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Overview of some radiative transfer issues in simulation of unwanted fires

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Abstract

Fire is an extremely complex phenomenon that is responsible for loss of human life and considerable property and environmental damages every year around the world. Significant progress during the last few decades in modeling of pool, compartment (enclosure), urban and outdoor (i.e., forest and woodland) fires has manifested in improved understanding of fire phenomenology, fire-safety regulations and fire-fighting techniques. Recent research efforts to develop numerical CFD (computational fluid dynamics) models for simulating fire phenomena from first principles are discussed. Since both thermal and oxygen-limited feedback processes can affect fire dynamics, quantitative description of fire development requires understanding of materials, turbulence, chemical kinetics, heat and mass transfer, radiation, and other important physical processes. Focus in the discussion is on radiative transfer (one of the most complex and time consuming process) in numerical simulation of large pool, compartment, urban and outdoor fires. The overview discusses current trends and identifies the outstanding problems requiring research attention.

Keywords: Unwanted fires; Fire simulation; Radiative transfer

1. Introduction

Every year unwanted building, urban, industrial and outdoor fires are responsible for loss of human life and considerable property as well as environmental damage [1]. Fire safety and control of unwanted fires represents a major scientific and technical challenge for the 21st century. This challenge in the study of fire, which is a primitive and uncontrolled form of combustion, is primarily motivated by safety considerations, and considerable progress has been made during the past few decades. The progress is being reflected in journals such as Fire Safety Journal, Combustion and Flame, and Combustion Science and Technology as well as International Symposium on Fire Safety Science, Symposium (International) on Combustion and others.

Numerous important topics frequently addressed in the fire safety literature include, but are not limited to, combustion phenomena, heat (and mass) release during fire, modeling aimed to improve understanding of physicochemical mechanisms, models for fire mitigation methods, sensors and their placement for detecting fires, development of experimental techniques for laboratory simulation of fires, experiments aimed for obtaining data to validate models, practical (operational) tools for prediction of fire spread, etc. The fields of fire science and fire protection technology are very broad, have grown rapidly, and cannot be covered in this brief account. For example, thermal radiation modeling in fire safety codes in Australia, France, Russia, United Kingdom and United States has been recently reviewed by Sacadura [2].

The knowledge and mitigation of fire risk depend on the understanding of complex phenomena involved in a fire, particularly the aerodynamic, chemical and thermal phenomena that govern the development and the propagation. Advancement of efficient methods of fire detection and control require full understanding of these phenomena. Reference is made to the published literature for the discussion of fire dynamics fundamentals [1,3,4].

Over the last few decades the phenomenological understanding of fires has increased greatly. In the process to understand the underlying coupling between momentum and scalar combustion, heat and mass as well as radiation transport, the focus of research has shifted from the engineering application of correlation based methods such as zone models to solution of conservation equations by numerical (CFD-based) techniques.

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These CFD based methods can simulate the global features of fires but are highly dependent on the small-scale processes modeled. The large body of literature on modeling has been discussed in recent reviews [2–7] and will not be repeated. The discussion in this overview will be limited to simulation of unwanted fires and more specifically to some of the issues needing to be addressed in modeling physicochemical processes in selected fires. Even in this limited context, it is not possible to be comprehensive and cite all of the worthwhile contributions to the field.

The nature of fire dynamics simulations using CFD in which radiative transfer is an important or a dominant mode of energy transport have limited the complexity of the radiative transfer models [8–11]. The dependence of the radiation characteristics of the combustion products (i.e., mainly composed of molecular gases and soot particles), chemical kinetics, and temperature makes the calculations intimately coupled to the temperature and chemistry. In addition, the spectral nature of radiation makes the treatment of radiative transfer extremely difficult and time-consuming. Owing to the great variety of fire situations, the very broad range of physical processes taking place in fires, and the very limited nature of this account, the focus of this discussion is on the state-of-the-art of radiative transfer in fire simulations. The overview should be considered as an update of the more comprehensive account by Sacadura [2]. One must note that in the discussion to follow the emphasis is on radiative transfer in small fires which can be treated as being homogeneous or equivalent homogeneous medium. Large (woodland and urban) fires are heterogeneous and have multiple (micro-, macro-, and mesoscopic) scales. Depending on the type of problem of interest and the choice of scales, radiative transfer cannot be analyzed using the same models. Such problems are beyond scope of serious discussion in this paper.

2. Overview of fire phenomelogy

The complexity of fires is the result of intimate coupling of the relevant physicochemical processes, nature of fuel, environment as well as numerous parameters controlling the fire. The global description of a diffusion flame leads to a simple equation [1,5],

$$\text{fuel} + s\,\text{oxidizer} \rightarrow \text{products} + \text{heat release} \tag{1}$$

where s is the stoichiometric ratio. Fire is an uncontrolled form of combustion and according to the above relation, the chemical reaction of fuel and oxidizer results in products of combustion (gases, soot, etc.) and heat generation. A simple schematic representation of a fire in the absence of extinguishment, say, by water spray or mist is given in Fig. 1. While the gasified fuel burns, additional fuel is being formed as liquid, solid and particle beds of combustible materials are being heated by conduction, convection and radiation. Thermal radiation from combustion products (gases, soot and particles) as well as enclosure walls (if any) "feeds" the fire. A number of complex physical and chemical processes such as turbulent flow, mass transfer, chemical reactions, heat transfer (molecular diffusion, advection and radiation) occur simultaneously but can not be shown in the diagram. In numerical fire dynamics simulations of pool, compartment, building and outdoor fires the transport processes have been modeled [7,11]. As a concrete example, three recent studies on small, medium and large scale pool fires are listed in Table 1, and the modeling approaches employed are identified.

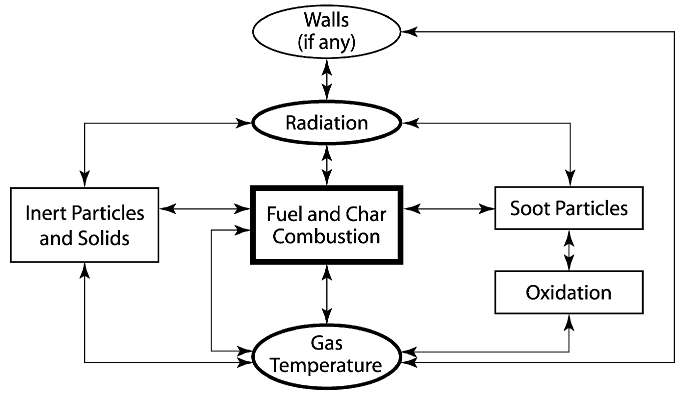

Fig. 1. Schematic representation of physical/chemical processes during a fire.

A special set of governing equations for fire simulations coded in the FDS (Fire Dynamics Simulator) [11] has been employed by Xin et al. [12] to study a small (7.1 cm diameter methane/air turbulent diffusion flame. The turbulent stresses were approximated with the Smogorinsky's model. A mixture fraction based combustion model was employed, and the state relationships were based on opposed flame calculations. The reaction mechanism included GRI-Mech 2.11 with 49 species and 279 elementary reactions [13]. The radiant energy loss was accounted for by arbitrarily assuming it to be 10% of the chemical heat release rate. NIST's FDS [11] does not explicitly

Table 1
Treatment of processes in some recent simulations of pool fires

Source	Momentum	Turbulence	Chemistry	Radiation
Xin et al. [12]	Special equations developed for FDS [11]	Turbulent stress approximated by Smogorinsky model	Mixture fraction	Arbitrary, 10% of chemical heat release
Wen et al. [14]	Filtered momentum equations	Smogorinsky's eddy viscosity model	Laminar flamlet and mixture fraction	Gray, finite-volume
Greiner and Suo-Antilla [15]	Reynolds-averaged Navier–Stokes RANS-based	Eddy diffusivity	User input file for different fuels	Gray diffusion treatment

solve the energy equation, but uses it to determine the divergence of the velocity field. Comparisons between the predicted and measured velocities, mixture fractions and temperatures showed that the mixture fraction based combustion model captured well both the qualitative and quantitative fire behavior. In an earlier simulation of a small scale pool fire, a simpler combustion model has been used [16]. The study has demonstrated that the LES approach with the modified laminar flamlet model (MLFM), accounting for six bands of gaseous radiation, is capable of capturing the fine details and unique characteristics of small pool fires.

A medium-scale methanol pool fire has been simulated by Wen et al. [14]. Favre-filtered velocity, mass species concentration and enthalpy equations are solved. The Smogorinsky's eddy viscosity model is used as the SGS (subgrid-scale) turbulence model. The subgrid-scale combustion model is based on the laminar flamlet approach along with the default mixture fraction combustion model for comparison. The finite-volume-based radiative transfer equation is solved on the band basis by considering soot as the most important combustion product controlling thermal radiation from the fire and hot smoke. No details are provided about the band models, except to mention that a simple band-mean absorption coefficients were used in the computations. The work has demonstrated the capability of the FDS model to yield reliable predictions of most important parameters of pool fires, but it also revealed some limitations. The experimental data for mean temperature and velocity distributions were in reasonably good agreement with the predictions, and air entrainment was captured by the velocity fluctuations.

The proprietary ISIS-3D CFD/radiation heat transfer computer code has recently been used by Greiner and Suo-Antilla [15] to simulate heat transfer from large (19 m diameter JP8 fuel) pool fires to engulfed packages for risk studies. The ISIS-3D solves the three-dimensional mass, momentum (Navier–Stokes), energy and species conservation equations using a variable density version of the PISO [17] pressure-based solution algorithm. The semiempirical combustion chemistry model in ISIS-3D is defined by the user through an input file that can be varied for different fuels. The radiation heat transfer model for large optically dense pool fires employs the Rosseland diffusion approximation [5]. ISIS-3D model cannot be considered as a fully predictive simulation and should not be used outside the range of conditions in which its parameters are determined (JP8 pool fires larger than 2 m). The reaction rate and radiation transfer models have been validated against only a few experiments (acquired in a 6-m square pool fire under light wind conditions).

This brief discussion of three representative (small, medium and large scale) pool fire simulations has provided the current state-of-the-art in modeling some of the important physical processes in fires. Some submodels of the FDS are realistic whereas others are primitive. While turbulence/chemistry interactions are being accounted for in most of the simulations, turbulence/radiation interaction has not been considered in any of the simulations discussed. In some models radiative transfer has been treated in a very simple manner [12] and in others [14] there is inconsistency between the spectral integration or averaging and definition of the band-mean absorption coefficients of the combustion products. Reference is made to accounts of compartment [7,18–20] and woodland [21,22] fire modeling with their special and unique simulation features. Fire suppression using water sprays to attenuate radiation by water droplets has special requirements and is an active area of research [23].

3. Radiative transfer in fire dynamics simulation

Accurate numerical simulation of an unwanted hydrocarbon fire is important for consideration of the thermal hazard to humans, facilities and equipment. The cost and accuracy of a large fire simulation is strongly dependent on the choice of a numerical model for solving the radiative transfer equation (RTE) governing radiation (i.e., a single term) in the conservation of the thermal energy equation [1,2,6,7]. However, it should be mentioned that the RTE requires the radiating medium to be homogeneous and continuous (i.e., gas or gas-particle mixture). In large scale (i.e., forest and urban) fires with strong hetrogeneities consisting of multiple phases (i.e., gases, solids, decomposing fuels, burning embers, etc.) radiative transfer in such physically complex systems can not be described by radiative properties and radiation intensity (i.e., a field quantity) as in the RTE. Since the focus of the present discussion is on radiative transfer in simple fires, the RTE and the difficulties in its solution are briefly reviewed.

The radiative transfer equation is a mathematical statement of the conservation of spectral radiant energy applied to a solid angle $d\Omega$ of radiatively participating (i.e., absorbing, emitting and scattering) medium propagating in a given direction $\mathbf{s}$. Radiation traversing along a path is attenuated by absorption and scattering and is enhanced by emission and by in-scattering from all other directions. In the absence of turbulence/radiation interaction and the purposes of this discussion, it is adequate to focus on the following form of the time-independent, incoherent scattering RTE [5,24,25] for radiative transfer calculations in engineering systems,

$$\mathbf{s}\cdot\nabla I_\lambda(\mathbf{r},\mathbf{s}) = -(\kappa_\lambda+\sigma_\lambda)I_\lambda(\mathbf{r},\mathbf{s}) + \kappa_\lambda I_{b\lambda}\big[T(\mathbf{r})\big] + \frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} I_\lambda(\mathbf{r},\mathbf{s}')\Phi_\lambda(\mathbf{s}'\to\mathbf{s})\,d\Omega' \tag{2}$$

where $I_\lambda(\mathbf{r},\mathbf{s})$ is the spectral intensity of radiation (radiance) at location $\mathbf{r}$ in direction $\mathbf{s}$. The scattering phase function $\Phi_\lambda(\mathbf{s}'\to\mathbf{s})\,d\Omega'/4\pi$ represents the probability that radiation propagating in direction $\mathbf{s}'$ and confined in the solid angle $d\Omega'$ is scattered into direction $\mathbf{s}$ confined to solid angle $d\Omega$. The first term on the right-hand side of Eq. (2) accounts for attenuation of radiation by absorption and scattering, the second for gain by emission, and the last term for gain by in-scattering. In the above equation, κ_λ and σ_λ are the spectral absorption and scattering coefficients, respectively, and $I_{b\lambda}(T)$ is Planck's function.

Integration of Eq. (2) over all directions ($\Omega = 4\pi$) and over the entire spectrum ($0 < \lambda < \infty$) results in the conservation of total radiant energy,

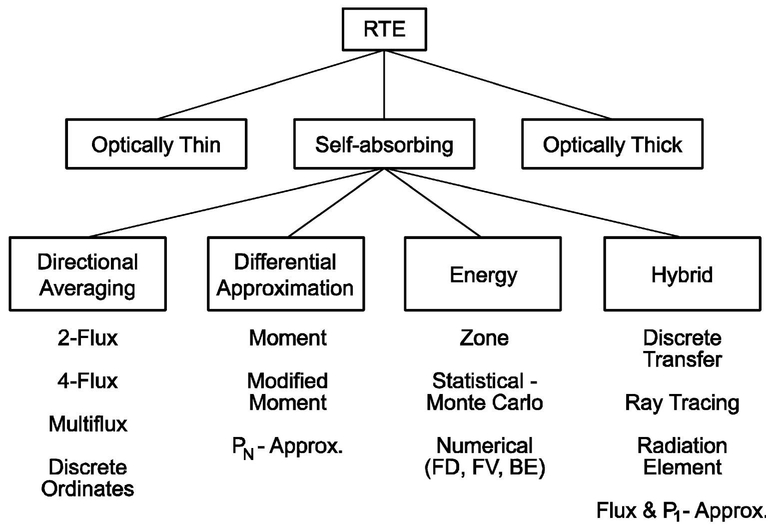

Fig. 2. Solution methods for the radiative transfer equation (RTE).

$$\nabla \cdot \int_0^\infty \mathbf{F}_\lambda(\mathbf{r})\,\mathrm{d}\lambda = \nabla \cdot \mathbf{F} = \int_0^\infty \kappa_\lambda \left[4\pi I_{b\lambda}(T) - G_\lambda\right] \mathrm{d}\lambda \tag{3}$$

where the radiation flux vector $\mathbf{F}_\lambda$ is defined as

$$\mathbf{F}_\lambda(\mathbf{r}) = \int_{\Omega=4\pi} I_\lambda(\mathbf{r},\mathbf{s})\mathbf{s}\,\mathrm{d}\Omega \tag{4}$$

and the spectral irradiance G_λ is defined as

$$G_\lambda(\mathbf{r}) = \int_{\Omega=4\pi} I_\lambda(\mathbf{r},\mathbf{s})\,\mathrm{d}\Omega \tag{5}$$

Note that there is no convective term in Eq. (3) since radiation propagates independently of the local material velocity [5]. The divergence of the radiation flux vector ($\nabla \cdot \mathbf{F}$) must be included in the thermal energy equation for calculating the velocity, temperature and species concentration fields in a moving medium [1,5,7]. Calculation of this source/sink term in the energy equation presents one of the major computational difficulties when predicting the flame structure and the performance of combustion or fire systems. Computation of combustion chemistry including quenching and turbulence/chemistry interaction is another. Capturing laminar buoyant instabilities that dominate the dynamics of buoyancy induced turbulence and feedback of heat between the flame and the burning fuel (i.e., fuel gasification) are additional important considerations in the numerical simulation of fire dynamics.

The RTE, Eq. (2), is complicated by the fact that, in addition to the three-dimensional space variables and indirectly the time (because the temperature and radiating species concentrations vary with time), integration over all directions is necessary at each point in the fire domain. Furthermore, integration over the entire spectrum or some type of appropriate averaging is required. Moreover, since the spectral radiation characteristics (i.e., absorption by gases and soot particles, scattering and extinction coefficients of the fuel, products and fire fighting agent such as water spray), depend on both the local radiating species (including soot particles) concentrations and temperature, radiative transfer is intimately coupled to the chemical kinetics of the flame. In summary, not only the method for solving the RTE, but modeling the radiation characteristics of the combustion products (gases and particulates) and the radiating species concentrations are necessary. It is well recognized [2] that in most hydrocarbon fires soot emission of radiation dominates gaseous emission, and therefore knowledge of soot volume fraction or soot particle concentration is essential in simulating the behavior of unwanted fires. In brief, calculation of radiative transfer requires two types of models: (1) models to account for directional nature of radiation, and (2) models to describe the spectral nature of radiation of the reactants and combustion products.

3.1. RTE solution methods

Descriptions of methods for solving the RTE are available in the heat transfer textbooks [24,25]. The commonly used methods for solving the (spectral) RTE are depicted graphically in Fig. 2. The self-absorbing situation falls between the optically thin and thick limiting cases. These two approximations are the simplest forms of the RTE, and are therefore easiest to adopt for solving the total thermal energy equation [5]. The self-absorbing domain is the most difficult to handle mathematically, but it is the most commonly encountered in typical fires.

Some of the methods for solving the RTE that are suitable for numerical simulation of fires are discussed in recent accounts [5,26]. Descriptions of methods for solving the RTE are available in heat transfer textbooks [24,25]. The most commonly used methods for solving the RTE in computational fluid dynamics based models are the discrete transfer (DTM), discrete ordinates (DOM), differential approximation (DAM) (i.e., moment, spherical harmonies, etc.), Monte Carlo (MCM) and ray tracing (RTM) methods. It should be pointed out that MCM is a statistical method, and RTM is a purely numerical approach, and they do not require the RTE presented in this section, but understanding of radiation physics is needed. In order to reduce the computational effort, the calculations are usually performed on a gray or at most band basis. Probably the most comprehensive comparison of methods for solving the RTE has been reported by Jensen et al. [26]. For a 2 m diameter JP-8 pool fire six methods for solving the RTE in an absorbing-emitting, non-scattering gray medium were used, and the radiative fluxes as well as the radiative flux divergences [see Eq. (3)] were compared. Soot was considered to be the dominant radiating species and local Planck mean absorption coefficients were used in the calculations.

Reference is made to Jensen et al. [26] for an up to date discussion of the literature and extensive results. The detailed findings and conclusions cannot be summarized here. Suffice it to say that the DAM with M_1 closure is judged to be the best compromise between accuracy and computational effort based on comparison with the reference (MCM and RTM) solutions. No justification has been provided in the paper for neglecting the absorption by combustion gases in comparison with the soot. In addition, use of the Planck mean absorption coefficient is inconsistent with emission and absorption of radiation, see right-hand side of Eq. (3). At least two local mean absorption coefficients (i.e., one for emission and one for absorption) need to be employed [5] to obtain reliable radiative transfer predictions for small and medium scale fire. There is a need for research to determine under what optical and radiation field conditions a single mean absorption coefficient would be sufficient to characterize radiative transfer in fires.

3.2. Radiation characteristics of gases

Determination of the radiation characteristics of combustion gases requires consideration the spectral absorption coefficients and the concentrations of the principal absorbing–emitting species such as CO_2, H_2O, CO and others. The spectral absorption coefficient of gases is very complex, containing a very large number ($\sim 10^4$–10^6) lines [27]. The necessity to simulate radiative transfer in nonhomogeneous and nonisothermal mixture of gases makes it impractical to carry out line-by-line calculations. To overcome these difficulties models ranging from narrow band, correlated-k (CK) (and its extensions), weighted-sum-of-gray gases and numerous others have been developed and detailed accounts are available [5,24–27]. A recent account by Sacadura [2] discusses the application of these models in fire simulations and fire safety.

Since fires are inhomogeneous systems, most of the models mentioned in the preceding paragraph cannot be directly used in the solution of the RTE, Eq. (3), and instead the spectral absorption coefficient κ_λ needs to be determined. To facilitate integration of the radiant energy quantities (i.e., flux, flux divergence) a number of mean absorption coefficients such as the Planck, Rosseland, Patch, incident and others have been defined [5,24,25]. Unfortunately, only the Planck and Rosseland mean absorption coefficients are local radiation “properties” and are uniquely defined for the optically thin and thick limiting cases, respectively. Use of these mean coefficients in situations other than for which they have been determined is inconsistent with the physics and is a questionable practice.

3.3. Radiation characteristics of soot

Soot is considered as an important if not the dominant combustion product controlling thermal radiation from fire and hot smoke. A recent overview of theories for soot aggregate formation is available [28], and the importance of soot radiation in fires has been discussed [2,29]. In the small particle limit of the Mie theory, the spectral absorption coefficient of soot κ_λ can be approximated by [5,24]

$$\kappa_\lambda/(f_v/\lambda) = F_\lambda(\tilde{m}_\lambda) = 36\pi n_\lambda k_\lambda / \left[(n_\lambda^2 - k_\lambda^2 + 2)^2 + (2n_\lambda k_\lambda)^2\right] \tag{6}$$

where f_v is the local soot volume fraction and n_λ and k_λ are the real and imaginary parts of the complex index of refraction. Hence, if the soot volume fraction and the spectral complex index of refraction m_λ $(= n_\lambda - ik_\lambda)$ are known, the spectral absorption coefficient can be calculated from Eq. (6). In the Rayleigh (small particle) limit, the scattering coefficient is negligible in comparison to the absorption coefficient [5], and the RTE, Eq. (2), can be greatly simplified.

Soot formation and oxidation models available in the literature have recently been reviewed by Lautenberger et al. [28]. The models range from very simple to sophisticated. For example, Porterie and Loraud [18,19] used a two-equation model which accounts for soot inception, growth, agglomeration and oxidation processes to predict the soot volume fraction f_v. A soot formation and oxidation model that considers only the phenomena essential for obtaining sufficiently accurate predictions of soot concentrations to make CFD calculations of flame radiation from non-premixed flames of an arbitrary hydrocarbon fuel feasible has been recently developed and subjected to an initial calibration [28]. The soot model has been incorporated within modified version of FDS [11] and used for a comparison of predicted and measured temperatures, soot volume fractions and velocities in laminar ethylene, propylene and propane flames. Due to the drastic simplifications and approximations made in construction of the model further research (theoretical experimental and computational) is needed to refine the model and extend it to realistic fire situations.

Measurements of the dimensionless extinction coefficient of soot from a flame zone and overfire regions of 2 m JP-8 pool fires have recently been reported [30]. The predicted extinction coefficients were 20–30% smaller than the extinction data at 635 nm using commonly accepted values of the index of refraction of soot, but agreed well with the experiments using the more recent value ($m_\lambda = 1.99 - 0.89i$). This emphasizes the need for accurate measurements of the optical properties for interpretation of optical diagnostics and validation of fire dynamics models. An additional complexity in modeling woodland fires (for example) is the need to account for burning embers that are lofted by a fire’s buoyant plume and transported ahead of the main fire [31]. In this situation there is a need not only to account for gas and soot radiation but also for radiation from solid wood particles and tree branches under pyrolysis and char oxidation conditions.

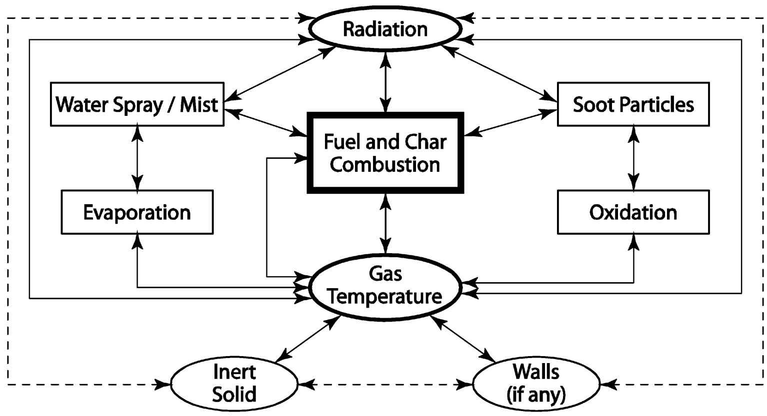

Fig. 3. Schematic representation of processes during fire extinguishment using water sprays.

3.4. Radiation characteristics of water sprays

Preheating of combustible materials ahead of the flame front by thermal radiation increases the rate of flame spread. Water-based suppression systems, which take advantage of water sprays (mist), can reduce the fire spread by attenuating thermal radiation and reducing the availability of oxygen needed for combustion. A simple schematic diagram of the processes occurring in a water-based fire suppression scheme is illustrated in Fig. 3. Heat and mass transfer processes during char formation and oxidation are not shown in the diagram but are implied. Water droplets in sprays attenuate radiation, and the spray/mist entering the flame affects radiation heat transfer rate of the fuel. Hence, there is an intimate coupling between the fuel burning (fire spread) rate, spray and radiative transfer. Recent discussions of modeling radiative transfer in fires using water sprays are available [23,32,33], including extensive citation of relevant prior work. The spectral radiation characteristics of monodisperse and polydisperse water sprays (needed as data input in the solution of the RTE), have been predicted [23,34] based on the Mie theory. Simple semi-empirical correlations based on the mean water droplet diameter have been developed for the spectral extinction coefficient and the single scattering albedo [34]. The results reported can be used in radiative transfer submodels of CFD codes modeling fire suppression using water sprays/mists [23,32].

Very recently a comprehensive model for radiative transfer in water sprays has been described [23]. The model predicts the spectral radiation characteristics of the polydisperse water sprays. The turbulent flow is modeled using a low Mach number large eddy simulation, and the liquid droplets are tracked using a Lagrangian approach. The most important absorption (six) bands of H_2O and CO_2 (the most important gaseous species in fire simulations) are used. A finite volume method is employed for solving the RTE. The simulations of two validation scenarios revealed that the model can predict radiation attenuation by water sprays when the hydrodynamic interaction of droplets is weak. However, modeling of interacting sprays would require an implementation of the droplet coalescence model and this would increase the cost of the flow calculation.

3.5. Radiative transfer in heterogeneous media

The RTE given in this section is appropriate for homogeneous or nearly homogeneous media. Use of the RTE for calculation of radiative transfer in large scale (i.e., urban or woodland) fires with strong hetrogeneities presents major conceptual and computational challenges. Probably the most complete formulation for multiphase modeling, which takes into account the detailed fire behavior in heterogeneous combustible (i.e., reactive and radiative) media so far, has been proposed by Larini et al. [35]. In the multiphase model the basic physical mechanisms and strong coupling between the phases due to mass, momentum, energy and radiative transfers are considered. Unfortunately, the model is computationally very intensive. In order to create an operational management tool able to describe the spread of forest fire and to help fire fighters make appropriate decisions when dealing with multiple fires, the general approach was abandoned and some special models have been developed [36–38]. For example, in the simplified model of fire dynamics by Simeoni et al. [37] radiative transfer modes from the flame were poorly represented, and the formulation did not describe adequately the combined effects of steep slope and high wind.

Even though this limited account does not discuss woodland (forest) or large urban fires, the choice of the scale in such fires is a challenge when modeling the dynamics of hetrogeneous fires. Radiative transfer on microscopic, macroscopic or mesoscopic scales cannot be described by the same RTE solution. Handling of such large scale fires in a realistic manner needs fundamentally new approaches.

4. Concluding remarks

Significant progress has been made during the last few decades in the numerical simulation of unwanted fires using CFD techniques based on physical/chemical models. The discussion in the overview focused on radiative transfer, an important energy transfer mode, which owing to directional and spectral nature, turns out to be the most time-consuming to calculate numerically.

There is a need to improve the effectiveness, reliability and accuracy of radiative energy transfer in CFD models simulating fire behavior, particularly for fire situations in which thermal radiation is an important and/or dominant mode of energy transport.

One of the biggest impediments preventing increased usage of CFD-based fire dynamics models is the limited experimental data base and our limited ability to use data from bench-scale fire tests for model validation.

Reliable methods have been developed for solving numerically the RTE and evaluate radiant energy quantities of interest, but the calculations require compatible radiation characteristics of fuel and combustion products which are time-dependent. These characteristics are functions of both radiating species concentrations and temperature, and, if the calculations are being performed on gray or band-based models, they also depend on the radiation field.

Lack of reliable models for soot formation/oxidation kinetics and uncertainties in the spectral optical constants of soot present a challenge in the overall prediction of the spectral absorption coefficient for radiation dominated fires which exhibit significant continuum radiation.

Available numerical and experimental results have shown that in chemically reacting and radiating flames the neglect of turbulence/radiation interaction can result in significant underprediction of radiant energy quantities even in nonluminous flames [39,40]. This suggests that for more accurate and realistic modeling of fire dynamics the turbulence/radiation interaction would have to be considered for intensely radiating fires.

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