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Radiation Heat Transfer Calculations**

S.L. Chang, B. Golchert, and M. Petrick
Argonne National Laboratory
Argonne, IL 60439

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The Effect of the Number of Wavebands Used in Spectral Radiation Heat Transfer Calculations

by

S.L. Chang, B. Golchert, and M. Petrick

Argonne National Laboratory

9700 S. Cass Avenue ES/362

Argonne, IL 60439

(630)-252-6518, (630)-252-6955, (630)-252-5960

Fax: (630)-252-5210

slchang@anl.gov, bgolchert@anl.gov, mpetrick@anl.gov

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ABSTRACT

A spectral radiation heat transfer model that conserves emitted and absorbed energy has been developed and used to model the combustion space of an industrial glass furnace. This comprehensive radiation heat transfer model coupled with a computational fluid dynamics (CFD) code was used to investigate the effect of spectral dependencies on the computed results. The results of this work clearly indicate the need for a spectral approach as opposed to a gray body approach since the gray body approach (one waveband) severely underestimates the energy emitted via radiation.

NOMENCLATURE

A	total band absorptance ($1/\mu\text{m}$)	c	speed of light (m/s)
f	species concentration (kg of species/kg of mixture)	f_v	soot volume fraction
h	enthalpy (J/kg) or Planck's constant	k	reaction rate or Boltzmann's constant
L	optical length (m)	n, n_k	optical constants
q_r	radiation heat flux (J/m^2)	S	source term in conservation equation (4)
T	temperature (K)	t	time (s)
u	velocity (m/s)	x_i	Cartesian coordinates, $i=1, 2, \text{ and } 3$

Greek Symbols

χ	optical variable defined in Eq.(7)	Γ	diffusivity (m^2/s)
λ	wavelength (μm)	σ	Stefan-Boltzmann constant
ξ	general flow property ($1, u_i, h, \text{ and } f_i$)	ρ	density (kg/m^3)
κ	volumetric absorptivity		

Subscripts

s subspecies

INTRODUCTION

The rapid advance in the performance of computers has made possible a concurrent advance in computational approaches to complex combustion systems of practical interest such as a glass furnace. These furnaces use the intense heat (mainly radiation) from the combustion of fuel and air/oxygen to melt sand and cullet (scrap glass) into glass products such as pane glass, TV glass, fiberglass, container glass, and light bulbs. Since the melting of glass is energy intensive, an improvement in the performance (efficiency) of a glass furnace can save energy and reduce pollutant and greenhouse gas emissions. Computational fluid dynamic (CFD) simulations can be used as a tool to improve the performance of a glass furnace. Since the heat from combustion (mostly radiation) drives the melting of the glass and a significant portion of the spectra of the radiation can penetrate into the glass flow, a CFD model needs to include a comprehensive radiation heat transfer model. Radiation heat transfer modeling in a CFD simulation started with simplified conductive-type approach. Recently, more rigorous treatments such as discrete ordinate methods (Fiveland, 1987) were introduced. The discrete ordinate approach includes gray-body emission, absorption, and transmission but can have severe numerical instability problems. A

consortium of five glass companies, two universities, and Argonne National Laboratory was formed to develop a rigorous, coupled glass furnace simulation that included advanced radiation modeling. This paper utilized the advanced radiation heat transfer model to investigate the spectral dependence of radiation heat transfer.

THEORETICAL APPROACH

A sketch of a glass furnace is shown in Figure 1. Fuel (natural gas or diesel fuel) and oxidizer (air or oxygen) are injected into the furnace and burnt. The heat of burning raises the gas temperature well above the melting temperature of the glass batch material (about 1400K). Because of the high temperature environment in the furnace, radiation becomes the dominant heat transfer mode and a significant amount of pollutant (i.e., NO_x) can be produced. Therefore, the coupling of fluid dynamics, combustion reaction, radiation heat transfer, and pollutant kinetics is essential for computational modeling of the combustion space of a furnace.

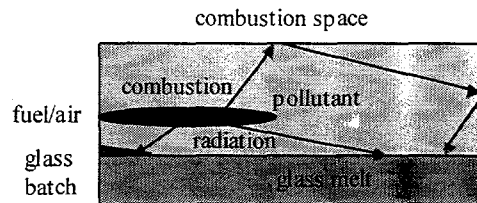


Figure 1 Sketch of a Simple Glass Furnace

A CFD code, ICOMFLO, was developed to simulate the combustion space of glass furnaces. The simulation consists of three major computational steps. The code first computes the major flow properties of the combustion flow in the furnace by assuming a uniform radiation heat flux in the space. In this step, pressure, temperature, density, velocity, and species concentrations are locally computed. A combustion model of the major species is needed in this step to establish an initial temperature field. Next, a kinetic model of the product species (or called subspecies) is used to calculate the formation and transport of the subspecies based on the major flow properties computed in the first step. Then, a radiation heat transfer model is used to calculate local net radiation heat flux (the balance of emission and absorption) based on the temperature and pressure calculated in the first step and the species concentrations calculated in the second step. The radiation participating media in a glass furnace include carbon dioxide, water vapor, and soot in the combustion space and glass in the glass melt flow. The energy absorbed in the crown of the furnace is used to calculate the surface temperature and this surface temperature is then used to calculate the surface emissive energy along with the reflected thermal energy. Since radiative emission and absorption of these media depend strongly on wavelength of the radiation, a spectral radiation heat transfer model is used. The spectral radiation heat transfer model divides the spectrum into a set of wavebands. This work focuses on the effect of the number of wavebands used to represent the spectrum.

Formulation of Hydrodynamic Flow with Combustion

In the first step of the calculation, major flow properties are computed with a highly reduced combustion model. The primary information required from the combustion model for the flow computation is the heat of combustion and mixture molecular weight change due to combustion, which affects mixture density through the equation of state. The flow is a mixture of many species. The species selected for the first-step calculation include nitrogen, fuel, oxygen, and two lumped products.

In the next step, pressure, temperature, velocity, density, and species concentrations are calculated from the conservation equations of mass, momentum, and enthalpy, the transport equation of species, and the equations of state. The equations of mass, momentum, enthalpy, and species are all elliptic-type partial differential equations. For convenience in numerical formulation, these equations are arranged in a common form, Eq.(1).

$$\sum_{i=1}^3 \frac{\partial}{\partial x_i} (\rho u_i \xi - \Gamma_\xi \frac{\partial \xi}{\partial x_i}) = S_\xi \quad (1)$$

in which ξ is a general flow property, x_i , $i=1,3$ are coordinates, u_i , $i=1,3$ are velocity components. Γ is effective diffusivity (calculated from both laminar and turbulent viscosities), and S_ξ is the sum of source terms. The general flow property is a scalar, a velocity component, an enthalpy, or a species concentration for the equations of mass, momentum, enthalpy, and species, respectively. Turbulent diffusivity and the source terms are derived from separate phenomenological models.

The combustion in a glass furnace produces many combustion products including CO_2 , H_2O , CO , NO , and soot. These products or subspecies are transported by the combustion flow whose major properties have been computed in the previous step. Thus, the transport of these combustion products can be formulated and calculated based on the computed flow properties. The subspecies transport equations can be derived as,

$$\sum_{i=1}^3 \frac{\partial}{\partial x_i} (\rho u_i f_{s,i} - \Gamma_{f_{s,i}} \frac{\partial f_{s,i}}{\partial x_i}) = S_{f_{s,i}} \quad (2)$$

in which $f_{s,i}$ is the unknown subspecies concentration, and the other flow properties including density, velocity, and diffusivity are calculated in the previous step. The formation of these subspecies can be determined from a set of detailed or reduced kinetics. The subspecies calculation includes soot. A soot model that accounts for the formation and oxidation of soot was developed.

In this study of glass furnace, seven gaseous species, CH_4 , O_2 , N_2 , CO_2 , H_2O , CO , and NO , are considered in the subspecies calculation. A validated five step kinetic mechanism for methane burning and NO formation (Nicol, et al. 1998) is used. The source terms of the subspecies transport equation can be obtained from the reaction rates in this reduced kinetic model. Once the solution of the transport equations is converged, the concentrations of CO_2 and H_2O are then used in the computation of radiation heat transfer.

Formulation of Spectral Radiation Heat Transfer

By assuming the scattering effect in the combustion flow is negligible, the radiative transport equation is basically the balance of emissive and absorption powers. Local net radiation heat power can be obtained by adding the absorbed energy of the incoming radiation from all other locations and subtracting the emitted energy for every wavelength. From which a radiative transport equation, Eq.(3), can be derived.

$$q_r(x, y, z) = \int_0^\infty \left[\int_0^\infty \kappa'_\lambda e'_{b\lambda}(T') e^{-\int \kappa''_v dv'} dv' \right] - \kappa_\lambda e_{b\lambda}(T) d\lambda \quad (3)$$

in which T is temperature, κ_λ is spectral volumetric absorptivity, and $e_{b\lambda}$ is the black body radiation function. The radiative transport equation (RTE) needs to be solved together with the CFD flow equations to determine the temperature field. In the combustion flow of the glass furnace, the radiatively participating media include mainly H_2O , CO_2 , and soot. The spectral volumetric absorptivity of these media will be determined from a gas and a soot radiation model.

Gas Radiation Model

Radiation from the H_2O and CO_2 species is not gray but in various wavelength bands with various intensities. H_2O radiation has five bands, centered at the wavelength of 1.38, 1.87, 2.7, 6.3, and 20 μm , and CO_2 radiation has six bands, 2.0, 2.7, 4.3, 9.4, 10.4, and 15 μm .

Edwards and Balakrishnan (1974) introduced a procedure to calculate total band absorptance by using a wide band model. For each band of the gas radiation, species concentrations, pressure and temperature are used to determine a set of semi-empirical parameters: the integrated band intensity, the bandwidth parameter, and the line width parameter. Then, a semi-empirical correlation is used to calculate the total band absorptance from these parameters. The total band absorptance is defined as,

$$A_i = \int_{\text{band } i} [1 - \exp(-k_\lambda L)] d(1/\lambda) \quad (4)$$

As can be seen in Eq.(4), the total band absorptance is a function of the volumetric absorptivity, which is a function of wavelength. Chang and Rhee (1986) converted the total band absorptance of gas radiation to spectral volume absorptivity for a calculation of the radiation heat transfer from diesel combustion. Their approach is used here to calculate spectral radiation heat transfer from a glass furnace.

Soot Radiation Model

Soot radiation also depends on wavelength. As the scattering is negligible, Rayleigh-limit expression of the soot volume absorptance $\kappa_{s\lambda}$, Eq.(5), can be used.

$$\kappa_{s\lambda} = \frac{36n^2k(\pi/\lambda)f_v}{[n^2(1+k^2)+2]^2 + 4n^4k^2} \quad (5)$$

Eq.(5) shows that soot volume absorptance is proportional to soot volume fraction f_v , and inversely proportional to the wavelength. However, the optical refraction indices, n and k , are also weak functions of wavelength. A dispersion model based on the classical electromagnetic theory is found to fit the experimental data by choosing appropriate constants.

NUMERICAL SCHEME

In a previous section, the set of governing equations used to solve for the velocity, pressure, density, temperature, and species concentration of the major species in the combustion space of a glass furnace was presented. ICOMFLO adopts a control volume approach to convert these governing equations to algebraic equations on a staggered, discretized grid system. The algebraic equations are solved iteratively with proper boundary conditions. In the calculations, Patankar's SIMPLER computational scheme (1980) is used to solve the pressure linked momentum equations. In this computer code, a calculation is considered to have converged if the local and global mass balances are smaller than a set of predetermined criteria. For this simulation, convergence criteria, defined by average mass residual of all computational cells, are 10^{-12} (in dimensionless form, normalized by the gas mass flow rate).

The subspecies are not solved in the first-step flow calculation to avoid numerical stiffness problems. After the first-step calculation, the transport equations of these kinetic subspecies is then solved for using the pre-determined flow field. Free from the interactions of the pressure and velocity fluctuations, the calculation of the partially de-coupled species transport equations becomes very stable numerically.

RTE is hard to solve with a CFD code because a CFD code is generally formulated for a Cartesian coordinate system and RTE is most suitable for the spherical coordinate system. Many existing methods make engineering approximations in order to simplify the most general RTE. However, these simplifications often create situations where an energy balance is not maintained. An advanced approach has been developed that allows the solving of the RTE in a Cartesian coordinate system and guarantees the integrity of the energy balance between emitting and absorbing powers.

The RTE solution routine divides the radiation heat flux into bands of wavelength. The blackbody radiation function can be discretized in the wavelength domain by using a closed form solution developed by Chang and Rhee [1983].

$$\frac{e_b(0-\chi)}{n^2\sigma T^4} = 1 - \frac{15}{\pi^4} \sum_{k=1}^{\infty} \left[\frac{e^{-k\chi}}{k} \left(\chi^3 + \frac{3\chi^2}{k} + \frac{6\chi}{k^2} + \frac{6}{k^3} \right) \right] \quad (6)$$

in which
$$\chi = \frac{hc/k}{n\lambda T} \quad (7)$$

For each wavelength band, a calculation is performed to balance the emitted and absorbed energy. For each node in the CFD grid system, emitted energy from a node is calculated. Then, this emitted energy is traced along the optical paths of all angles. The energy absorbed in every node (including the wall surface node) is calculated and added to the absorption energy of the initial node. In three dimensions, the emitted energy leaving the node is divided into six solid angle directions (plus and minus x_1 , plus and minus x_2 , and plus and minus x_3).

Once the total amount of energy absorbed in the crown is calculated, an iterative routine is used to determine the corresponding wall temperature and surface radiation. This routine accounts for the heat transfer effects (convective) on both sides of the wall, the heat transfer due to conduction (inside the wall), the reflection of thermal radiation incident to the wall, and the emissive radiation from the wall (based on the calculated wall temperature).

CODE VALIDATION

The code was set up to model a portion of a glass furnace on which experimental measurements were taken (Newbold et al., 1977). This is only a qualitative validation since the exact geometry and operating conditions were not explicitly given in the article. The actual configuration of the furnace contains a

number of burners with fuel/oxidizer entering on one side of the furnace and exiting out the other side. For this work, only one burner is simulated in order to focus on the capabilities of the newly developed computational models. The dimensions of the furnace are 11 m in the direction of the flow, 2.6 m high and 3.6 m wide. The computational results reproduce the general flow field that was measured in the furnace. In addition, the computed temperature and species concentrations match fairly well with the experimental results.

RESULTS AND DISCUSSION

This furnace burns natural gas with air that has been preheated to 1400 K. The burners are modeled as concentric tubes with the fuel being injected on the inner tube and the oxidizer being injected in outside tube. The furnace operates with a significant amount of excess oxygen. ICOMFLO calculates the flow property distributions and radiation heat transfer inside the furnace.

This paper is focusing on the discussion of the spectral effects of the radiation model. The radiation model requires the input of the local temperature and gaseous species distribution. Figure 2 shows a temperature distribution in the combustion space of the glass furnace. The figure shows a cutaway view of the furnace with the inlet to the burners being on the left and the exhaust being on the right. A plume shape flame structure is shown in the figure.

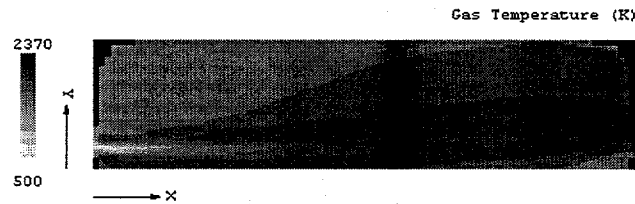


Figure 2: Temperature Distribution in the Combustion Space of the Glass Furnace

With this information along with the local molar concentrations of water vapor and carbon dioxide, the spectral radiation heat transfer equation may now be solved. Figure 3 shows computed net radiation heat flux in the same cross-section of the furnace. The net radiation heat flux is highly non-uniform and appears to have strong dependency on the flame structure.

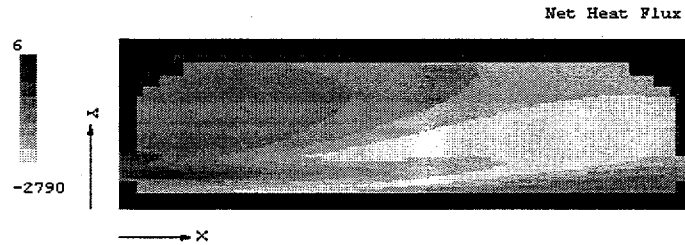


Figure 3: Net Radiation Heat Transfer Rate in the Combustion Space of the Glass Furnace

However, the method for selecting both the number of wavebands and the relative width of each waveband can have an influence on the total amount of absorbed energy. As was mentioned earlier, assuming one waveband corresponds to the gray-body approximation. This assumption does indeed simplify the radiation calculation but there might be a trade-off in the accuracy of the solution. To determine the effect of the number of wavebands on the calculated absorbed heat flux, a series of computational trials were performed for the same input data (geometry, local temperature, and local species concentration). Figure 4 compare absorption heat flux at a location in the combustion space. Clearly, absorption heat transfer is highly spectral dependent. Figure 5 also gives an indication of the minimum number of 'acceptable' wavebands based on a predetermined accuracy margin. Making the gray-body assumption can underestimate the amount of the radiation heat flux about 10 %. Thus, after five or six equally spaced wavebands, the increase in accuracy becomes less and less. Since additional wavebands directly correlates to additional execution time, the choice of the number of wavebands (overall accuracy of the radiation calculation) has to be balanced by reasonable execution times.

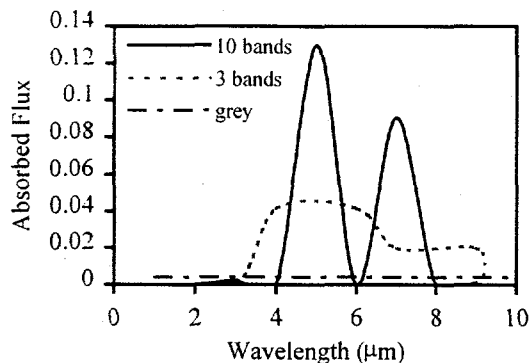


Figure 4: Radiation Absorption at a Location of Various Waveband Calculations

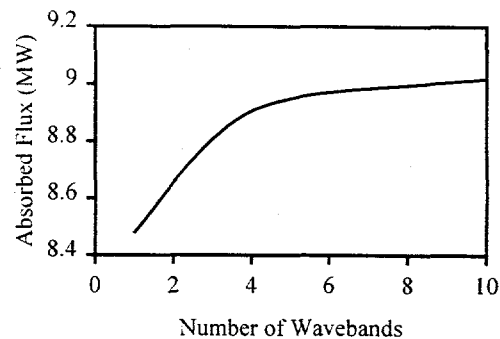


Figure 5: Total Absorbed Flux as a Function of the Number of Wavebands

While the wavebands chosen for the sensitivity trials presented in Figure 5 were all equally spaced, care must be taken when selecting the cutoffs between bands. Since the gaseous species have eleven wavelengths where the radiation emission is strong, it is advisable to avoid placing a waveband cutoff on or near one of these wavelengths. For example, if one were select six wavebands and then to equally space these wavebands, one of the wave bands would fall in a region very near one of the gaseous species wavelengths. When this occurs, the model will overestimate the radiation heat flux; it is similar to 'double counting' the effect of the gaseous wavelengths. For this particular example, the formulation will predict an absorbed heat flux that would be ten percent higher than the calculated heat flux using ten bands.

SUMMARY

The sensitivity of the calculated radiation heat flux to the discretization of the thermal energy spectrum was demonstrated. It was shown that the gray-body approximation underestimates the radiation heat flux by about ten percent. Further, it was shown that how the spectrum is split into wavebands could have a significant effect on the calculated heat flux. The selection of cutoffs between wavebands should not occur near the strongly radiating wavelengths of the gaseous species. This work shows the necessity of implementing a proper spectral radiation heat flux model in order to calculate accurate heat fluxes.

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