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Development of a multiphase photon Monte Carlo method for spray combustion and its application in high-pressure conditions

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ABSTRACT

In this work the development of a multiphase photon Monte Carlo (PMC) method with a focus on resolving radiative heat transfer in combustion simulations is presented. The multiphase PMC solver can account for description of participating media in both Lagrangian and Eulerian frameworks. The solver is validated against exact solutions in several one-dimensional configurations. The developed solver is then applied to Diesel spray combustions, where liquid spray droplets are assumed to be cold, nonemitting, large, and isotropically scattering. Several formulations for radiative properties of the Diesel spray are first explored. The PMC solver has then been coupled with the multiphase spray combustion solver in OpenFOAM and the coupled solver is used for simulations of high pressure Diesel spray combustion. It was found that in typical Diesel spray combustion applications, such as in an internal combustion engine, impact of radiation on the evolution of the liquid spray was insignificant. Although the impact of radiation on the spray was minimal, nongray spectral properties and the assumption of semi-transparency for Diesel spray were found to impact the radiative transfer significantly, while impact of scattering was marginal. Spray radiation was also found not to have much effect on global combustion characteristics in high-pressure engine-relevant configurations. However, a small but noticeable effect on minor species distribution relevant to pollutant formation was observed.

1. Introduction

High-fidelity combustion simulations require accurate modeling of turbulence, chemistry, and radiative heat transfer. Each of these processes is mathematically complex and computationally expensive. These processes closely interact with each other. Hence, to resolve accurate physics of a combustion system each of these three processes should be modeled with comparable fidelity. However, due to the small influence of radiation on small scale laboratory flames and due to the computational complexity of radiation solvers, radiation modeling in combustion simulations is usually less sophisticated than flow or chemistry modeling. Although such simplification may be satisfactory for simple and small geometries at atmospheric pressure, it is generally not appropriate for practical combustion systems.

Combustion processes in many practical systems are heterogeneous; for example, coal furnaces or internal combustion engines (ICEs). It is the presence of the discrete phase that makes multiphase radiation modeling a hurdle in such combustion simulations. Multiphase radiation modeling involves models for both the continuum carrier or gas phase and the discrete dispersed or particulate phase. The optical regime of particulates depends on their size, complex index of refraction, and the irradiating wavelength. Wide variability in these parameters makes accurate radiation modeling in particulate media a daunting task. While a large body of work exists on modeling radiation for dispersed and particulate media [1–5], not many studies have been done on radiation in the context of multiphase combustion, and even fewer studies focused on multiphase radiation in high-pressure spray combustion.

In spray combustion, the thickness of the reaction zone and droplet diameter are often of the same order, thereby making flame dynamics very sensitive to spray evolution [6]. Evolution of spray, on the other hand, is sensitive to heating of the spray due to convection and radiation. In a single droplet study Godsave [7] estimated that for large benzene droplets, radiation could contribute as much as 20% of the heat of evaporation in the presence of hot surroundings. For a monodisperse spray in an inert atmosphere, Sazhin et al. [8] reported a small but noticeable effect of radiation on Diesel droplet surface temperature and evaporation rate, particularly for larger droplets. In single droplet studies in microgravity [9] and in low-pressure [10], radiation has also been shown to affect droplet evaporation rate under certain conditions. For

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hydrocarbon fuels Tseng and Viskanta [11] showed that depending on the relative rate of heat transfer due to radiation and convection, evaporation of droplets is affected by radiation in a combustion environment. They also showed that for n-heptane droplets of 100 μm diameter, radiative heating could be as high as 15% of convective heating in presence of 1000 K surroundings.

For an order-of-magnitude analysis of relative heat transfer rates due to convection and radiation, we assumed a motionless droplet with diameter of $d = 20$ μm and uniform temperature of $T = 300$ K in a unit volume of still ambiance of radiatively inert gas at $T_\infty = 800$ K in a closed chamber whose walls are black and hot (same temperature as the surrounding combustion gas). If one assumes the droplet to be large and opaque with an absorption efficiency of $Q_{abs} = 0.95$, and it being uniformly irradiated with radiation from a black surrounding at $T_{comb} = 2000$ K. The approximate convective and radiative heat transfer rates for the droplet, respectively, would be

$$S_{conv} \approx \frac{Nu \times k}{d} \pi d^2 (T_\infty - T), \quad (1)$$

$$S_{rad} \approx Q_{abs} \pi \frac{d^2}{4} \sigma T_{comb}^4, \quad (2)$$

where Nu is the Nusselt number, σ is the Stefan-Boltzmann constant, and k is the conductivity of the droplet. Assuming a droplet moving with the surrounding gas (*i.e.*, no relative velocity, hence, $Nu = 2$) and a liquid fuel conductivity of $k \approx 10^{-2}$ Wm^{-1} K^{-1}, one obtains $S_{rad}/S_{conv} \approx 0.4$. This indicates that under some conditions radiative and convective heat transfer could be comparable. Although in practical high pressure spray combustion systems this ratio, S_{rad}/S_{conv}, is expected to be small because of the high rate of convective heat transfer owing to high injection velocity, it is important to confirm the impact of multiphase radiation in such conditions with a rigorous quantitative analysis.

Several studies have been carried out on the effects of radiation in the context of fire and quenching by spray or mist [12–20]. Some spray combustion studies, such as [21,22], had included radiation but only for the gas-phase. Very few studies were in the context of spray combustion that included multiphase radiation. Based on the findings of [11], Watanabe et al. [23] investigated the impact of radiation in spray combustion in a laminar counterflow n-heptane flame using a discrete ordinates method (DOM) for radiation. They found that consideration of the spray in the radiation model does not affect the temperature field substantially, but affects soot production. Building on [23], recently Fujita et al. [24] performed a simulation of a jet flame with n-decane as liquid spray fuel coupled with multiphase radiation calculations using a narrow band model and a DOM solver. There appears to have been very few studies that considered multiphase radiation in the context of practical spray combustion systems, such as ICEs. Very recently, El-Asrag et al. [25] performed a coupled large eddy simulation of a Diesel engine with optically thin multiphase radiation.

The primary goals of this work are to develop an accurate and efficient multiphase radiation solver suitable for combustion simulations, to evaluate accuracy, applicability, and sensitivity of various optical models for radiation formulation of Diesel fuel in spray combustions. To that end, a multiphase photon Monte Carlo (PMC) method is developed for accurate analysis of radiative heat transfer coupled with flow and combustion in the presence of a discrete phase, specifically, liquid fuel spray. This solver is then used to evaluate impact of multiphase radiation in spray combustion in an engine-relevant condition. Although the solver is developed with high-pressure Diesel spray in mind, it can be used, with minor modifications, for any coupled combustion simulations where a discrete phase is present.

The broader goal of the current work is to advance the understanding of the spray combustion dynamics in engines. Several studies have shown importance of radiation in engine [26–30]. In most previous studies without radiation, turbulence, chemistry, and spray models are usually "tuned" to match global experimental data such as spray penetration length and ignition delay on a case-by-case basis. Instead of tuning the spray, combustion, or turbulence models, in this work we used standard versions of these models as available in the literature and focused specifically at the quantitative evaluation of the effect of multiphase radiation on spray.

The solver developed in the current work was implemented on the open source OpenFOAM [31], utilizing its built-in spray modeling capabilities. The developed multiphase PMC solver is designed to handle both a Lagrangian and a Eulerian description of the discrete phase. In this article we first discuss the models for radiative property calculations for the discrete phase, followed by a description of the Eulerian-PMC and the Lagrangian-PMC schemes developed and used in the current study. Then we present validation studies and sensitivity studies for the optical models used in modeling spray radiation properties. The multiphase PMC scheme is then used to evaluate the effect of radiation on the evolution of the spray and the impact of including the spray in radiation calculations in configurations relevant to an internal combustion engines. It is emphasized here that the primary motivation of this work is to develop a multiphase radiation model, and not to investigate spray, chemistry, and combustion models, or their interaction directly.

2. Calculation of radiative properties of droplets

Radiative properties of a droplet of radius a, when interacting with a ray of wavelength λ, are governed by three nondimensional parameters: (i) complex index of refraction, $m = n - ik$; (ii) size parameter, $x = 2\pi a/\lambda$; and (iii) clearance-to-wavelength ratio, c/λ. Here we assume independent scattering ($c/\lambda \gg 1$), thereby removing the effect of clearance-to-wavelength ratio from the formulation. Absorption and scattering potential of a droplet is expressed in terms of efficiency factors. Efficiency factors for absorption, scattering, and extinction for a droplet of radius a are given as [32]

$$Q_{abs} = \frac{C_{abs}}{\pi a^2}, \quad Q_{sca} = \frac{C_{sca}}{\pi a^2}, \quad Q_{ext} = \frac{C_{ext}}{\pi a^2} = \frac{C_{abs} + C_{sca}}{\pi a^2}, \quad (3)$$

where C_{abs}, C_{sca}, and C_{ext} are absorption, scattering, and extinction cross-sections, respectively.

Calculation of radiative properties of droplet involves (i) evaluation of spectral variation of complex index of refraction of the liquid fuel and (ii) formulation for absorption and scattering efficiencies of droplets. In this work we explore several models and formulations for both of these aspects of droplet radiative properties.

2.1. Complex index of refraction of liquid fuel

The choice of liquid spray of the current study is Diesel fuel. Because of the complexity of real fuel, n-heptane is often used as a surrogate in both experimental studies and numerical simulations of Diesel combustions. Surrogates are determined by matching various properties such as density, evaporation characteristics, C/H ratio, ignition timing, sooting propensity, etc. with the target fuel. Choice of surrogate fuel usually depends on the focus of the application at hand, for example, the surrogate to study global characteristics of an engine may be different than surrogate used to look specifically at the emission characteristics. Common Diesel surrogates such as n-heptane, n-decane, n-dodecane, and various