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INFLUENCE OF PARTICLES SIZE AND CONCENTRATION IN PARTICLES CLOUD RADIATION BY MIE THEORY

Dusan N. Trivic Department of Thermal Engineering and Energy Research Institute of Nuclear Sciences "Vinca" P.O. Box 522 11001 Belgrade Yugoslavia

> Bojan Djordjevic and Zeljko Grbavcic Faculty of Technology and Metallurgy Karnegijeva 4 11000 Belgrade Yugoslavia

ABSTRACT

The effects of mean diameter of particles and of particles concentration, for particles cloud, on the radiative heat flux have been analyzed by a mathematical model. The mathematical model for the radiation of particulate media on the surrounding walls, for 3-D rectangular geometry has been developed. The model is based on the Hottel-Cohen Zone Method for the analysis of radiative heat transfer. Total View Factors for radiative exchange have been evaluated by the Monte Carlo Method. Mie Theory has been used for the determination of the radiative properties of particles cloud in the enclosure. Parameters defining the radiative properties by Mie equations are: particles shape, mean diameter of particles, complex refractive index of particles material, density of material, particles concentration and the wavelength of incident radiation. The particles considered have been of spherical shape.

In the zone method, the enclosure and its surrounding surfaces are divided into a number of volume and surface zones, each of which is assumed to have uniform properties. A radiative energy balance is written on each zone giving the net radiative heat transfer between that zone and every other volume and surface zone in the system. The Monte Carlo Method is based on probability and statistics. The concept of energy bundles is introduced to simulate the actual physical process of radiation. A statistically meaningful number of energy bundles are followed from initial points of emission through randomly determined paths until the final points of absorption on the system. The mathematical and physical background of the interaction between incident radiation and a single solid particle is the solution of Maxwell's wave equations. Gustav Mie solved Maxwell,s wave equations with the appropriate boundary conditions for single cylindrical and spherical particles and the resulting equations are called the Mie equations.

The main objectives of the study are: To link numerically Hottel-Cohen zone method and Monte Carlo Method with Mie equations and to create an original 3-D computer code for the prediction of heat flux distribution. Using the code, as the results, the distribution of net radiative heat flux on the surfaces of a cube have been predicted for various values of mean diameter of particles and of particles concentration. The parametric study has been carried out keeping constant: complex refractive index of particles material and density of material. The wavelength of incident radiation was varied as well. It has been concluded, inter alia, that the larger is the mass concentration of particles the higher is the radiative heat flux transferred to the surfaces. The influence of particles diameter on the heat flux is not straight forward and it depends on the wavelength of incident radiation.

INTRODUCTION

Mathematical modelling of particles radiation within a boiler furnace is very complex due to several reasons. First of all there are more different types of particles. In a pulverized coal fired furnace, for example, the particles consist of chair, soot and ash. Each of these species has its own physical properties as, inter alia, complex refractive index and density. Also the concentrations and the sizes of particles, for each of the species, vary within the enclosure. Besides that the complex refractive index varies to some extent with the wavelength of incident radiation and Foster and Haworth (1968) gave some data for carbons and coals. The radiative properties of a suspension of particles, as absorption and scattering coefficients and the scattering albedo, depend on the wavelength of the incident radiation. Thus the radiative heat coming from particles cloud should be considered as a function of wavelength as well.

To carry out the radiation modelling of each particle species for more different particle concentrations and for various particle sizes, simultaneously taking into account the variation of complex refractive index and of the radiative properties of a suspension of particles with the wavelength is a difficult task. It also will take, for an industrial furnace, tremendous amount of computer memory and of computation time, despite the existence of very powerful computer systems nowadays. The difficulties arise as well due to the unknown input data for the predictions, as the distribution of particle concentrations and sizes (granulations) within the furnace. Their evaluation or measurement are not easy. The question is whether it is worth while to develop a large and numerically very complex code which will use uncertain input data.

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Various researchers performed the modelling of particles radiation with various approximations. Trivic (1987) and Steward and Trivic (1989) carried out the modelling of only one dominant particle species as alumina, ash or soot, neglecting the presence of others. They also took an uniform concentration within the whole enclosure and considered that all particles had only one value of mean particle diameter. Their predictions, as well, did not take into account the variation of complex refractive index and of the radiative properties of particles suspension with the wavelength.

Tong and Scocypec (1992) gave a summary of the comparison of the results predicted by several participating authors for a specified radiative heat transfer problem. The idea was to assess the capability at that time (1992) for solving non-gray, anisotropically scattering multidimensional radiation problems. The problems were relevant to the modelling of heat transfer in coal-fired furnaces. The authors applied their own methods to solve the problems. The problems were specified, among other things, for particles suspensions of 30-µm spherical carbon particles. So the size of particles was kept constant in those cases. Also Mie solution was used.

The differences between cases done by Trivic (1987) and Steward and Trivic (1989) at one side and done by Tong and Scocypec (1992) at the other side are the following. The radiative properties (scattering and extinction efficiencies) for the cases performed by Trivic and Steward were evaluated for λ_m , i.e. only for one single value of wavelength. Tong and Scocypec were evaluated the radiative properties of particles suspensions for 21 values of wavelength in the wavelength region between 1.0 and 12.0 µm inclusively, having the increment of 0.5 µm.

Also in cases done in Tong and Scocypec's paper a nonhomogeneous problem for the particles concentration was specified where the carbon particles were distributed in the enclosure according to the given mathematical expression. Five different solution methods were applied by four groups of researchers in Tong and Scocypec's paper to solve variously specified radiative heat transfer problems. Only one group solved nonhomogeneous particles concentration problem.

OBJECTIVES OF THE STUDY

The objective of the study is to develop mathematical model which predicts the heat flux distribution of the particles cloud on the surrounding walls in a 3-D rectangular geometry by Mie Theory. Mie Theory means that only the cases where particles size parameters are not much larger than 1.0 and not much smaller than 1.0 were considered. The goal of the paper was to analyze the influence of particles concentration and particles mean diameter on the heat flux distribution as well. The influence of wavelength of incident radiation is taken into account. Thus only the radiation of one species (particles suspension of soot) with one concentration and with one particles diameter at one wave length of incident radiation is considered here at a time. Hence, the mixture of various particles species (simultaneous radiation of soot, ash etc, of various concentrations and diameters) is not analyzed. An additional simplification is that the cases considered are without the presence of grey or non grey gas.

Compared to real situation in furnaces, it is an idealized situation, but the objectives are to study the effects of particles parameters. So in this study the homogenous and monochromatic or spectral conditions are considered. Also, the model was developed with the intention that it could be used as a "building block" in an analysis of the radiation process of particulate media. Based on the structure of this model, the complex codes for particles suspensions radiation for nonhomogeneous cases within the wavelength regions could be developed.

GEOMETRY AND INPUT DATA

The geometry under consideration is shown in Fig. 1. It is a cube having the dimension of edge 1.0 m. For the purpose of numerical analysis of radiative heat transfer, (the Hottel and Cohen Zone Method is used) each cube edge is divided into ten increments. The length of an increment is 0.1 m. It gives for each side of the cube 10x10=100 and for whole cube 6x100=600 surface zones. The number of volume zones is 10x10x10=1000. All surfaces are grey and diffuse having the emissivity 0.855. The enclosure contains particles suspension of soot.

The enclosure contains particles suspension of soot with an emissive equal to 10.0 Wm2. The emissive power of wall surfaces is equal to 1.0 Wm². With all surfaces having the same emissive power and with uniform emissive power of the medium within the enclosure, the system is symmetric. It means that the heat flux distribution on each cube side should have be the same. This is one of more ways for code testing. The complex refractive index of soot is taken equal to n=2.29-1.49i and the density of soot material p=2003.0 kgm3 and these values were used by Trivic (1987) and Steward and Trivic (1989). These input values are constant throughout all predictions. The shape of particles are spheres. The input data which varied were: particles diameters having the values: 0.5, 1.0, 5.0 and 15.0 µm; the concentrations of solid particles in mass per unit volume with values 1.22, 2.44 and 4.88 gm³ and the wavelength of incident radiation having values 3.0, 4.0 and 5.0 µm.



Figure 1. Enclosure geometry and its zoning

THE BASIC EQUATIONS OF ZONE METHOD

For the zone method, developed by Hottel and Cohen (1958) and discussed by Hottel and Sarofim (1972), the enclosure and its surrounding surfaces are divided into a number of volume and surface zones, each assumed to have uniform properties as temperature, concentration etc. A radiative energy balance is written on each zone giving the net radiative heat transfer between that zone and every other volume and surface zone in the system. This energy balance on a given surface zone "i", considering radiative interaction between surface zones "i" and all other surface zones "j" and volume zones "k" in the enclosure takes the form D. N. Trivic - B. Djordjevic - Z. Grbavcic: Influence of particles size and concentration in particles

$$Q_{s,j(net)} = \sum_{j} \overline{S_j S_i} E_{s,j} + \sum_{k} \overline{G_k S_i} E_{g,k} - \varepsilon_i A_i E_{s,j}$$
(1)

Here the expression $Q_{4,\underline{N}(\underline{n}\underline{n})}$ is the net heat flowrate on the surface zones, and $\overline{S_jS_i}$ and $\overline{G_kS_i}$ are the total interchange areas. Similarly, an energy balance for a volume zone can be expressed

$$Q_{g,i(nei)} = \sum_{j} \overline{S_j G_i} E_{s,j} + \sum_{k} \overline{G_k G_i} E_{g,k} - 4 \kappa_a V_i E_{g,j}$$
(2)

as

where $Q_{g,i(net)}$ is the net heat flowrate in the volume zones, or in other words the volumetric heat source (or heat sink). The expressions $\overline{S_IG_i}$ and $\overline{G_kG_i}$ are the total interchange areas.

MONTE CARLO METHOD FOR TOTAL INTERCHANGE AREAS CALCULATION

The Monte Carlo Method is based on probability and statistics. The concept of energy bundles is introduced to simulate the actual physical process of radiation and is discussed by Siegel and Howell (1972). A statistically meaningful number of energy bundles are followed from initial points of emission through randomly determined paths until the final points of absorption on the system.

The definition of total view factor, f_{ij}, is introduced, which is the ratio of the number of bundles absorbed in zone "j" and originally emitted from zone "i", to the total number of bundles released from zone "i". The total interchange areas can be expressed in the following form:

$$\overline{G_i S_j} = 4 \kappa_a V_i f_{ij}$$
(3)
$$\overline{G_i G_j} = 4 \kappa_a V_i f_{ij}$$
(4)
$$\overline{S_i S_i} = A_i \varepsilon_i f_{ij}$$
(5)

$$\overline{S_i G_j} = A_i \varepsilon_i f_{ij} \tag{6}$$

This is the link between Monte Carlo and Hottel-Cohen Zone methods. The Total Interchange Areas can be calculated by the Determinant Method as well given by Hottel and Cohen (1958) and by Hottel and Sarofim (1972), but Monte Carlo Method is very convenient for non-isotropically scattering media as it is the particles suspension.

The random paths are formulated by following randomly generated decisions. The cumulative distribution function R(\$) is taken to be a random number R. Once the random number R is generated, the required values for the appropriate variable § (which can be coordinates of the points, angles of direction or surface emissivities etc) is calculated from the available relation R(5). Different cumulative distribution functions are used for different variables, such as coordinates of the emission points, the angles determining the direction of emission or the maximum distance of travel. The methods of obtaining these cumulative distribution function are discussed in reference [7]. Every time a decision is necessary a random number in the interval 0.0 to 1.0 is generated. The Monte Carlo relations used in the absence of solid particles were used and reported by Steward and Canon (1971), by Carmichael (1979) and by Kocaefe (1982). The method adapted for the calculation of the radiative interchange involving the scattering by solid particles was reported by Whalen (1972), Guruz (1973) and by Steward and Guruz (1973).

RADIATIVE PROPERTIES OF SOLID PARTICLES

In early furnace calculations, the emissivity of a radiant gas mixture containing solid particles was estimated by empirical relations, reported by Hottel and Sarofim (1972). A rigorous theory of radiative infrared waves interacting with solid particles was developed for several simple particles geometries reported by Van de Hulst (1975). Application of this theory on furnaces modelling, done by Guruz (1973), has given useful results.

Radiation from a cloud of solid particles in a enclosure can be considered as volume radiation. However, the physical phenomena involved are completely different from those in gas radiation. The radiation incident on a solid particle is partly absorbed and partly scattered. The absorption is interrelated to the emissivity by Kirchoff's Law. The scattering is a dispersion of part of the incident radiant energy in different directions. The mathematical and physical background of the interaction between incident radiation and a single solid particle is the solution of Maxwell's wave equations. The solution to this problem was first obtained by Gustav Mie. It was reported by Chromey (1960) and by Van de Hulst (1975). Mie solved Maxwell,s wave equations with the appropriate boundary conditions for single cylindrical and spherical particles. The resulting equations are called the Mie equations and are discussed by Chu at all (1957), Chromey (1960), Deirmedian at all (1961), Hottel and Sarofim (1972) and Modest (1993).

The interaction of a single solid particle with radiation incident on it depends on several dimensionless quantities. These quantities are: the particles shape, the complex refractive index, m=n-ki; the size parameter, s_p, defined as the ratio of a characteristic particle dimension to the wavelength of incident radiation and the number of particles per unit volume. Knowing these quantities and using the Mie equations, the scattering and absorption coefficients, σ_a and κ_a , and the angular distribution function, $f(\alpha)$, can be calculated. The interference among individual particles in a suspension can be neglected when the particles are more then three radii apart, discussed by Siegel and Howell (1972). Radiative properties of the cloud of particles from this category can be determined from the number of solid particles per unit volume in the gas phase.

The resulting quantities of interest for radiative heat transfer calculations are: the scattering albedo w, defined as the fraction of attenuated energy that is scattered by the particle; the absorption and scattering efficiencies X, and X, defined as the ratios of the cross section of these phenomena to the geometrical cross section of the particle; and the angular distribution function $f(\alpha)$, defined as the fraction of the scattered radiant energy directed into a unite solid angle in the direction of the scattering angle α , measured from the forward direction.

The absorption and scattering coefficients, $\kappa_i(\lambda)$ and $\sigma_i(\lambda)$ of a suspension of spherical particles are given by:

$$\kappa_{a}(\lambda) = \frac{3C_{p}X_{a}(\lambda)}{2\rho_{a}D_{a}}$$
(7)

$$\sigma_s(\lambda) = \frac{3C_p X_s(\lambda)}{2\rho D_s} \tag{8}$$

Here C_p is the concentration of solid particles in mass per unit volume, ρ_p is the ultimate density of the solid and D_p is the mean particle diameter of the suspension.

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The number of solid particles per unit volume can be expressed in terms of mass concentration of particles in the gas phase and the ultimate density of the solids. For solid particles suspended in a nonradiant gas, the attenuation of a beam along a straight line is due to absorption and scattering by the solid particles only. In this case, the total extinction coefficient of the medium is given by:

$$\kappa_e(\lambda) = \kappa_a(\lambda) + \sigma_s(\lambda) \tag{9}$$

The scattering albedo, $\omega(\lambda)$ is given by:

$$\omega(\lambda) = \frac{\sigma_i(\lambda)}{\kappa_e(\lambda)} \tag{10}$$

These radiative properties are strongly dependent on the wavelength of the incident radiation and a strict calculation requires the evaluation of these properties as a function of wavelength. However, the gray gas approximation brings simplification and saves a significant amount of computer memory and of computation time. Therefore, a mean wavelength, λ_{m} , representing the spectral distribution of the incident radiant energy was introduced. This wavelength may be calculated from the equal energy division relation for blackbody radiation:

$$\lambda_m T = 4107.0 \ (\mu m \circ K)$$
 (11)

The above radiative properties, the absorption and scattering coefficients and the scattering albedo can be evaluated at this wavelength.

On the assumption that a suspension of solid particles can be treated as a gray gas, the emissivity and absorptivity of the volume of suspension was taken as:

$$\varepsilon_n = \alpha_n = I - e^{(-\kappa_n L_m)} \tag{12}$$

Experimental data on the particle suspension is required for calculating the above quantities in any given circumstance for a particular furnace chamber.

To create the computer code, mathematical formalism and operations based on Mie Theory were carried out for the development of several subroutines. Those subroutines were used for the calculations of: scattering phase function, complex amplitude functions, Mie scattering coefficients, Ricatti-Bessel and Ricatti-Hankel functions and there first derivatives, Legendre Polynomials etc.

The link between Mie Theory and Monte Carlo Method for particle radiation and anisotropic scattering was performed by the following way. Also, this is the difference between non-scattering and scattering media. Once an energy bundle, or photon, hits a volume zone containing particles suspension, it can be either absorbed or scattered. That is checked by Monte Carlo method, discussed by Trivic (1987). If the bundle is scattered, two angles should be calculated: the scattering angle and the angle between plane of incident beam and plane of scattering beam. The direction of the scattered bundle defined by these two angles, is in a different, new, coordinate system. This direction is transformed into the original, old, coordinate system by trigonometrical relations. The scattered bundle whose direction is defined in the original coordinate system is considered now as a new emitted bundle. It is followed through all scatters and reflections until its final point of absorption.

This is a very good example how a problem of physics is exactly interpreted by an appropriate mathematical tool. More details on Mie Theory-Monte Carlo link is given by Trivic (1987).

PREDICTIONS PERFORMED AND PRESENTATION OF RESULTS

The series of predictions were carried out and for each of 600 surface zones the net radiative heat flux was calculated. Only ten values of heat flux for the index k=6, Fig. 1, were used for plotting the diagrams for comparisons. The heat fluxes for the surfaces zones at the i=1 cube side, for k=5 and k=6 have identical (or very close values) because of the system symmetry.

The number of predictions performed here are 20, and the results are presented in six Figures having the numbers from 2 to 7 inclusively.



Figure 2. Net heat flux for various particles sizes at wavelength 3.0 µm.

As was mentioned previously, the calculations were done only for soot. It means that the complex refractive index and the density of material were kept constant for all calculation cases. In Figures 2, 3 and 4 the wavelengths of incident radiation were 3, 4 and 5 respectively, the mass concentration was constant and equal to 1.22 gm³. The variation of net heat flux with particles diameters along the zones designated in Fig. 1 on x surface (for i=1, k=6 and j=1,2,...10) are presented in these Figures. Only the heat flux predicted on these surface zones is considered in all other Figures (Figures 5, 6 and 7). The influence of particles mass concentration on the radiative heat flux for wavelengths of incident radiation 3, 4 and 5 μ m is shown in Figures 5, 6 and 7 respectively, where the particle diameter is constant with the value of 5.0 μ m. These are the results only some of the parametric studies done.



Figure 3. Net heat flux for various particles sizes at wavelength 4.0 μm



Figure 4. Net heat flux for various particles sizes at wavelength $5.0 \ \mu m$.

DISCUSSION

From the diagrams in Fig. 2 for the wavelength of incident radiation equal to 3.0 μ m, it was found that the larger is particle diameter the smaller the net radiative heat fluxes. This is only in Fig. 2, but it is not the case in Figures 3 and 4, where the λ values are 4.0 and 5.0 respectively. In these Figures 3 and 4 can be seen that the largest values of heat flux are for the particles diameter of 1.0 μ m. Thus the variation of heat flux with particles diameter is not straight forward and depends on the wavelength of incident radiation.







Figure 6. Net heat flux for various particles mass concentrations at wavelength 4.0 μ m.

Something similar or a kind of paradox has been found by Lee and Tien (1980) and discussed and presented by Modest (1993), but their research was done for very small soot particles which obey Rayleigh theory. For a simplified analysis of radiative heat transfer related to particulate media, it was desirable to use suitably defined

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Figure 7. Net heat flux for various particles mass concentrations at wavelength 5.0 μm.

mean absorption and extinction coefficients such as Planck-mean and Roseland-mean. The extinction coefficient for very small soot particles, so that the Rayleigh theory applies for all particles and relevant wavelengths, can be described by an algebraic equation and this is presented by Modest (1993). The results for absorption and extinction coefficients calculated in a region of wavelength and presented by graphs by Lee and Tien (1980) and by Modest (1993), show the following. In a region of wavelength (for smaller values of wavelength) the smaller sizes of particles gave larger absorption and extinction coefficients. In an other wavelength region (for larger values of wavelength) is vice versa, i.e. the smaller particles gave the smaller absorption coefficients than the particles with larger diameter which gave higher values of absorption coefficients. In their relatively simplified algebraic equation absorption coefficient, inter alia, has reciprocal relation to wavelength and does not have maximum.

Our analysis in this paper is mathematically rigorous and follows Mie theory. Predictions done here are for particle size parameters less than 20. We can expect that there is a particular value of particle size parameter which will give the highest (maximal) value of heat flux.

Analyzing the graphs in Figures 5, 6 and 7 it can be seen that the larger is the particle mass concentration, the larger is the net radiative heat flux. This is logical and understandable. Keeping all others parameters constant, the larger mass concentration of particles means the larger number of particles and that does increase the absorption and extinction coefficients.

CONCLUSIONS

The computer code for particles radiation by Mie theory in 3-D rectangular geometry is developed. (Some subroutines of the code were separately tested, e.g. the prediction of scattering phase function and of scattering and extinction efficiencies are in excellent agreement with the values given in literature.) The code is capable of predicting heat flux distribution. It shows sensitivity to different input values of various particles parameters.

It was concluded that the increase of particles mass concentration increases the net radiative heat flux transferred to the surrounding surfaces. The influence of particles diameter on the heat flux, under the conditions that the other particles parameters were constant, is rather complex and it depends on the wavelength of incident radiation. For a particular wavelength there is a value of particle size which gives the highest heat flux. This value should be determined either by numerical experiments (i.e. by the series of calculations) or by rigorous mathematical analysis of the Mic equations. The future research work related to this area should be directed towards these investigations.

NOMENCLATURE

A	surface area (area) [m2]	
C.'	mass concentration of solid particles [kg/m ³]	
D.	solid particle diameter [m]	
E.	emissive power of surface zone [W m ³]	
E.	emissive power of volume zone [W m ²]	
6	total view factor, fraction of the radiant energy emitted	
.4	by zone "i" that is absorbed by zone "i", expressed as a	
	fraction of actual emission from "i" (dimensionless)	
f(a)	angular distribution function, fraction of the scattered	
	energy directed into a unit solid angle in the direction	
of	scattering angle α (dimensionless)	
GS	total interchange area between volume zone "k" and	
0101	surface zone "i" [m ²]	
aa	total interchange area between volume zones "k" and	
";"	[m ²]	
	imaginary unit =>	
	solid narticles abcomtion coefficient [m ⁻¹]	
-	solid particles autinction coefficient [m ⁻¹]	
2	mean beam length of an enclosure [m]	
100	complex refractive index	
n	real part of complex refractive index	
k	imaginary part of complex refractive index	
0	net radiative heat flowrate to volume zone "i" [W]	
Outres	net radiative heat flowrate to surface zone "i" [W]	
R	random number	
2.2	total interchange area between surface zones "j" and "i"	
0,0,	())	
0.0	[m]	
S_jG_i	total interchange area between surface zone j and	
	volume zone "i" [m ²]	
Т	temperature [K]	
V	volume [m']	
X,	absorption efficiency	
х,	scattering efficiency	

Greek letters

α,

εį

Ep X

 σ_s

absorptivity of	particles suspension
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- emissivity of surface zone "i"
- emissivity of particles suspension
- wavelength [m]
- λ_m wavelength at blackbody equal energy division [m]
- ρ_p density of particles material [kg/m³]
 - solid particles scattering coefficient [m1]
- ω scattering albedo

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