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# Soot in Combustion Simulations

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## Abstract

Soot is the dominant source of radiative heat transfer from most practical flames. A review is presented of historical, empirical modelling approaches for estimating heat flux from fires and flames. These historical methods have drawn on empiricism to address the role of soot while seeking methods for including the multi-scale effects of soot formation and flame structure. Both soot concentration and flame temperature have been seen to be local phenomena with dimensions on the order of the diffusion and chemical (Batchelor) scales of the flame. The correlation between the local soot volume fraction and the local temperature field is needed for determining the radiant heat flux from the flame. By using high performance computers (hundreds to thousands of processors) Large Eddy Simulations (LES) can resolve structures on the scale of the pool diameter in pool flires. Thus, air engulfment and visible flame structure are resolved. Manifolds for the gas-phase chemistry, soot formation, particle growth, soot diffusive/ thermophoretic transport are used to bridge the Batchelor and resolved (LES) scales.

## 1. Introduction

Soot formation and oxidation in combustion is a multiscale, multiphysics problem. For example, one combustion flame application in which the role of soot is predominant is in the study of hydrocarbon pool fires from the stand-point of fire prevention, safety and extinction. Realistic simulations of fires that adequately represent the relevant physical processes such as turbulent reacting flows, heat transfer and chemistry can provide valuable insights into the fire and flame physics. Thermal radiation is often the dominant mode of heat transfer in these flames. Water vapour, carbon dioxide and soot are the major sources of radiation from a fire. To numerically estimate the radiation field in and around a fire, accurate representations of the flame shape, size and the composition and temperature fields are necessary. While significant progress has been made to accurately predict via combustion modelling, the temperature, $CO_2$ and $H_2O$ fields as well as the radiation from these gases [1-5], obtaining accurate estimates of the soot concentrations, its temperature as well as its radiative properties remains a challenging undertaking. This is particularly important, because in general, soot particulates contribute the most to flame radiation.

This paper first, briefly reviews semi-empirical modelling approaches that have been employed to estimate the radiation field from hydrocarbon pool fires for a historical perspective. These approaches have often been employed by the fire community for providing immediate and practical engineering solutions for estimating the radiation hazards. The inability of these approaches to explain some experimental observations is pointed out. Obtaining accurate concentrations of soot and capturing the fire dynamics correctly are shown to be pivotal to overcoming these shortcomings and for obtaining valuable insights into experimental observations. The increase in computing power along with an increased understanding of the fire and soot physics has led to the development of sophisticated numerical approaches that may help to better describe the dynamics of the fire. Then, the remainder of the paper introduces a method to bridge the Batchelor and resolved scales in a large eddy simulation (LES) of fires. This bridging is based on estimating parameterized manifolds for the soot formation and transport at the Batchelor scale soot formation and transport processes [6].

## 2. Historical modelling approaches

Historically, flame radiation has been estimated invoking the assumption of a homogeneous flame. In this assumption, turbulent flames have been assumed to have homogeneous gaseous and soot concentrations at some "effective radiation temperature." Various semi-empirical approaches for estimating the radiation field in and around hydrocarbon pool fires have been reviewed by De Ris [7] and Mudan [8].

To estimate the radiation from a homogeneous flame one needs to know the flame shape and size, an effective radiation temperature and the flame absorption coefficient/flame emissivity. A conical [7] or cylindrical [8] flame shape is usually assumed over a circular pool. A flame height can either be estimated through photographs [7] or from the burning rate of the fuel. The non-dimensional flame height (flame height to pool diameter ratio) has been found to correlate well with a non-dimensional mass burning rate [8, 9]. Correlations relating the angle of tilt of the flame from the vertical to wind velocity are also available [7]. Once the shape and size of the fire is calculated, the radiative characteristics of the fire need to be determined. The radiative properties of the flame are often estimated in the form of grey absorption coefficients or grey emissivities by assuming a homogenous mixture of CO2, H2O and soot. The determination of an effective flame temperature is described in [7, 10]. For many years the paper by Modak [11] served as a reference for the homogeneous flame modelling approach. In that study, the radiative fluxes to a burning surface and to the surroundings were computed from a horizontal homogeneous pool fire of a specified shape. The results obtained were in good agreement with experimentally measured fluxes. Zone models constitute an approach more sophisticated than the homogeneous flame approximation. These models divide the domain of interest into zones and describe the basic equations of mass, momentum and energy transfer in a control-volume sense for each zone and also account for the interactions between different zones [12]. However, zone models have mainly been used to simulate enclosure fire phenomena and are not discussed further in this paper.

An important shortcoming of the homogeneous model is that the effective flame temperatures of many liquid fuels are still not known [8]. Second, radiative fluxes to the pool surface and even at locations away from the fire are likely to be influenced by the assumed flame size and shape through its dependence on geometric view factor [8]. Numerical estimates of the radiative heat fluxes to the pool surface from 30 cm diameter pool fires employing the homogeneous model were found to be higher than the experimental values by 40% by De Ris [7].

Most of this error was attributed to assuming a conical shape to the flame.

Another shortcoming of the homogeneous model is its inability to predict the radiative feedback to the pool surface, particularly in large pool fires. Obtaining accurate estimates of the radiative fluxes to the pool surface is important to determining the burning rates of the fuels. Hottel [13] was able to explain the trends in the burning rates of liquid fuels by relating the rate of heat transfer from the fire to the pool to the rate of fuel vaporization. The cooler unburnt sooty pyrolysis gases near the fuel surface in large fires may block part of the flame radiation from reaching the surface. Radiation blockage has been shown to significantly affect the fuel burning rates in pool fires at diameters greater than 1m [14]. Shinotake et al. [14] observed that the experimentally measured radiative fluxes to the pool, increased with increase in diameter but quickly saturated compared to the external fluxes. They explained these observations in terms of radiation blockage by performing simple two-layer model calculations with conical outer-shapes. An outer cone represented the radiative characteristics of the fire and an inner cone represented the vapour dome of pyrolysis gases. An assumption of a homogeneous flame failed to capture the observed trends in heat fluxes. The two-layer model calculations however, were found to be very sensitive to the adopted soot concentrations and soot temperatures in the flame as well as the vapour dome. Measurements in very large pool fires also show significant gradients in the radiative heat fluxes to the pool surface, which are likely to result in significant gradients in the fuel vaporization rates within the pool [15].

The fire hazard of a fuel is characterized to an important extent by the total radiative output of a fire to its surroundings. The fraction of combustion energy that has been radiated to the surroundings ($\chi_R$) is an important parameter that provides insight into classifying the flammability of the combustion materials. This fraction cannot be estimated theoretically, and is normally estimated using measured radiometer data. However, the radiation fraction ($\chi_R$) in certain fuels has been observed to decrease with increase in pool diameter due to smoke obscuration which results in a significant reduction in the recorded radiation [8, 16]. Experimentally measured mean surface emissive power (which is proportional to $\chi_R$) for different fuel pool fires at different diameters is shown in Figure 1.

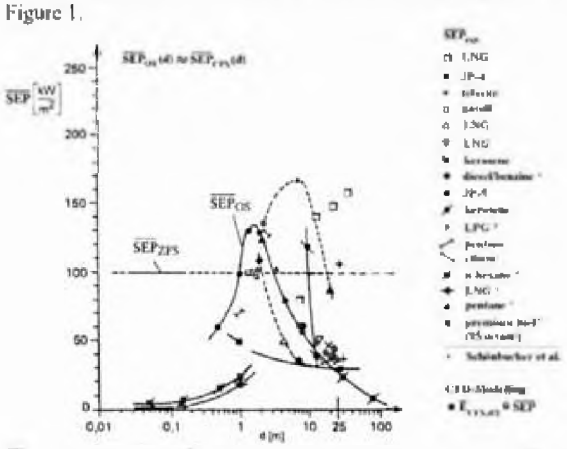


Figure 1: Experimentally measured mean surface emissive power for different pool fires at different diameters (reproduced with permission from Prof. Dr. A. Schönbucher, University of Duisburg-Essen, Institute of Technical Chemistry, Essen, Germany).

The mean surface emissive power for many hydrocarbon pool fires is seen to decrease with increase in pool diameter due to smoke obscuration. Although, a systematic methodology to reliably address this phenomenon is not yet available, some explanations have been proposed. The vapour dome of large fires may contain pyrolyzed fuel vapours, which are at moderate temperatures relative to the reaction zones. Poor mixing and/or the slow entrainment of this stream with the air stream may result in the formation of long lived, fuel rich eddies that contain the fuel-rich but un-oxidized fuel [17]. The smaller fluid strain rates associated with this process can reduce the diffusion rates and give more time for the fuel to pyrolyze and form larger soot particles (smoke) that take longer to oxidize. Klassen and Gore [9] measured transient emission and absorption properties in pool fires of different fuels and sizes with a maximum pool size of diameter 1m. They observed a relatively cold layer of soot particles near the fuel surface. Comparing their absorption and emission measurements they also showed that a large portion of the soot particles are at relatively low temperatures and do not contribute to emission. Therefore, it is important not only to understand the chemical phenomena that lead to the formation of soot but also the local transport phenomena that determine the distributions of soot and its temperature within a flame. The local soot concentration is a result of a time evolved history of local production, oxidation, convective and diffusive (thermophoretic) transport processes [18]. In fact, in laminar diffusion flames the peak soot concentrations have been found to be slightly offset from where the peak temperature was located [19]. This is shown in Figure 2, for a laminar diffusion $C_2H_2$ flame.

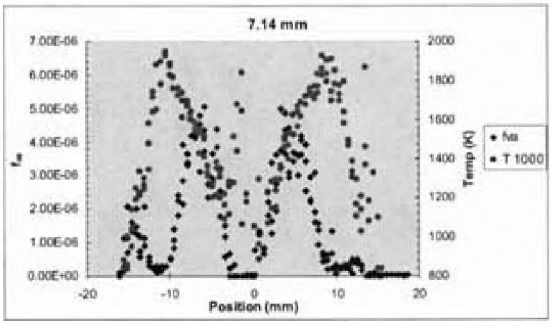


Figure 2: Radial profiles of soot concentration and temperature at an axial height of 7.14 mm in a laminar $C_2H_2$ diffusion flame (Fig. 27 of Ref. [19]).

The radiant emission from a flame is linearly dependent on the soot concentration and is dependent on the soot temperature to the fourth power. This indicates that maximum emission occurs at a region between the maximum flame temperature and maximum soot concentration. Hence, the temperature and axial placements of the soot volume fractions are critical in calculating the effective flame temperature across flame fronts.

Clearly, in order to reliably address these phenomena (radiation blockage, smoke obscuration and the location of soot near the flame front) requires basic developments in the modelling of air entrainment and soot formation that go beyond the homogeneous modelling approach [20]. The past two decades have seen an increasing use of computational fluid dynamics (CFD)-based models to study fire phenomena. The difficulty of applying CFD to fires lies in the fact that the physical processes associated with the fire are characterized by a wide range of continuum length scales and their corresponding time

scales. However, the important features of the fire physics can be captured by resolving the large length and time scales that are responsible for controlling the dynamics of the fire [21, 22]. In this regard, LES methods appear to be very promising to capture the flame processes occurring on the scale of the flame (the resolved scale). In fact, LES is expected to emerge as the most prevailing methodology for studying fires due to its ability to render realistic, time-resolved flow of gases, heat and smoke throughout the domain [23]. In order to spatially resolve the important flow characteristics in a fire, grids containing $10^6$ to $10^8$ computational cells are used at every time step associated with the LES calculation. Massively parallel computations (hundreds to thousands of processors) are required to perform this task. Computational "Frameworks" and "Problem Solving Environments" (PSEs) make the tasks of parallelization, load balancing, data-structure management, and scaling (the computational work scales with the number of processors) efficient. We have developed the Uintah Computational Framework (UCF)[24] for a pool fire application. The parallelization is carried out employing a domain-decomposition strategy. Fully coupled simulations of pool fires have been performed with more than $200^3$ computational cells. A snapshot of one such simulation of a one meter diameter methane pool fire is shown in Figure 3.

Figure 3: Snap shot image of the volume rendered temperature field during a transient simulation of a 1m diameter methane pool fire. Warm colors represent higher temperatures, cooler colors represent cooler temperatures.

In Figure 3 it can be seen that the turbulent momentum field results in the entrainment of air deep into the fire plume that results in an increase in the combustion surface area. Although, the entrainment of air by large scale structures increases the surface area, these circumstances also lead to large regions of segregated fuel rich pockets that grows large amounts of soot. Figure 4 shows the computed soot field that accompanies the temperature field shown in Figure 3.

Figure 4: Snap shot image of the volume rendered soot volume fraction field during a transient simulation of a 1m diameter methane pool fire. The grey color scale wither darker grey represents higher soot volume factions, lighter gray represents lower soot volume fractions.

This LES approach has been employed to model radiative heat transfer in LES calculations of a wide range of diameters of methane pool fires. Predictions of the radiation fraction ($\chi_R$) with different radiation models were found to compare well with experimental observations [25]. The next step is to extend these calculations to more sooty fuel fires. Approaches for bridging the Batchelor scale soot formation and transport processes to the resolved LES scale computations through identification of parameterized manifolds are discussed next.

## 3. Soot modelling in fire simulations

The production of soot in a flame is a chemically controlled phenomenon where low molecular weight gaseous hydrocarbons like acetylene grow to solid carbon particles in just a few milliseconds. Recent advances in modelling soot formation and burnout in combustion systems were surveyed by Kennedy [26]. The soot formation process can be divided into particle inception, surface growth and oxidation. The formation of aromatic hydrocarbons from aliphatic hydrocarbons constitutes the first step in soot formation. The aromatic species grow by the addition of other aromatic and smaller alkyl species to form larger polycyclic aromatic hydrocarbons (PAH). The continued growth of the PAH leads eventually to the smallest identifiable soot particles. PAH and

their formation pathways have been thought to be the key ingredients in modelling soot production [27]. The net amount of soot produced has been thought to be linearly dependent on the rate of soot inception based on the assumption that the surface growth rates were linearly dependent on the available surface area which in turn depends on the total number of particles that were created during nucleation. The growth of soot particles after particle inception occurs by the physical process of collisional coagulation and the chemical process of surface growth where gas phase material and PAH are added through chemical reactions with the active sites on the soot particles. Agglomeration occurs during the later stages of combustion. Finally, soot oxidation occurs primarily due to the attack by oxygen containing species like $O_2$, OH, O, $H_2O$ and $CO_2$. Modelling soot formation in turbulent diffusion flames remains a challenge due to the complex chemical mechanisms and long time scales governing soot formation. Second, the presence of soot in strongly sooting flames can significantly alter the flame chemistry by being a sink for important species such as OH and acetylene, by being a source for CO during oxidation, as well as by altering the heat release profile through radiative heat loss. Due to this bidirectional coupling between the soot field and the flame field, it cannot be effectively post-processed on established flame fields as has been done with modelling other pollutants such as $NO_X$.

In combustion modelling of turbulent diffusion flames, the instantaneous thermochemical state of the gaseous mixture and the species of interest are often expressed as a function of a conserved scalar variable called the mixture fraction (Z). The chemical equilibrium model or the flamelet model is often used to obtain this functional relationship. An essential aspect of the mixture fraction approximation is that all the species and energy diffuse at the same rate. However, soot is the product of a relatively slow reaction, is not in equilibrium and does not diffuse at the same rate as the molecular species. Hence, soot is not expected to correlate well with mixture fraction. Attempts to correlate the soot volume fraction with mixture fraction in calculations of turbulent diffusion flames have been carried out previously with limited success [28]. From measurements carried out in co-flow diffusion flames, Kennedy et al. [29], modelled the nucleation rate to be a function of mixture fraction alone and showed that the surface growth process to be the controlling mechanism in determining total soot volume fractions. For example, hydrocarbon pool fires are known to have high concentrations of soot. Under these circumstances, the surface growth processes are likely to be more important than the others [26].

Most of the modelling of soot in combustion simulations of diffusion flames has been done through semi-empirical approaches [26]. Most of these approaches usually lead to the development of rate equations for reactions of soot precursors and soot particles with a simple description of the chemistry and solving transport equations for the soot number density and the mean mass concentration of soot (or the soot volume fraction) on the CFD grid. Usually, global four-step reaction schemes that account for soot nucleation, surface growth, coagulation, and oxidation, are employed, with the rates based on fuel concentrations and intermediate growth species. The soot number density and the soot volume fraction represent the first two moments of the soot particle distribution, and allow for the calculation of the mean particle size and surface area for surface reaction. Steady flamelet models (in favour of the equilibrium model) have often been employed to model the gas phase in these semi-empirical approaches, due to the need to predict minor radical species like OH which is an important constituent in the reaction scheme for oxidation of soot. Our approach to modelling soot formation and oxidation in CFD simulations is described next.

In the steady flamelet approach, the flamelet equations are solved to steady state [30]. However, slow chemical or physical processes such as NOx or soot formation cannot be accurately captured using the steady flamelet approach. To alleviate some of this shortcoming, the flamelet equations are solved in unsteady form using time as an additional parameter. The transient flamelet may now be thought of as moving through the computational grid in a Lagrangian sense. Now, this additional "time" parameter needs to be linked to the CFD grid. This may either be done by linking the flamelet time to the corresponding time on the CFD grid or by progress variable approaches [31]. Pitsch et al. [32] linked the flamelet time to axial position in a jet, based on the axial jet velocity and position. They applied this approach in a numerical simulation of soot formation in a turbulent C2H4 jet diffusion flame. The predicted soot volume fractions were shown to compare reasonably well with the measured data. In the progress variable approach, a scalar (or combination of scalars) that vary or correlate monotonically with the subgrid flamelet time is employed as the "time" parameter and transported on the CFD grid. This approach was first employed by Desam [33] to study $NO_X$ formation in turbulent non-premixed jet flames. We have used both these approaches of "linking" the "time" parameter in the unsteady flamelet equations to either the position on the CFD grid or to scalars that can be transported or modelled on the CFD grid.

Our objective is to simulate the combustion behaviour of real transportation fuels like JP-8. Real jet fuels are chemically complex and often blended from thousands of compounds that differ widely in their volatility, sooting propensities and heat of combustion. Consequently, fires from these fuel blends do not burn at a uniform rate. In the beginning, the burning rate is characteristic of the most volatile component and become increasingly characteristic of the less volatile components as the fractionation proceeds. A surrogate blend of six hydrocarbons was proposed by Violi et al. [34] that adequately captured the distillation and sooting characteristics of a practical JP-8 fuel. A detailed reaction network for the surrogate fuel was then proposed by Zhang [35]. The model also unified kinetic models that were available for some of the individual components of the surrogate. The model development thereby provided a methodology for generating new combustion mechanisms for larger paraffin fuels (that are important constituents in the surrogate) and enable the prediction of soot precursors during their oxidation. A mathematical sub-model based on the technique of Frenklach and co-workers [36] was then developed to describe the particle dynamic processes of nucleation, coagulation, surface growth, surface condensation and oxidation. The sub-model led to improved predictions of some of the physical and chemical characteristics associated with soot formation than reported previously.

The process of polymerization of PAH leading to soot formation is associated with a wide range of timescales. The intramolecular processes that can occur on a particle surface can take place in pico- or nanoseconds compared to the formation of the first soot precursors that occurs in milliseconds. Violi et al. [37, 38] presented a novel methodology to bridge these time scales. The methodology involved alternating between Molecular Dynamics (MD) calculations (for the intermolecular relaxation processes) and a Kinetic Monte Carlo (KMC) (for the long time scale processes) during the course of a simulation. The fully integrated KMC/MD code in conjunction with high-level quantum chemical

calculations was used to carry out simulations of structures of soot precursors containing hundreds of carbon atoms. This methodology is a reflection of the "patch dynamics" outlined in Kevrekidis et al. [39], where results from simulations of microscopic descriptions (Eg: MD) that are carried in small computational domains over small time steps may be employed to advance macroscopic simulations that are carried over large times on larger computational domains.

## 4. Concluding remarks

Due to the complexities associated with understanding fire behaviour, the reliability of predictive tools developed for the fire protection engineering community depends on the amount of physics that has gone into the model development. The advent of faster computers and physical insights has led to the development of sophisticated, physics based models. The capability now exists to capture important characteristics of the pool fire flame, plume structure and air entrainment. These models have been able to predict thermal radiation from low-sooting pool fires like methane [25, 40]. However, extending these capabilities to sooty pool fires depends to a large extent on obtaining accurate distributions of soot in the fire.

In recent years, soot modelling has been attacked with very detailed descriptions of the soot physics and chemistry. However, reduced mechanisms and semi-empirical approaches are currently necessary to reduce the problem to a scope that can be handled by codes that treat turbulent reacting flows. The applicability of empirical and semi-empirical prediction methods is naturally limited to a certain range of conditions. Hence, the parameters like rates of surface growth processes, and those of oxidation by $O_2$ and OH are often adjusted in these approaches to fit the experimental data [26]. Consequently, improvements in soot modelling will be greatly determined by the measurement of elementary rate constants.

Validation efforts are necessary to help certify the adequacy of the numerical models for simulating fires. Fortunately, there is a lot of experimental data and experimental observations in the literature that can help support the development and validation of soot and radiation models in pool fire simulations [9, 41, 42]. However, due to the difficulties associated with directly measuring soot concentrations, the soot volume fractions are usually determined from attenuation studies after assuming the values of the optical constants (radiative properties) of soot. The structure of soot and its radiative and optical properties have extensively studied by Faeth and coworkers [43, 44]. Therefore, while comparing simulations with experiments, it is important that the optical constants in the numerical modelling of the soot property be the same as those employed in the experiments to deduce the soot volume fractions.

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