00	2.8748964655861227E+00	2.0233481196129666E+00
1.7335796769488281E+00	2.1670345075075819E+00	2.6656650739201924E+00	2.5348083076054269E+00
1.8465702897953542E+00	2.2806857455601133E+00	2.3836431650979804E+00	1.8916704641754902E+00
2.2492777627333851E+00	1.9697771509506923E+00	1.9185859643382477E+00	2.0647553807313277E+00
1.8396702431554521E+00	1.8970965894767555E+00	1.9060960000626819E+00	1.7812601518557754E+00
1.8459667115067508E+00	1.7964872713037749E+00	1.7434920541339163E+00	1.7755756244265282E+00
1.7220238513424393E+00	1.7072165805503485E+00	1.7072340217932980E+00	1.6697625094031214E+00
1.6632165384444662E+00	1.6479088250149301E+00	1.6284769977387299E+00	1.6170327978599270E+00
1.2425579913243484E-03	2.0855465008502574E-02	2.7837705686586695E-01	9.5929363328062656E-01
2.1036186500758984E+00	3.0635383358986443E+00	3.6582042847669261E+00	4.2380929590302276E+00
4.2276897482005538E+00	3.4193865609023111E+00	2.2922830657913984E+00	1.8384677480675984E+00
2.1806454288243451E+00	2.7341503263781393E+00	2.9255503485665559E+00	2.1569366283842104E+00
2.2352325284850529E+00	2.5629172500632826E+00	2.1128666328999524E+00	2.2486022351436517E+00
2.1183864616163262E+00	2.2717805202074595E+00	2.2162404121901420E+00	2.1394011904789787E+00
2.1702321463444756E+00	2.1600450288696500E+00	2.1456429224027795E+00	2.1417478399375107E+00
2.1198574385896869E+00	2.1283251545326842E+00	2.1319428965043303E+00	2.1050172390311297E+00
2.1076231147369686E+00	2.1188407549514352E+00	2.1007406482556719E+00	2.0965408518368753E+00
2.1005965643434785E+00	2.0942792755765627E+00	2.0927052564857060E+00	2.0889667705781645E+00
4.7264240491454027E-04	1.8689407342246549E-02	2.7268906318410097E-01	9.4768804256255046E-01
2.0862543827475241E+00	3.0386976703287973E+00	3.6297387966363992E+00	4.2029152542979951E+00
4.1846501297353855E+00	3.3670749211103721E+00	2.2282137393833032E+00	1.7637304670852847E+00
2.0922195628361364E+00	2.6382568921650034E+00	2.8190579938751688E+00	2.0351834393136987E+00
2.1034452550207559E+00	2.4231298944050770E+00	1.9631985898870368E+00	2.0848192249680415E+00
1.9293343949725741E+00	2.0642618719899479E+00	1.9858846561234815E+00	1.8889290296972798E+00
1.9000267183030743E+00	1.8711176145314337E+00	1.8382641110468616E+00	1.8169627866787641E+00
1.7792544243029638E+00	1.7700822486985306E+00	1.7571749417328448E+00	1.7146652200066628E+00
1.7022187751483357E+00	1.6978204603827702E+00	1.6666066447945775E+00	1.6485747046324550E+00
1.6393562581890557E+00	1.6201359381335401E+00	1.6061101456271099E+00	1.5900856668216283E+00
1.5848282616997581E-03	3.1572890942123510E-02	4.0305140751478247E-01	1.3945623386528831E+00
2.4439971363519546E+00	3.5753319187765453E+00	4.2174477687651635E+00	4.1783266423955618E+00
3.8268536651347120E+00	2.7224888456878067E+00	1.8726678609899909E+00	2.0811302733724744E+00
2.7172479964613037E+00	2.9111378873873979E+00	2.4858984258589727E+00	2.0858383801699225E+00
2.5820216932677296E+00	2.1105977657580137E+00	2.2933947669753252E+00	2.3232361622494189E+00
2.3199565120952435E+00	2.1857342238153170E+00	2.1323422709721505E+00	2.1580556786165963E+00
2.1667932162677892E+00	2.1450439811214230E+00	2.1374137499003485E+00	2.1372007070781405E+00
2.1204464921236195E+00	2.1041418346777765E+00	2.1092962720737329E+00	2.1180944681526022E+00
2.1092724610676470E+00	2.0957276448169746E+00	2.0922299967139835E+00	2.0948522113076042E+00
2.0919075478718545E+00	2.0875780624648121E+00	2.0871078577229856E+00	2.0849170070879941E+00
7.3574556773432895E-04	2.9123334722981113E-02	3.9642593296244205E-01	1.3799604640043475E+00
2.4248517323748926E+00	3.5487958716362304E+00	4.1827000390048417E+00	4.1373183531137299E+00
3.7825883068610939E+00	2.6618346928564645E+00	1.8010040937157117E+00	1.9989353348404242E+00
2.6229496454532053E+00	2.8050789714967839E+00	2.3719611915717591E+00	1.9581918298065060E+00
2.4467776298237705E+00	1.9621361775587487E+00	2.1309075817092573E+00	2.1450093947495223E+00
2.1188278026315097E+00	1.9618525861339733E+00	1.8843944189034780E+00	1.8895247918138296E+00

1.8774598351021561E+00	1.8357897781699535E+00	1.8086178908199428E+00	1.7902032989085728E+00
1.7557807285932372E+00	1.7214214404572470E+00	1.7098346539313365E+00	1.7024407319168386E+00
1.6779692289979196E+00	1.6486005714832386E+00	1.6309105053773374E+00	1.6195163872387650E+00
1.6028258640336355E+00	1.5853191720532704E+00	1.5719091437594654E+00	1.5574027527120813E+00
1.9964985936799053E-03	4.3444129933858627E-02	5.2270931807991727E-01	1.8082829150699877E+00
2.9003036609237536E+00	3.6998131747167791E+00	4.1772023564291150E+00	4.1704268984285875E+00
3.6588528149264157E+00	2.1140019810097752E+00	1.8636477542609720E+00	2.5274111596361601E+00
2.9594034134107132E+00	2.5918179532539645E+00	2.0511686891052774E+00	2.4573028844722522E+00
2.3081457416436129E+00	2.1714054332818740E+00	2.4147101789932330E+00	2.0594010477851690E+00
2.1031358156087827E+00	2.1936554609759651E+00	2.2394173782446929E+00	2.2166630731273340E+00
2.1611470728993627E+00	2.1135952941820668E+00	2.0978528248795767E+00	2.1080729890993357E+00
2.1203155715218300E+00	2.1209757929602291E+00	2.1119089874232388E+00	2.1019998590974907E+00
2.0975109703996067E+00	2.0968500425765595E+00	2.0940224949360111E+00	2.0876340490746372E+00
2.0809796477449063E+00	2.0782821375307163E+00	2.0800878734134471E+00	2.0829561454515253E+00
1.0253794178693709E-03	4.0581612924272994E-02	5.1476969071119938E-01	1.7909044382647386E+00
2.8758155789637696E+00	3.6699270557953581E+00	4.1407443003503854E+00	4.1252165563359116E+00
3.6010385858840408E+00	2.0472753201540792E+00	1.7867569538175847E+00	2.4286501745073408E+00
2.8515478953334807E+00	2.4743187879254598E+00	1.9259944530166646E+00	2.3246819341851754E+00
2.1507745956170861E+00	2.0038349031396701E+00	2.2319461795960827E+00	1.8631713884428542E+00
1.8819327950177804E+00	1.9460635099201860E+00	1.9673255587429530E+00	1.9210692102407709E+00
1.8420901559489538E+00	1.7725582386832890E+00	1.7371470092468888E+00	1.7269090115639023E+00
1.7203637264831564E+00	1.7024055182522331E+00	1.6756040271988610E+00	1.6482224645256327E+00
1.6273476039223493E+00	1.6107550495294820E+00	1.5930381720717264E+00	1.5720223337423294E+00
1.5510538942309855E+00	1.5347527170893502E+00	1.5234172323966251E+00	1.5137901431806511E+00
2.4401479801579983E-03	5.6447540993011615E-02	6.3842657306535255E-01	2.0824980128185602E+00
3.3845657002678475E+00	4.0946746309391635E+00	4.1400105450811990E+00	3.6878707708406746E+00
2.9948751876476516E+00	1.9563401040584825E+00	2.1242773144525176E+00	2.8091345103966474E+00
2.8131461190026243E+00	2.1943084222916216E+00	2.0073625410163145E+00	2.6234708880956958E+00
2.0390941244131127E+00	2.4398106241085835E+00	2.1086283631930081E+00	2.3006410590952253E+00
2.1988559840418467E+00	2.1305224482743799E+00	2.1079751116782330E+00	2.1057018659761626E+00
2.1119833994129005E+00	2.1199787277917754E+00	2.1239153831990110E+00	2.1204317818199687E+00
2.1126573672761841E+00	2.1043824834255695E+00	2.0976199507998206E+00	2.0939845130195751E+00
2.0932932751466198E+00	2.0935707876474292E+00	2.0937051845391133E+00	2.0916773394423105E+00
2.0877203453680546E+00	2.0826232176153754E+00	2.0776374462479326E+00	2.0737288199467621E+00
1.3448064461479008E-03	5.3156520693337241E-02	6.2904340311736429E-01	2.0635966821187255E+00
3.3555243824475727E+00	4.0572049243802280E+00	4.0949441138794356E+00	3.6376413601088076E+00
2.9394628036812849E+00	1.8809895156230272E+00	2.0290213904614394E+00	2.7038905022174911E+00
2.6955858953871203E+00	2.0662750667953049E+00	1.8692291951501758E+00	2.4692714804816611E+00
1.8763095969707866E+00	2.2565347842223371E+00	1.9085132615253124E+00	2.0868043007377954E+00
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1.7648618297565397E+00	1.7503008296047224E+00	1.7317353748670890E+00	1.7073377793128248E+00
1.6796101815718179E+00	1.6516604750031434E+00	1.6264119752502584E+00	1.6052973447606542E+00
1.5874437037509750E+00	1.5715737847352766E+00	1.5558865500885992E+00	1.5388865930604352E+00
1.5206569675722963E+00	1.5018205553331507E+00	1.4836584347296471E+00	1.4669378461159459E+00
3.1398554166809332E-03	7.7330804882602050E-02	8.0991295549045350E-01	2.3072244463152929E+00
3.6343037843991488E+00	4.2966273416977634E+00	4.1809335282056761E+00	3.5005906853610123E+00
2.6558352275539230E+00	1.8585069238026244E+00	2.5163666374269256E+00	2.9583001259830177E+00
2.4116064112346134E+00	2.0007441547950480E+00	2.3339160359756250E+00	2.3055047622174243E+00
2.2572079086509751E+00	2.2531461389909841E+00	2.2134627075095854E+00	2.2218381833714371E+00
2.1950855791317814E+00	2.1778262083744431E+00	2.1606149833574180E+00	2.1458089876023827E+00
2.1344905890912225E+00	2.1250436689876122E+00	2.1167031116815935E+00	2.1095726642757717E+00
2.1031015092118794E+00	2.0982386560205657E+00	2.0936289014405989E+00	2.0900401196094740E+00
2.0868523795272234E+00	2.0839185131934306E+00	2.0816735565668889E+00	2.0796411373838222E+00
2.0777452918312975E+00	2.0759691860561569E+00	2.0743017741464764E+00	2.0726440672419666E+00
1.8636352908459927E-03	7.3399845477945841E-02	7.9814026169936758E-01	2.2863050403896481E+00
3.6028716449853078E+00	4.2552949060984409E+00	4.1294019217257523E+00	3.4376169100054668E+00
2.5823223539338738E+00	1.7680179668296956E+00	2.4103837656880867E+00	2.8361579125578289E+00
2.2760562169972398E+00	1.8567397043840093E+00	2.1836565597106339E+00	2.1401264442002179E+00
2.0701753060910608E+00	2.0467448688942489E+00	1.9905051924353308E+00	1.9828656588857447E+00

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1.7495117103908260E+00	1.7150429287931717E+00	1.6832303487896321E+00	1.6536459587484333E+00
1.6261891472807244E+00	1.6009054292649110E+00	1.5770002615816987E+00	1.5550496602920800E+00
1.5343960092409421E+00	1.5150004006490627E+00	1.4968691277496771E+00	1.4797088519671580E+00
1.4634232629489754E+00	1.4479779150982570E+00	1.4332765587808243E+00	1.4191455996674600E+00
4.1179136806331418E-03	1.0718763497751273E-01	1.0557439965716553E+00	2.6030438978863928E+00
3.7663316067021246E+00	4.1039241824466197E+00	3.6545223713943509E+00	2.8204900301691129E+00
2.0974473148979627E+00	2.0385053439230956E+00	2.8807718024491411E+00	2.6442431787054290E+00
2.0203515819944853E+00	2.2345903085920309E+00	2.6021491415295115E+00	2.0481368839712526E+00
2.4319177024310648E+00	2.1086933095413931E+00	2.2914790860214689E+00	2.1587714363354822E+00
2.1859683160478367E+00	2.1870719709982001E+00	2.1709149666273793E+00	2.1498557344976081E+00
2.1299963042864490E+00	2.1183555679000734E+00	2.1124170740612955E+00	2.1101796514096618E+00
2.1074777604689148E+00	2.1025933884002894E+00	2.0955009721915969E+00	2.0881564083291195E+00
2.0821391781424152E+00	2.0783948199092532E+00	2.0762861785472206E+00	2.0750238220838697E+00
2.0735387718074771E+00	2.0713808110918199E+00	2.0687122302710637E+00	2.0661396593486390E+00
2.6199984190087735E-03	1.0244445062905312E-01	1.0404861201482491E+00	2.5773432734750896E+00
3.7293291095338112E+00	4.0549887152793076E+00	3.5939628297493615E+00	2.7483104421761131E+00
2.0134810382139161E+00	1.9340959171296530E+00	2.7587108834767480E+00	2.5089860239730810E+00
1.8703740093295718E+00	2.0793134657027057E+00	2.4354429885473565E+00	1.8607066705553672E+00
2.2202211012230042E+00	1.8777265728192136E+00	2.0420938358619023E+00	1.8894043630875073E+00
1.8810496776082486E+00	1.8477656659366324E+00	1.8013048771104807E+00	1.7499034360267611E+00
1.7023077573201930E+00	1.6641306830486637E+00	1.6334134891600756E+00	1.6076739861092231E+00
1.5829914784395758E+00	1.5570003877267908E+00	1.5302926829240786E+00	1.5042821011514587E+00
1.4806413839548174E+00	1.4601737148936567E+00	1.4423793617988236E+00	1.4262331615542476E+00
1.4107220666805784E+00	1.3951982499526447E+00	1.3799027494421561E+00	1.3655016445114412E+00
5.3144760879864830E-03	1.4563148689276911E-01	1.3912588340873961E+00	3.1353528599908258E+00
4.2528660675848480E+00	4.2576209769260434E+00	3.3956175150071144E+00	2.3686444609067085E+00
1.8184650808232556E+00	2.4425359843231473E+00	2.9147686013671854E+00	2.1983399225780778E+00
2.0899431496959151E+00	2.6010953816064082E+00	2.3750457999022738E+00	2.3306833290164608E+00
2.1084435472005287E+00	2.3528492357452415E+00	2.1028179673598371E+00	2.2367904508143766E+00
2.1365184817427689E+00	2.1144927591517630E+00	2.1301340825289872E+00	2.1337621473691533E+00
2.1202445225975572E+00	2.1114769829727122E+00	2.1105218717873884E+00	2.1047654668234639E+00
2.0926459957528993E+00	2.0832567469425149E+00	2.0830361558478176E+00	2.0853205244599939E+00
2.0832556137650404E+00	2.0779709927325092E+00	2.0742814858715577E+00	2.0725083664118253E+00
2.0699334015891713E+00	2.0665312219178515E+00	2.0647007733049323E+00	2.0647077454070829E+00
3.6277433955899268E-03	1.4014146663572363E-01	1.3723907520656662E+00	3.1029859337522048E+00
4.2069718229849551E+00	4.1993840907562259E+00	3.3270649628200366E+00	2.2912962502507992E+00
1.7309131849251340E+00	2.3282719877575797E+00	2.7815493349777811E+00	2.0468831442857605E+00
1.9304336404527624E+00	2.4281081348477596E+00	2.1965634711849003E+00	2.1245808250166038E+00
1.8794956990466172E+00	2.1030335331714887E+00	1.8314238514916445E+00	1.9451228801386358E+00
1.8065460909624664E+00	1.7489587050508555E+00	1.7307543804786496E+00	1.7029897679625663E+00
1.6606159704834775E+00	1.6245112354401290E+00	1.5979127924424041E+00	1.5681003709131569E+00
1.5332859176894105E+00	1.5029318656852066E+00	1.4827851381507280E+00	1.4663833421240735E+00
1.4468228229883977E+00	1.4250913834936478E+00	1.4059033891670338E+00	1.3896448483007402E+00
1.3733605876468338E+00	1.3571179378616687E+00	1.3432191815008527E+00	1.3319236100398473E+00
6.8345303759274048E-03	1.9634028327484318E-01	1.7962201789448871E+00	3.5983523329605669E+00
4.2388598434282736E+00	3.7048771823380431E+00	2.7803927961333277E+00	2.0347770699484689E+00
1.9184450646762843E+00	2.8242596051561972E+00	2.5873475086515820E+00	1.9916668895449934E+00
2.4738107446867050E+00	2.4765659025293152E+00	2.0541120748207504E+00	2.4020537482269440E+00
2.2215617408322559E+00	2.1205643509924723E+00	2.2840279494423648E+00	2.1406207017316037E+00
2.2005477995698848E+00	2.1464095920890771E+00	2.1187341160950073E+00	2.1198743319435072E+00
2.1099778729605423E+00	2.1096878450024565E+00	2.1035562996340338E+00	2.0870319754851496E+00
2.0879321675461089E+00	2.0912805162968708E+00	2.0815215981796551E+00	2.0763466126074195E+00
2.0762835331934286E+00	2.0732661896509659E+00	2.0717018610174973E+00	2.0689691640168109E+00
2.0645823681271643E+00	2.0646089174100011E+00	2.0643500989514436E+00	2.0604471806091067E+00
5.0223319264676887E-03	1.9027265548270708E-01	1.7751552630072238E+00	3.5640516954642125E+00
4.1942046851390486E+00	3.6482610755971843E+00	2.7052552474155234E+00	1.9449464082544992E+00
1.8195967056869056E+00	2.7037552709078705E+00	2.4479591218056926E+00	1.8376953004472096E+00
2.3131402391080536E+00	2.3029370152171014E+00	1.8676346051169523E+00	2.1867971626588227E+00

1.9834717251255580E+00	1.8612084200871919E+00	2.0012355975798930E+00	1.8370523682364173E+00
1.8573422923682239E+00	1.7665420076907832E+00	1.7035447679378808E+00	1.6731724367790615E+00
1.6334120569813131E+00	1.6052876557773890E+00	1.5730456579287690E+00	1.5321858224164955E+00
1.5103098533644517E+00	1.4924178247609396E+00	1.4627855737547195E+00	1.4390601438683368E+00
1.4215596319763959E+00	1.4022374334000183E+00	1.3854512317995242E+00	1.3685026376435749E+00
1.3508049213087392E+00	1.3382955391300815E+00	1.3263301279851214E+00	1.3113803256407981E+00
8.3031303814828060E-03	2.4359465389505996E-01	2.0649146232664153E+00	3.6774040320397199E+00
4.0659626451994635E+00	3.6659519289884623E+00	2.4920950920066582E+00	1.7469174917771577E+00
2.0653081313372175E+00	2.9989496184385893E+00	2.2462506812604084E+00	2.1042301492851658E+00
2.6447611479749442E+00	2.1679915295505605E+00	2.1488831617233957E+00	2.1192609175637140E+00
2.3796208276869590E+00	2.1647483837378569E+00	2.0948059918069055E+00	2.2621416457257073E+00
2.0816815863886022E+00	2.1542810030705031E+00	2.1483208030086796E+00	2.0821825925877770E+00
2.1279492750972864E+00	2.1008231562515496E+00	2.0842591397137675E+00	2.1010792104101803E+00
2.0820695648117216E+00	2.0808298480803127E+00	2.0812588960488925E+00	2.0748978044041499E+00
2.0726575200549506E+00	2.0699117817008958E+00	2.0697456358714170E+00	2.0639881195672833E+00
2.0640361377617458E+00	2.0637827062916392E+00	2.0577027227776172E+00	2.0601001777456567E+00
6.3837824754859078E-03	2.3703175360400000E-01	2.0432224230020752E+00	3.6437085051693945E+00
4.0177536501009206E+00	3.5945227283205297E+00	2.4153154634774761E+00	1.6652481349721824E+00
1.9535265435267091E+00	2.8784666230282570E+00	2.0964435257197667E+00	1.9570240999744228E+00
2.4753992879867810E+00	1.9901845344263176E+00	1.9553727668394933E+00	1.9003260343738981E+00
2.1343346190372832E+00	1.8946083428577243E+00	1.8027313903355895E+00	1.9487529232427530E+00
1.7269077707824301E+00	1.7617499053656864E+00	1.7211099601931572E+00	1.6216203565890908E+00
1.6374906104750502E+00	1.5819410693147413E+00	1.5391840249972104E+00	1.5317134634680525E+00
1.4896074083575306E+00	1.4671966574307596E+00	1.4478514287879432E+00	1.4230086074992185E+00
1.4035933300945513E+00	1.3847683332649157E+00	1.3695552752023179E+00	1.3497633040970898E+00
1.3367702487009405E+00	1.3243611292470960E+00	1.3069061644093238E+00	1.2986579008069119E+00
9.9966109829360272E-03	2.9445467975618628E-01	2.2287303194554613E+00	3.7353593928594506E+00
4.2721170536822299E+00	3.2548133240224932E+00	2.0664230790062730E+00	1.8968478285540287E+00
2.3065237056531305E+00	2.8943363323769966E+00	2.0329159810364987E+00	2.4069452984971478E+00
2.4835935328314371E+00	2.0356308927602784E+00	2.4001105607124731E+00	2.0851462516987591E+00
2.1747110099719200E+00	2.2991518594240721E+00	2.1653476215063114E+00	2.0978981383048598E+00
2.1812260459196628E+00	2.1184665870169246E+00	2.1220380898907192E+00	2.1148543366023000E+00
2.1023355597648390E+00	2.0960466773273776E+00	2.0962791413958088E+00	2.0819018234059552E+00
2.0883479246875449E+00	2.0761569349972970E+00	2.0773758651178307E+00	2.0735296403640930E+00
2.0691712239793207E+00	2.0690959986219992E+00	2.0650690749115594E+00	2.0633767125120737E+00
2.0623386587692139E+00	2.0589984661148129E+00	2.0587520150817316E+00	2.0565181933787606E+00
7.9348504237141890E-03	2.8727073066378139E-01	2.2066123919821141E+00	3.6991197109241822E+00
4.2145883860872368E+00	3.1896935319709780E+00	1.9863839975314710E+00	1.7950783854888412E+00
2.2036275084774100E+00	2.7597894419201152E+00	1.8837093137099084E+00	2.2414299080879823E+00
2.3118535110967207E+00	1.8502542394489290E+00	2.1948316018757241E+00	1.8522410789642956E+00
1.9193093335136382E+00	2.0174618032852902E+00	1.8615211531943152E+00	1.7702805954820615E+00
1.8118932326186945E+00	1.7097904489157563E+00	1.6770339470937863E+00	1.6361324777317221E+00
1.5932028434270753E+00	1.5584077574985513E+00	1.5320600417897667E+00	1.4929424773035058E+00
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1.3813979026744558E+00	1.3656082428053611E+00	1.3469810095423733E+00	1.3316896883057672E+00
1.3180193667129909E+00	1.3029469492773744E+00	1.2918343211555763E+00	1.2794310303823442E+00
1.1916612563992060E-02	3.4759610874796382E-01	2.3476809804512402E+00	3.9666538228500543E+00
4.1893722043725194E+00	2.7408049192381361E+00	2.0750750019358302E+00	1.9010455147752228E+00
2.5958140037460971E+00	2.6397780164012707E+00	1.9458308107053131E+00	2.5851510687379253E+00
2.2547141034563780E+00	2.1512983073920231E+00	2.4689124701268454E+00	2.2767632729630574E+00
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2.1079079205285765E+00	2.1568734457770979E+00	2.0906503507595819E+00	2.1304230790419552E+00
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2.0661685528870555E+00	2.0667363207850480E+00	2.0633686820388664E+00	2.0611593006282782E+00
2.0604781071472762E+00	2.0568649997039619E+00	2.0575514683546734E+00	2.0535522579247587E+00
9.6387017129226232E-03	3.3952477370938688E-01	2.3240954916471392E+00	3.9235202751120726E+00
4.1313248987992823E+00	2.6722218526218078E+00	1.9765065185144481E+00	1.8068214346247387E+00
2.4637857276161257E+00	2.4937388029265803E+00	1.7945866177598619E+00	2.4222755984953914E+00

2.0702169452557402E+00	1.9462947339225507E+00	2.2485162955785389E+00	2.0295333883299334E+00
1.7885982265773595E+00	1.8444240419022468E+00	1.9440297653041601E+00	1.8471227997033510E+00
1.7145070746381896E+00	1.7229625238368069E+00	1.6188347683518285E+00	1.6241976886500065E+00
1.5438017684498688E+00	1.5438865402602848E+00	1.4821292966837789E+00	1.4771723160500601E+00
1.4313023428079381E+00	1.4215396558907674E+00	1.3879327443356733E+00	1.3752465316031628E+00
1.3510459944785174E+00	1.3364711706226955E+00	1.3191299105328400E+00	1.3040393463779267E+00
1.2914753819184037E+00	1.2768392607002910E+00	1.2673881431036995E+00	1.2540941312109344E+00
1.4413403580546102E-02	4.1198098475517714E-01	2.4999309279927706E+00	4.3106493814447822E+00
3.7392383868183923E+00	2.6867389696505568E+00	1.7867326017790257E+00	2.1930491290530232E+00
2.8287936914740159E+00	2.3924774765368126E+00	2.1516564406787220E+00	2.6080215595079719E+00
2.0568666042472961E+00	2.3799374609878337E+00	2.2607288826972916E+00	2.3558300362370095E+00
2.2488900212794367E+00	2.1171300411059071E+00	2.1060097187759830E+00	2.1660840447640894E+00
2.1474822232050310E+00	2.1109495799829809E+00	2.1185383304158965E+00	2.1042125101494702E+00
2.0964010527240635E+00	2.0897973114604369E+00	2.0903691433359199E+00	2.0764853237350529E+00
2.0819202188726509E+00	2.0725387764319110E+00	2.0714304864935951E+00	2.0687189533114907E+00
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2.0571737345259855E+00	2.0569288635626055E+00	2.0536703065856843E+00	2.0534729448435138E+00
1.1873924261516461E-02	4.0281525042598043E-01	2.4733590399127263E+00	4.2608344808115115E+00
3.6793831708505307E+00	2.5974055701291974E+00	1.6930855881606943E+00	2.0724043447448031E+00
2.6970305871868900E+00	2.2401318410877367E+00	1.9774071842748406E+00	2.4199020127358204E+00
1.8555941722680076E+00	2.1597887379460161E+00	2.0246816970872290E+00	2.0912293358196825E+00
1.9532507049359968E+00	1.7943973309258114E+00	1.7567734039486869E+00	1.7914600190320906E+00
1.7260433078442157E+00	1.6475205251408176E+00	1.6166705331588629E+00	1.5672156264125148E+00
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1.4103432992378166E+00	1.3805718311962227E+00	1.3608818338265896E+00	1.3411069075454449E+00
1.3228744401980956E+00	1.3054209346712993E+00	1.2916454262384964E+00	1.2768672193472199E+00
1.2637248121643179E+00	1.2535229248748789E+00	1.2411115874764014E+00	1.2324325778537968E+00
1.7581744806155951E-02	4.8834075843846597E-01	2.7525709775491416E+00	4.3304811486876966E+00
3.6048545024920822E+00	2.2086899531918687E+00	1.9350959744070833E+00	2.3945824632186556E+00
2.9753503165619954E+00	2.1688184172974343E+00	2.3877176155904789E+00	2.3818420516644476E+00
2.1005659209973349E+00	2.4603770467935577E+00	2.0532769208518702E+00	2.1611215560730823E+00
2.2647303755942776E+00	2.2737502001558791E+00	2.1999588445698581E+00	2.1131748561939165E+00
2.1013969654536271E+00	2.1560145414867979E+00	2.1030075488212896E+00	2.0850058875934954E+00
2.1056369360495784E+00	2.0888535010071498E+00	2.0778697864855249E+00	2.0812334632158063E+00
2.0752966763630671E+00	2.0717950315972282E+00	2.0685637864365725E+00	2.0647930707674389E+00
2.0654213484820461E+00	2.0612698897317236E+00	2.0574451918121315E+00	2.0589590862460341E+00
2.0560887221432562E+00	2.0525577718821366E+00	2.0532923802460239E+00	2.0516385384328060E+00
1.4737609830103865E-02	4.7786531963782358E-01	2.7209897732051815E+00	4.2793216813648840E+00
3.5265378455248388E+00	2.1257055109118839E+00	1.8141727172254061E+00	2.2738677817132609E+00
2.8354063957059727E+00	1.9920867386795771E+00	2.2162939152961143E+00	2.1867833054266455E+00
1.8830417536576780E+00	2.2239529641012918E+00	1.7983114757234351E+00	1.8738189962522682E+00
1.9465139696171461E+00	1.9266711778118517E+00	1.8240458134693414E+00	1.7124024163858722E+00
1.6508160584541742E+00	1.6615856740430037E+00	1.5691234195940220E+00	1.5154735526358025E+00
1.5038494079335607E+00	1.4577635667554141E+00	1.4205185609776068E+00	1.3999593303835796E+00
1.3724932531940359E+00	1.3494112525407929E+00	1.3283658399515030E+00	1.3085429273594578E+00
1.2945409292535339E+00	1.2771731580507397E+00	1.2613244069879914E+00	1.2519752215967306E+00
1.2392136172375525E+00	1.2267606595110632E+00	1.2193599759991409E+00	1.2103437500740488E+00
2.0551633025814871E-02	5.5448681904161312E-01	3.0480060444681158E+00	4.1464061199991704E+00
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2.8951994404751362E+00	1.9890764888574903E+00	2.5885415987812759E+00	2.1680865300810059E+00
2.2969255123494392E+00	2.3003670848734910E+00	2.1216434947072176E+00	2.0676822849712235E+00
2.0955457369676780E+00	2.1544570553154418E+00	2.1971211138528615E+00	2.2062972568419319E+00
2.1376338172405394E+00	2.0869086316463985E+00	2.1003843593992659E+00	2.1103697130067323E+00
2.0938997227554044E+00	2.0817795340997067E+00	2.0806231710498402E+00	2.0766002448682994E+00
2.0721745148807846E+00	2.0715325134824178E+00	2.0684463385902747E+00	2.0623131225480762E+00
2.0603051968081094E+00	2.0612335996794870E+00	2.0589031636743371E+00	2.0548723017404229E+00
2.0534281546607098E+00	2.0530617118165417E+00	2.0513803903938888E+00	2.0496353207410207E+00
1.7446074123244344E-02	5.4284211973464491E-01	3.0113283444438448E+00	4.0933669201393164E+00
3.4577146502266025E+00	1.9265978481778911E+00	1.8148091070251691E+00	2.5470564192565375E+00

2.7425418858145467E+00	1.8171560011795886E+00	2.3964465182014711E+00	1.9590001185352888E+00
2.0649338661967778E+00	2.0482081777362402E+00	1.8521764841832029E+00	1.7646644605785693E+00
1.7584543233253109E+00	1.7868584395438272E+00	1.8016442443854452E+00	1.7825624321284128E+00
1.6643265132421630E+00	1.5684070937643817E+00	1.5417916247424563E+00	1.5157646786952785E+00
1.4670280524133428E+00	1.4261345115883052E+00	1.3989733916452500E+00	1.3717287202595885E+00
1.3462557426799342E+00	1.3268540219391873E+00	1.3068168288701130E+00	1.2854434152712786E+00
1.2697499853544694E+00	1.2583509766037346E+00	1.2449620937959498E+00	1.2309477847858361E+00
1.2205366581149546E+00	1.2120755095505991E+00	1.2031393710475344E+00	1.1948737474842943E+00
2.4157349622180198E-02	6.2967764491168243E-01	3.3788623655386307E+00	4.0659410113561298E+00
3.0489708424439157E+00	2.0174054225143863E+00	2.1135511682921853E+00	2.8394993768757084E+00
2.8545418592426821E+00	1.9893458067310184E+00	2.6360486115970758E+00	2.0353788235232315E+00
2.4519047750287264E+00	2.0999896310453545E+00	2.3134156510640893E+00	2.2038606711703399E+00
2.1288210407034920E+00	2.0914556684421116E+00	2.0819496787463367E+00	2.0896540834393345E+00
2.1235834540078629E+00	2.1359186378994357E+00	2.1192619345491837E+00	2.0954407732206710E+00
2.0825434359682218E+00	2.0801163076188676E+00	2.0789056957475989E+00	2.0745359536569095E+00
2.0697008047476673E+00	2.0674799215490061E+00	2.0667086953708202E+00	2.0645262458490148E+00
2.0604209890791352E+00	2.0565516358346470E+00	2.0546584014011180E+00	2.0541508430385358E+00
2.0533600956103744E+00	2.0516345042737849E+00	2.0496800702916778E+00	2.0482421446208585E+00
2.0756102119035384E-02	6.1664825793146116E-01	3.3374696370393586E+00	4.0049633375059042E+00
2.9720455643943677E+00	1.9055492104303593E+00	1.9742701465697574E+00	2.6936244661975386E+00
2.6976759279960039E+00	1.8043950940654911E+00	2.4326175284726017E+00	1.8130705641916860E+00
2.2067785695868496E+00	1.8324056814352041E+00	2.0296330690109077E+00	1.8820271626896088E+00
1.7732996145199376E+00	1.7036698592604378E+00	1.6632846292070598E+00	1.6427342494318526E+00
1.6251815905515576E+00	1.5921682558328623E+00	1.5349406924895945E+00	1.4752240107648968E+00
1.4304430817733989E+00	1.3995278807834504E+00	1.3729664484252184E+00	1.3460320656485054E+00
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1.2510787502848584E+00	1.2358882007589311E+00	1.2239083654806540E+00	1.2144008549207816E+00
1.2055929432297880E+00	1.1967244645786965E+00	1.1884267905958661E+00	1.1812869825086687E+00
2.9185065055535357E-02	7.2804643619381249E-01	3.6258418186679235E+00	4.2748736777076379E+00
2.7265466028263843E+00	1.7643222564284806E+00	2.3394263171824425E+00	2.9556458402285739E+00
2.5880858162767817E+00	2.1844903007932608E+00	2.4657674784824355E+00	2.1209805883197075E+00
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2.0688626488706081E+00	2.0648345617858674E+00	2.0619511897000429E+00	2.0599112145883440E+00
2.0582327051788463E+00	2.0565262118546568E+00	2.0546359856266561E+00	2.0526385877613627E+00
2.0507185518694224E+00	2.0490432219744608E+00	2.0476676719716456E+00	2.0465310419925182E+00
2.5402343894417336E-02	7.1310194080833955E-01	3.5816650632922924E+00	4.2005314541508003E+00
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2.4085760191331871E+00	1.9878067284152412E+00	2.2518330720957946E+00	1.8811994134819956E+00
2.1367957545304637E+00	1.8084434215872882E+00	2.0414657205538549E+00	1.9524287238976457E+00
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1.6032826498595947E+00	1.5351824455495802E+00	1.4834886282376776E+00	1.4423636149315111E+00
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1.2955127065426510E+00	1.2748449113550655E+00	1.2572688834013412E+00	1.2422617949073596E+00
1.2291594775930916E+00	1.2173989437068167E+00	1.2065999336240583E+00	1.1967754430622066E+00
1.1879980579713876E+00	1.1802403725239956E+00	1.1734826635046995E+00	1.1676287105542960E+00
3.9424431388266234E-02	9.3090429300637467E-01	3.7083576186965717E+00	3.8738193201345625E+00
2.2938311463500445E+00	1.9558325891627262E+00	2.7605607889535748E+00	2.7905972127425436E+00
2.1336411940052713E+00	2.5401271663057603E+00	2.1161958850445863E+00	2.4169805596834188E+00
2.1098750374271757E+00	2.3282112733719695E+00	2.1201317021172619E+00	2.1326399405685001E+00
2.1399379656379467E+00	2.1419791248507645E+00	2.1373152402125766E+00	2.1284998872998950E+00
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2.0481742087580761E+00	2.0469487659216208E+00	2.0457293700269319E+00	2.0444181953579079E+00
3.5532120607314831E-02	9.1443149880035712E-01	3.6669651014884099E+00	3.8081641093501544E+00

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1.9653311841921759E+00	2.3502323552231066E+00	1.9020610798455495E+00	2.1773648050925254E+00
1.8481136575652026E+00	2.0471851381451756E+00	1.8176080782483368E+00	1.7909291751799539E+00
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1.2269811325584137E+00	1.2152316109229542E+00	1.2044367485307790E+00	1.1947466681433225E+00
1.1863357613355121E+00	1.1790255833238863E+00	1.1724667626945566E+00	1.1664321298156031E+00
5.7100553348343630E-02	1.2917603147455188E+00	4.1135732667803495E+00	3.5118664288981574E+00
1.9368752157733209E+00	2.3771128872876215E+00	2.9220639296203461E+00	2.3177109185158068E+00
2.0592997216977103E+00	2.4575416869422813E+00	2.2484889633467904E+00	2.1849846941446613E+00
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2.1378787431214228E+00	2.1293587062287553E+00	2.1284379582194997E+00	2.1166302932201759E+00
2.1020501275261272E+00	2.1037602508007947E+00	2.0873004439628811E+00	2.0815162636039921E+00
2.0742318224882497E+00	2.0717137552065861E+00	2.0688727610235911E+00	2.0636301642526957E+00
2.0609129118071623E+00	2.0573721980608455E+00	2.0562801552171730E+00	2.0537520560668492E+00
2.0515857309822700E+00	2.0495827851980115E+00	2.0478472875293194E+00	2.0468438573974974E+00
2.0451428861753276E+00	2.0439007714925661E+00	2.0424323823518815E+00	2.0414687837457297E+00
5.3051175350958726E-02	1.2728278375090589E+00	4.0669786207827503E+00	3.4372507997500428E+00
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2.0600704987971659E+00	1.8309842917408685E+00	1.9648842385034861E+00	1.8445244971119537E+00
1.7630149207767090E+00	1.7212748973294125E+00	1.6881429000710397E+00	1.6466681954544988E+00
1.5786556382587877E+00	1.5337468065976421E+00	1.4764013394115085E+00	1.4346908003482397E+00
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1.1843185027714012E+00	1.1769874759089263E+00	1.1701803599045422E+00	1.1645385215832835E+00
8.0540729324497268E-02	1.7410046060717952E+00	4.3105552464335126E+00	2.7945823762563200E+00
1.8927730812938091E+00	2.7994611716288280E+00	2.6682551083446682E+00	1.9822807786148355E+00
2.4432445090009671E+00	2.0719581975238945E+00	2.4247893982096906E+00	2.1849092221290691E+00
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2.1583159528841587E+00	2.1254851696761063E+00	2.1210417672441162E+00	2.1083344794385712E+00
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2.0709842171706994E+00	2.0677013161484119E+00	2.0634988508864285E+00	2.0601870754218252E+00
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2.0425488317063598E+00	2.0412575339754637E+00	2.0401488511447456E+00	2.0389818452919739E+00
7.6168715170621487E-02	1.7196939691686639E+00	4.2643277377046127E+00	2.7220564847944875E+00
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2.2754203467146192E+00	1.8832257742018168E+00	2.2067895734492327E+00	1.9448106215372216E+00
1.8902097290021547E+00	1.9952745017088029E+00	1.8185928755774010E+00	1.8420305288458914E+00
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1.5754969161194270E+00	1.5036362473476590E+00	1.4638798449451740E+00	1.4189534736468621E+00
1.3819156127430885E+00	1.3512067375356611E+00	1.3227522997362979E+00	1.2985283872906588E+00
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1.1060262175533413E-01	2.1110616886993725E+00	4.1067115437607589E+00	2.3887991207791623E+00
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1.2232293087681651E+00	1.2213016399298401E+00	2.1087312832115948E+00	2.1011140921775535E+00
2.0876942809605410E+00	2.0789458664656154E+00	2.0731605729862834E+00	2.0689473302439438E+00
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2.0513731274768343E+00	2.0487945478486247E+00	2.0467409311161582E+00	2.0450811290446698E+00
2.0436440897476853E+00	2.0422833417066681E+00	2.0409259443923284E+00	2.0395679742537949E+00
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1.9036626085829693E+00	1.9244649344925253E+00	1.8028103605547616E+00	1.7620365130590758E+00
1.6919284092271156E+00	1.6530687782963989E+00	1.6060139276750545E+00	1.5670048877456382E+00
1.4978394707177780E+00	1.4419923755823145E+00	1.3960488541401264E+00	1.3575283940751091E+00
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1.2309113263668590E+00	1.2150518016494072E+00	1.2016559040216284E+00	1.1903374093514867E+00
1.1806358775578756E+00	1.1722286695297193E+00	1.1648605682218565E+00	1.1583745155709348E+00
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