MATHEMATICAL MODELLING OF RADIATIVE HEAT TRANSFER IN COMBUSTION CHAMBERS

by

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Three main phenomena: fluid flow, chemical reactions and heat transfer comprise the processes in combustion chambers. The analysis and discussion of their mathematical modelling have been presented. The requirements of the industry, which make it important to obtain an accurate prediction of combustion chambers performances, have been stated. The modelling of radiation and of radiative properties of combustion products, the incorporation of turbulence as well as some recent modelling and a comparison with industrial tests have been reviewed. The up-to-date state of the art has been given. The latest needs of the industry for the modelling of these processes have been stated. More conclusions have been drawn. Inter alia, one of them is that the inflow of combustion gases at the adiabatic flame temperature at burners locations is a good approximation for the furnaces in large industrial and auxiliary boilers. The recommendations for further research in this field has been given. These can be generally grouped in three areas: (1) theoretical research, (2) experimental work, and (3) industrial application.

Introduction

Three-dimensional turbulent flow with combustion and radiation occurs in combustion chambers of various types used for many purposes. The combustion chamber can be defined as an enclosure in which fuel and air come into contact and combustion takes place, liberating the energy which is used as a heat or work output. Three main phenomena occur in combustion systems: fluid flow, chemical reactions and heat transfer.

There is a great interest in development and application of the mathematical model describing the processes within combustion systems. The requirements for increasing unit capacity and heat loading of industrial furnaces, for energy conservation, for process control by controlling temperature and heat flux distributions, for avoiding local overheating or underheating of the sink surface, make it important to obtain an accurate prediction of furnace performances. Examples of combustion systems are:

steam generators, refinery furnaces, cement kilns, glass furnaces, steel furnaces, internal combustion engines, gas turbine combustion chambers, rocket nozzles *etc*. Some furnaces are arranged so that departing gases pass to further heat exchange equipment. In these cases gas temperature and heat flux distributions at the furnace exit should be known with a certain degree of accuracy.

Radiation modelling

In many industrial furnaces, the primary interest is the amount of heat transferred from the combustion products to sink surfaces. The dominant mechanism of heat transfer in most combustion chambers is radiation. The exact solution of integro-differential equations describing the radiation is possible only for very simple cases. Several numerical methods are developed for radiative heat transfer as: Flux, Hottel and Cohen Zone, Monte Carlo, Discrete Ordinates, Discrete Transfer, Finite Volume *etc*.

Radiation models [1] suitable for incorporation in reactive fluid flow codes are extended to calculate radiation in enclosures containing obstacles of very small thickness. The discrete transfer, the discrete ordinates and the finite volume method are employed to predict the heat transfer in two-dimensional enclosures and the results are compared with zone method calculations, with the total exchange areas determined by Monte Carlo method. All the methods predicts similar heat fluxes, but the computational requirements are different. The discrete ordinates and the finite volume method are the most economical ones. An application to a utility boiler is also presented.

Radiative heat transfer in a square enclosure with a single vertical partition containing a gray emitting-absorbing medium is investigated [2]. The Monte Carlo and the discrete ordinates methods are used for that purpose. The influence of the length and location of the partition, the emissivity of the boundaries, the absorption coefficient and the temperature of the medium are discussed. It is shown that the region near the corner of the enclosure closer to the partition is protected from the highest incident heat fluxes. The influence of the baffle is larger when the medium is optically thin and the emissivity of the boundaries is high.

Radiation modelling is discussed in more detailed in paper [3].

For the flux method [4–8] the solid angle surrounding a differential volume element is divided into an even number of solid angles. Over each of these solid angles the radiative heat flux is assumed to be uniform but unequal in the various directions. An energy balance is written for the flux within each solid angle. The resulting equations are differential equations and this makes the flux method compatible with the numerical solutions of transport equations. Since the radiation is treated as a local phenomenon, this method often gives poor results except for the case of strongly absorbing media [9, 10].

For the zone method [8, 11, 12] the enclosure and its surrounding surfaces are divided into a number of volume and surface zones, each 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.

There are two different ways to integrate the zone method with the combustion distribution and the flow pattern.

(a) The combustion distribution and the flow patterns are known [13–21] from experimental data or empirical and semi-empirical equations. The total energy balance, consisting of sensible, chemical, convective and radiative energies *etc*., is written for each zone. This gives a set of simultaneous algebraic equations which are solved for zone temperatures.

(b) The transport equations are coupled with the zone method through a source-sink term in the energy equation [9, 22–26]. This term is the net radiative energy received by the zone calculated from the zone method.

In order to use the zone method the radiative interchange factors between all possible pairs of zones must be known. These factors are called "total interchange areas" and can be calculated by the Determinant Method [12, 19–21, 27] or by the Monte Carlo Method [8, 16, 28–31]. The latter method was used exclusively in studies [25, 26].

Early modelling of combustion chambers

In the early modelling of the processes in combustion chambers two simplified models were used: (1) a well-mixed furnace for which temperature and gas properties were uniform [12, 16] and (2) a plug-flow furnace for which fluid properties were assumed uniform in the transverse direction with only a variation in the longitudinal direction [12, 16, 32]. The oversimplification of the problem usually required certain empirical factors to obtain accurate results for such models. The calculations of furnace performance by these models are usually straightforward and relatively simple, however such calculations do not yield temperature and heat flux distributions.

Radiative properties of combustion products

An important aspect of the analysis of the radiative heat transfer is the determination of the radiative properties of combustion products. The combustion products which make the major contribution to radiative heat transfer are in most furnaces carbon dioxide and water vapor, and solid particles suspended in the gas. Emission and absorption of gaseous products occur in certain wavelength bands [11, 29], whereas the emission and absorption of solid particles are over the entire spectrum. Therefore, the gaseous products and solid particles require two different methods of analysis. There is detailed information on the radiative properties of carbon dioxide and water vapor in the literature [12, 33, 34]. However, the radiative properties of solid particles generated by combustion are not normally available because it is difficult to quantify the composition, structure and size distribution of such particles.

Different models for representing the radiative properties of carbon dioxide and water vapor mixtures have been formulated [9, 12, 13, 23, 32, 34]. In some cases the radiant emission is based on actual spectral behavior obtained from detailed spectroscopic data [33, 34]. Such detailed information is not convenient for heat transfer calculations in furnaces. In other models, the radiative properties of the combustion gas are represented by a sum of gray gases [11, 12]. This gives an important simplification to the heat transfer calculations.

A new gas radiative properties model was developed [9, 23, 29, 35–37] by the Department of Chemical Engineering at the University of New Brunswick, Fredericton, N. B., Canada. This model is based on spectral data of carbon dioxide and water vapor mixtures and can also be represented by the sum of gray gases. It was believed that the application of this model (Steward's model) to complex and detailed furnace calculations could increase the accuracy of the predictions of the heat transfer over a wide range of combustion gas compositions. Therefore, in study [25] two gas radiative properties models were used: (1) Hottel and Sarofim's model and (2) Steward's model.

A rigorous theory of interaction between infrared waves and solid particles was developed for several simple particle geometries [38]. The resulting set of equations, called the Mie equations [12, 38–41], enable the calculation of absorption and scattering coefficients, for given particle shape, particle size, complex refractive index, mass concentration, density of particles material and wavelength of the incident radiation. These relations were used to determine solid particle radiative properties in studies [25, 26].

The emissivity and absorptivity of a carbon dioxide water vapor mixture containing solid particles is calculated by adding the solid particle absorption coefficient to the absorption coefficient of each gray gas including the clear gas [16]. This is made possible by the fact that solid particles radiate over the entire spectrum, compared to the discontinuous radiation from gas molecules.

It is expected that the incorporation of the solid particle radiation will improve predictions in the large furnace chambers investigated.

A way of numerical incorporation of turbulence in some models

The turbulent flow within the combustion chambers was analyzed on the basis of the normal time averaged properties of the flow [42]. The turbulent transport processes are described in terms of an "effective" turbulent viscosity [43]. There are a number of different turbulence models [44] available for such calculations. Each of them has its particular merits, depending on the type of flow under consideration [45]. In several studies the kinetic energy-dissipation rate, or k-ε turbulence model, has been found to give a reliable description of turbulence in combustion systems [24, 46]. This turbulence model was mainly used in many studies.

Tennankore and Steward [24] have compared several turbulence models for predicting flow patterns within confined jets. They obtained a numerical solution of the differential equations governing isothermal and non-isothermal confined jets for three different models of the turbulence correlation terms. The model used were: (1) mixing length model, (2) k-l model and (3) k-ε model. A comparison of the predictions with experimental data taken in a confined jet system indicates that in the absence of a measured distribution of the kinetic energy of turbulence at the entrance section the mixing length model provided the best results for the isothermal case. For the non-isothermal jets, however, it was found that the *k-ε* model gives better predictions than the other two models in spite of the lack of measured distributions for the kinetic energy of turbulence at the entrance to the enclosure.

Past modelling

Many of previous models of combustion systems have used: (a) a sophisticated radiation analysis with combustion and flow pattern based on experimental data, empirical and semi-empirical equations or (b) a rigorous and detailed solution of the transport equations with a radiation analysis using the flux method.

Considerable work has been done in the field of detailed furnace modelling taking into account relevant phenomena.

Zanelli *et al.* [18] have calculated the spatial temperatures and heat flux distributions in a water-tube furnace of a 150 MW boiler. They used Hottel and Cohen's zone method of analysis. The flow pattern was estimated by geometrical consideration of the burner design and visual observation.

Hirose and Mitunaga [17] have developed a method of defining the distribution of gas temperature and radiant heat. They also used Hottel and Cohen's zone method. The flow pattern in a furnace was estimated, leaving aside a number of unknown factors of combustion and thermal characters of burned gas.

Steward and Guruz [15] have carried out a mathematical simulation of the heat transfer in a large modern boiler using the zone method of analysis. They used several semi-empirical flow patterns. The estimation of the combustion pattern was based on data of Maesava *et al.* [47]. The fraction of the fuel burned before a particular distance from the burner mouth was taken as the ratio of that distance to the total flame length. The total flame length was defined as that length in which stoichiometric mixing was complete. They introduced in their calculations the interaction of a solid particle with radiation incident on it. They also carried out the calculations of the total heat transferred in a large modern boiler by several simpler methods.

Whalen's study [28] had as its main objective the coupling of the transport equations for convective flows in combustion systems with the Monte Carlo method to calculate the radiative source term. The radiative interchange factors were calculated for the systems considered independent of the finite difference solution procedure. Since these interchange factors can reasonably be assumed to be independent of temperature, it was only necessary to perform this calculation once. The results were compared to the axisymmetrical two-dimensional experimental furnace of Osuwan [48]. The calculation of the total heat flux to the sink walls showed reasonable agreement with measured values. The vorticity and stream function equations were found to be unstable for some cases and no solution could be obtained.

A second major study of the Carmichael thesis [29] was the development of a generalized furnace model for the prediction of radiative and convective heat transfer from the combustion gases to the sink surface. The geometry of the generalized furnace was a rectangular parallelepiped. The dimensions of the furnace were variables as were the location and amount of the fuel and air input, combustion product output and the location of heat transfer surface. The furnace radiative interchange was determined from the Hottel and Cohen's zone method of analysis with radiative interchange factors calculated by the Monte Carlo technique. The flow and combustion patterns within the furnace were set as part of the input data. The solution for the temperature profile within the furnace and the heat flux distribution over the surface was obtained from the solution of a set of simultaneous nonlinear algebraic equations based on an energy balance derived for each individual zone. The model was developed with the intention that it could be used as a furnace "building blocks" in a system analysis approach of a chemical or metallurgical process.

Steward and Tennankore [22] have presented a mathematical simulation of a cylindrical combustion chamber based on the solution of the equations of motion, energy transport and mass transport of appropriate species. The set of finite difference equations was solved by a standard iterative technique. The radiative heat transport was calculated using the zone method of analysis and directly coupled to the finite difference technique. The emissivity and absorptivity of the carbon dioxide water vapor mixture was represented by three gray gases and one clear gas with temperature dependent weighting factors. The results were compared with experimental data from a laboratory test furnace.

Steward and Kocaefe [23] have developed a procedure for predicting the flow pattern, temperature and concentration distributions and heat flux patterns within furnace chambers. They coupled the finite difference solution of the fundamental equations of motion and transport of heat and mass with the zone or flux method representing radiative transfer. The radiative properties of the combustion gases were represented by various models. Results of the calculation were compared with experimental data from a test furnace. The zone method gave reasonably good predictions of the radiative heat flux on the combustion chamber wall. The predictions by the flux method were relatively poor.

Serag-Eldin and Spalding [46] presented a mathematical model for three-dimensional, swirling, recirculating, turbulent flows inside can combustion chambers. The model was restricted to single-phase, diffusion controlled combustion with negligible radiation heat transfer. The mathematical model comprises differential equations for: continuity, momentum, stagnation enthalpy, concentration, turbulence energy, its dissipation rate, and the mean square of concentration fluctuations. The simultaneous solutions of these equations by means of a finite-difference solution algorithm yielded the values of the variables at all internal grid nodes. The prediction procedure, composed of the mathematical model and its solution algorithm, was applied to predict the fields of variables within a representative can combustion chamber. The results were compared with corresponding measurements. The predicted results gave the same trends as the measured ones, but the quantitative agreement was not always acceptable. This was attributed to the combustion process not being truly diffusion-controlled for the experimental conditions investigated.

Patankar and Spalding [49] described the development of a computer program for the prediction of the flow, heat transfer, and combustion processes in a three-dimensional furnace. The mathematical model involves the solution of the differential equations for momentum, continuity, chemical species concentration, stagnation enthalpy, radiation fluxes, turbulence quantities, and concentration of particles of various size ranges. The mathematical framework was outlined in some detail, and the results of some recent calculations are presented. The conclusions of this work were that substantial progress had already been made toward the development of a computer model for the transfer processes in a furnace, and that further work was needed to validate the computer program and to refine the physical inputs.

Pai, Michelfelder and Spalding [50] described an exercise wherein the computations were based on a general procedure for the computation of three-dimensional flows with recirculation, combustion and heat transfer developed by Patankar and Spalding [51, 52]. The experiments were performed on the experimental rectangular furnace of the International Flame Research Foundation, Holland. At IFRF, the furnace trials were carried out to provide data with a calorimetric hearth for testing the mathematical model of the furnace. Computations and comparison with experiment were made for the case of a tunnel burner operating on natural gas, firing parallel to the hearth as well as inclined to the hearth at 25°. It was found that quite realistic predictions of flow and velocity patterns, temperature patterns and heat flux distributions were obtained with a single set of sub-models which describe the turbulent exchange of momentum, mass and radiative heat exchange. Discrepancies with measurements were found, but the results were encouraging.

Recent modelling and comparison with industrial tests

Robinson [10] has constructed a three-dimensional model of a large tangentially-fired furnace of the type used in power-station boilers. That model was based on a set of differential equations governing the transport of mass, momentum and energy, together with additional equations constituted of subsidiary models of the turbulence, chemical reaction and radiative heat transfer phenomena. The 13 governing differential equations were converted to finite-difference form and solved by an iterative procedure that utilizes the tridiagonal matrix algorithm. It was found that the computer memory limitations restricted the amount of geometric detail that could be included and prevented the use of a finite-difference grid having the desired fineness. The model was validated against experimental data acquired on two large furnaces. It was found that the model was successful in predicting several overall trends od furnace behavior but was inaccurate in predicting certain details.

Preliminary work on the coupling between the transport equations and the zone method of analysis was carried out for a two-dimensional system, a cylindrical-axisymmetrical test furnace [9, 22–24, 36]. In the meantime new and more efficient numerical schemes have been developed [53–55] so that a three dimensional system can now be considered.

The proper choice of algorithm, depending on the specific problem, is one of the crucial points in mathematical modelling and simulation. In the first part of the study [25], efforts were made to investigate and compare, for a simple combustion problem [56], some numerical schemes [25, 57] for the solution of partial differential equations.

It was found that the finite difference technique is the most advantageous in respect to computation time and accuracy for the problem considered. On the basis of the study [25], finite difference techniques were used for the numerical solution of the partial differential equations. An enhanced scheme for a finite difference technique [54] was used in the second part of that study, for the construction of the algorithm used for the solution of the transport equations which involved a k-ε turbulence model.

The equations of motion (Navier-Stokes equations) were defined in primitive variables. These, together with the turbulence equations, were solved by a "semi-implicit consistent" numerical scheme [54], with a time-like marching procedure.

Plant tests on the power station boilers of the New Brunswick Electric Power Commission (N. B. E. P. C.), N. B., Canada, were performed. The data were collected by the graduate students of the Department of Chemical Engineering at the University of New Brunswick, Fredericton, N. B., Canada. There is an available bank of data at this Department for almost every power station in the province New Brunswick in Canada.

For validation of the mathematical model in the study [25] the following tests were used:

(1) Test performed on Dalhousie Station, Dalhousie, New Brunswick, Canada, Unit No. 2, Load 220 MW, on July 23, 1982 [58].

(2) Test performed on Dalhousie Station, Dalhousie, New Brunswick, Canada, Unit No. 2, Load 160 MW, on March 25, 1986 [59].

(3) Test performed on Dalhousie Station, Dalhousie, New Brunswick, Canada, Unit No. 2, Load 106 MW, on July 22, 1982 [58].

(4) Test performed on Coleson Cove Station, Sent John, New Brunswick, Canada, Unit No. 1, Load 345 MW, on August 17, 1982 [58].

(5) Test performed on Coleson Cove Station, Sent John, New Brunswick, Canada, Unit No. 1, Load 240 MW, on August 19, 1982 [58].

(6) Test performed on Coleson Cove Station, Sent John, New Brunswick, Unit No. 1, Load 80 MW, on August 18, 1982 [58].

There was no report in the literature of mathematical model for three-dimensional turbulent flow with combustion and radiation, which has connected the zone method for radiative heat transfer and the transport equations. There was also no model reported previously which was general enough to be applied to two different physical systems, oil and pulverized coal fired furnaces. The study [25] presented calculations for both furnaces based on a single model.

Trivić's study [25] consisted of two related parts.

In the first part the Burke and Schumann combustion problem [56] was solved by three numerical techniques: finite difference, finite element and orthogonal collocation. The results were compared with the analytical solution. For this particular problem it was found that the finite difference method was the most efficient numerical scheme. This method was used exclusively for solving the transport equations in the second part of the study.

The second part consisted of developing a three-dimensional mathematical model for predicting turbulent flow with combustion and radiative heat transfer within a furnace chamber. The model consists of two sections: (1) the transport equations which are nonlinear partial differential equations solved by a finite difference scheme, and (2) the radiative heat transfer which was analyzed by the zone method. The link between these two sections is a source-sink term in the energy equation.

The radiative properties of combustion gases were represented by two different models: (1) Hottel and Sarofim's model and, (2) Steward's model.

The Monte Carlo method was used to evaluate total radiative interchange in the system between zones.

The Mie equations were used for the determination of the radiative properties of particles suspended in the combustion gases.

The mathematical model was validated against experimental data collected on two large furnaces:

(1) A tangentially pulverized coal fired boiler of 220 MW;

(2) An oil fired boiler of 345 MW, with symmetrically positioned burners at the front and rear wall.

The tests and calculations were performed for several loads for both boilers. The measured and predicted gas temperature and heat flux distributions within the boilers were compared. The results gave reasonable agreement between measurements and values predicted by the model.

A series of calculation with varying gas radiative property models, loads, types of fuel, excess air, burner tilt angles and several particle parameters were performed. The effects of these variables on the gas temperature and heat flux distributions within the furnace were studied.

Steward and Trivić studied the particle radiation in a pulverized-coal-fired boiler [26]. A mathematical model based on the fundamental equations of motion and energy transfer, and on the zone method for determining radiative heat-transfer, was developed for an operating 220 MW pulverized-coal-fired boiler. The model is capable of predicting velocity, temperature and heat-flux distributions for the three-dimensional combustion chamber. The calculated heat fluxes at the wall have been compared with experimental measurements taken on the boiler for three sets of operating conditions, and they indicate that confidence can be placed in the results.

If the particle size of the ash is assumed to be that mean particle size of the pulverized coal that is fired to the boiler (50 μm), the model indicates that the radiative heat transferred by the particles is negligible. If the ash particles are assumed to be one-tenth this size (5 μm) the model indicates that the radiative heat transfer is increased by more than 20%. The model also indicates that for the 5 μm particles the radiative transfer within the combustion chamber is significantly affected by the complex refractive index of the ash particles.

Trivić [60] has studied the temperature field within a separeted tube fin of water wall in a boiler furnace. The interaction by heat transfer between combustion gases-solid particles as one multiphase system and steam-water mixture as the other, through a rectangular metal wall, has been analyzed. A second order partial differential equation has been solved by a finite difference ADI scheme with variable iteration parameter. A series of computer programs for the temperature fields prediction within the metal has been developed in Decart 2-D system of coordinates.

It has been found that the temperatures of the fin considerably vary not only inside the metal but also along the fin surfaces. The concept of taking one uniform temperature of water walls as a boundary condition in the heat transfer analysis of the combustion gases-solid particles system in the furnace (so far widely used in many studies) should be reviewed.

Some current modelling concepts and recently used combustion models

Scot C. Hill and L. Douglas Smoot developed a model [61] for the simulation of particles laden, reacting, turbulent combustion systems. The model was based on an Eulerian framework for the gas fluid dynamics and on a Lagrangian framework for particle mechanics. It used equilibrium gas-phase chemistry and coupled turbulent flow field with chemical reactions. This coupling was done by integrating the equations over a probability density function (PDF). Radiative heat transfer was modelled by the discrete ordinate method (DOM). The model was tested by the comparisons of code predictions with experimental data collected in an 85 MWe pulverized-coal-fired utility boiler.

The comparisons of measured and predicted temperatures and of oxygen and carbon dioxide mole percent concentrations (dry) within the furnace were presented. Measured and predicted temperatures and species concentrations were in good agreement in most regions of the furnace, except in the burner and near-wall regions where further work was required.

The comparison of measured and predicted heat flux on the furnace walls were not presented in the paper.

The combustion model here was based on the following items. Gas-phase combustion chemistry was assumed that the gaseous reactions were limited by the mixing rates of reactants and not by the reaction kinetics; *i. e.* fast chemistry, mixing limited.

Chemical equilibrium was calculated by minimizing of Gibbs free energy coupled with turbulence using probability density function (PDF) and mixture fractions. Devolatilisation was considered by two-step model with particle swelling allowed. Chair oxidation was modeled by first order reactions where CO was primary product.

In spite of this very detailed combustion model the measured temperatures are much more uniform and considerably higher than the predicted values in the near-burner region of the combustion area.

Thus, increasing the complexity of gas combustion model does not mean that automatically the accuracy of the predictions will be improved as well.

It proved once more that the concept based on the inflow of combustion gases at the adiabatic flame temperature at burners locations [25, 26] is a good approximation for the large utility boiler.

Authors of the paper [61] expressed their opinion that the largest discrepancies in measured and predicted gas temperatures occurring near the furnace wall was caused by boundary conditions used in the code and that it required additional investigation.

Trivić has found [60] that the temperatures of the metal surfaces in the furnaces considerably vary and that the concept of taking one uniform value of temperature of water wall (of metal surfaces) as the boundary conditions should be reviewed.

L. Douglas Smoot [62] gave in 1997 current state-of-the-art, in the last decade, relating to fossil fuel combustion research done at the Advanced Combustion Engineering Research Center (ACERC) at Brigham Young University and at the University of Utah, in cooperation with other universities. The paper did not present the substantial contribution of other researches to recent advancement in the area. Smoot discussed, inter alia, new work in coal structure, coal reaction processes and rates and turbulent reacting flows. Particular attention in the paper among the other things has been paid to the following aspects as: fuel structure and reaction chemistry, devolatilisation submodel development, chair oxidation, fouling and slagging from fuels, air pollutant emissions, ash particle transport and deposition submodels, as well as the sub-model component integration and incorporation into main codes.

J. M. Jones *et al.* [63] stressed in their review paper that recently the attention was increasingly focused on the development and application of mathematical and chemical kinetic models to industrial combustion processes. They wrote, inter alia, that there were two very different numerical methods commonly used for the processes modelling: (1) Hottel and coworkers method [11, 12] based on heat balances calculation and (2) Spalding *et al.* [49–51] method based on Computational Fluid Dynamics (CFD). The merits and drawbacks at these two methods were discussed but the authors did not mention several papers where the link of these two methods were done [25, 26, 36] as well as the advantages and accuracy obtained by that link. Their paper critically assessed the status, capability and limitations, of current available models for application to coal fired industrial combustion plants. Making the list of the processes to be modelled, the authors, among other things, emphasized the following. For turbulent flow modelling continuity equation, Navier Stokes equations and k-ε, Algebraic Stress Model (ASM) and Reynolds Stress Model (RSM) were used. For gaseous combustion modelling the following models were used: (a) eddy break-up, (b) mixed-is-burnt, (c) mixture fraction and variance, (d) assumed Probability Density Function (PDF), (clipped Gaussian β function *etc.*), (e) enthalpy, (f) equation of state,(g) combustion model, flamelets, *etc.* and (h) NO_x model/soot/other pollutants. For oil spray combustion the models were: (i) continuous droplet model, (j) discrete droplet model, (k) evaporation, (l) combustion model and (m) NO_x soot/model. For coal combustion were considered the following models: (n) discrete particle model, (o) devolatilisation (single or two competing reactions), (p) chair oxidation, (q) volatile combustion model, NO_x/soot model and (r) slagging model. For thermal radiation the authors mentioned only two methods: (1) Discrete Transfer Method (DOM) and (2) Monte Carlo Method.

Fred C. Lokwood *et al.* in their study [64] presented the results of the predictions obtained by using a mathematical model of pulverized coal combustion. The authors carried aut the predictions for two swirl burners types and compared them with data collected in a large scale combustor. The furnace used was cylindrical and vertically oriented, 0.6 m in diameter and 3.0 m in length, down fired along its axis. Comparisons of measured and predicted oxygen concentration and gas temperature were presented. The predictions of one burner type were in goad agreement with data collected, while the performance of the other burner was less well reproduced. The sensitivities of the predictions to various of the model parameters were explored in an attempt to explain the sources of the discrepancies.

The change in particle temperature was calculated from the energy conservation equation. Coal devolatilisation was simulated by a first-order single reaction model with a given rate expression. The rate constant was given by Arrhenius expression. The volatile gases were represented by a single chemical species and are assumed to burn at a rate controlled by the small scale turbulence mixing.

The combustion of the char particles was governed by the external diffusion rate of oxygen to the particle surface and by chemical reaction presumed to be first-order in oxygen partial pressure and to occur entirely at the particle surface.

P. J. Coelho and M.G. Carvalho developed a three-dimensional mathematical model of a power station boiler [65]. The model was based on the numerical solution of the governing equations of mass, momentum and energy transfer and on transport equations of scalar quantities. The k-ε model of turbulence was used in this study. The authors applied the model to a 230 MWe power station boiler of the Portuguese Electricity Utility. The experimental data for that boiler were collected. The predictions and the measurements of the gas temperature and of chemical species concentrations were compared. The species considered were CO_2, CO and O_2. It was found that for a combustion model based on the chemical equilibrium assumption, the predicted concentrations of gas species were in good agreement with measured data. The temperature profiles had the correct trend, although the gas temperatures were unpredicted in the burner region. The authors used in their calculations three different grids to ensure that conclusions were not affected by the grid refinements. They found, for their particular calculations, although is not always the case, that the influence of grid refinement on the predictions was generally negligible, compared with the differences between predictions and measurements. The authors identified the situations where grid refinement might influence the prediction.

The air/fuel ratio and firing load were varied as well. It was found that these influences were successfully simulated, demonstrating the model ability for parametric studies. The results presented confirmed the predictive capabilities of the model and its possibility to be used for the design and optimization of boilers.

The combustion model applied in the paper assumed that the reaction rates are large enough that the chemical reactions occur instantaneously as soon as the reactants come into contact. Combustion was controlled by mixing and not by kinetic phenomena. The relation between the gas composition and the mixture fraction depended on the model used. Two different models were employed: simple chemically reacting system (SCRS) model and chemical equilibrium model, which was used in most of the cases. For the chemical equilibrium model it was assumed that chemical equilibrium prevailed and the instantaneous gas composition was calculated from the minimizing of the free Gibbs energy.

The mixture fraction fluctuations for turbulent flow were taken into account to calculate the mean values of the mass fractions, density and temperature. This was done by prescribing a clipped Gaussian shape for the mixture fraction probability density function.

The radiative heat transfer was calculated by the Discrete Transfer Model (DTM). This model is based on the solution of the radiative heat transfer equation along specified directions.

Conclusions

The study [25] shows that the inflow of combustion gases at the adiabatic flame temperature at burners locations seemed to be a good approximation for the type of combustion chambers as large industrial and auxiliary boilers. That study demonstrates that the model devloped within it can treat furnaces with widely differing operational characteristics. This model can be used to study the sensitivity of the heat transfer within the combustion chambers to various operating parameters.

Because the temperatures of the metal elements in the furnace considerably vary along the surfaces, the concept of taking one uniform temperature of water walls as a boundary condition should be reviewed.

The cases of the modelling of processes in the enclosures with obstacles as well as the modelling of complex and irregular geometries very often are requested by the industry. The existing mathematical models should be modified to be able to cope with those problems.

The future work in the modelling of processes in combustion chambers would go towards two different directions: (a) simple and (b) sophisticated modelling. It is necessary to develop the easy-to-use models which should contain all the complexities of the existing phenomena as turbulent flow, combustion and radiation and to be, at the same time, convenient for the operation by industry. This is a difficult task. Second direction is to abandon, one by one, previously stated approximations by incorporating more physics and using parallel processing. It means the larger numbers of zones, the modelling of very complicated and irregular geometries, the more realistic gas radiative properties models and the more complicated combustion models. The super computers make it possible.

Recommendations

Further research in this field can be developed in several different directions. These can be generally grouped into three areas: (1) theoretical research, (2) experimental work and (3) industrial application.

Theoretical research

Recommended theoretical research comprises the following items:

(a) Incorporation in the present model as [25] of differential equations describing the concentration of fuel, oxygen and combustion products and conduction of mathematical experiments with several expressions for the rate of the combustion reaction.

(b) Incorporation in the present model as [25] of other turbulence models and the conduction of numerical experiments to test their reliability. In the case of some specific combustion system, searching for new empirical parameters or model constants which will give a better prediction of measured values.

(c) Expanding of the present model as [25] by incorporating the radiation of several species of particles with different particle parameters such as particle size, mass concentration and complex refractive index. Assuming concentration of ash particles was uniform throughout the entire furnace does not seem to correspond to physical reality. The ash particles probably have a larger concentration in the burner region than in the upper part of the furnace.

(d) Application of the present model as [25] to the other combustion or radiation systems of rectangular geometry such as fluidized bed combustion chambers, copper or aluminium melting furnaces or steel reheating furnaces.

(e) The present study [25] and the mathematical model developed can be used as a pattern for the solution of other combustion reaction systems of different geometries (spherical or cylindrical) for various processes, boundary conditions and other situations.

(f) Numerical experiments with the present model [25] using a different number (or sizes) of zones in the radiative part and the control volumes in the transport equations part to determine the influence of such changes on the accuracy of the calculation procedure. The numerical experiments with different finite difference schemes can be conducted.

(g) Further work on the Steward's radiative gas properties model [37], particularly on the part related to the gas absorptivity.

Experimental work

Recommended experimental work comprises the following items:

Design and construction of a three-dimensional rectangular test furnace which can be fired, by gas, oil or pulverized coal, fully equipped with appropriate instrumentation could be undertaken. The facility for particle injection should be included.

The following studies can be conducted on this test furnace:

(a) Three-dimensional isothermal and non-isothermal flows.

(b) The flows with and without radiation and combustion.

(c) The particle radiation studies.

Industrial applications

Recommended industrial applications comprise the following items:

(a) The model [25] can be used for furnace design calculations.

For any rectangular, "box shape", geometry furnace and for chosen (1) burners and heat sink surfaces locations and (2) input data which consist of type and amount of fuel, amount of air, the temperatures of the sink surfaces: the velocity, pressure, temperature and heat flux distributions can be calculated. One of the recommendations for further work can be the modification and rewriting of that model [25] in a convenient operative form to satisfy a user's specific furnace design requirement.

(b) Modification of the present mathematical model [25] for on-line use according to the specific requirements of the users in industry.

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