

Assessing the Importance of Radiative Heat Transfer for ECN Spray A Using the Transported PDF Method

Muhammad Aqib Chishty, Michele Bolla, and Evatt Hawkes
The University of New South Wales

Yuanjiang Pei
Argonne National Laboratory

Sanghoon Kook
The University of New South Wales

ABSTRACT

The importance of radiative heat transfer on the combustion and soot formation characteristics under nominal ECN Spray A conditions has been studied numerically. The liquid *n*-dodecane fuel is injected with 1500 bar fuel pressure into the constant volume chamber at different ambient conditions. Radiation from both gas-phase as well as soot particles has been included and assumed as gray. Three different solvers for the radiative transfer equation have been employed: the discrete ordinate method, the spherical-harmonics method and the optically thin assumption. The radiation models have been coupled with the transported probability density function method for turbulent reactive flows and soot, where unresolved turbulent fluctuations in temperature and composition are included and therefore capturing turbulence-chemistry-soot-radiation interactions.

Results show that the gas-phase (mostly CO₂ and H₂O species) has a higher contribution to the net radiation heat transfer compared to soot. The effect of radiation absorption was found to be important and the typical radiation time scale is observed to overlap with the long injection duration, leading to a moderate influence on the temperature distribution. The flame lift-off length is not affected by radiation and differences in soot formation are perceivable but only minor. The performance of the DOM and P1 models is comparable, whereas the optically thin assumption leads to a higher cooling effect. It is anticipated that NO_x formation rates are expected to be influenced by radiative heat transfer in a more pronounced manner.

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INTRODUCTION

The Engine Combustion Network (ECN) is a collaborative multiinstitution experimental and numerical framework which seeks to improve the understanding of engine combustion. Researchers from all over the world work on well-defined target conditions, in particular on the so-called Spray A test case - a 90 μm diesel-type single-hole injector operated with *n*-dodecane. Extensive research has been reported for inner-nozzle flows, liquid evaporation, fuel-air mixing, ignition and combustion up to soot formation - refer to [1] for more details. On the other hand, radiation heat transfer has obtained limited attention experimentally [2] and to the best of our knowledge there is no modeling work exploring the role of radiation heat transfer in the context of Spray A.

The situation for atmospheric laboratory jet-flames (e.g. in the context of the TNF Workshop series [3]) is considerably more mature. On the one hand, the importance of turbulence-chemistry interaction and the related need to be modelled has been

demonstrated more than a decade ago [4,5,6,7,8,9,10]. On the other hand, the role of radiation has already been extensively assessed and radiation models are routinely included in numerical simulations [10,11,12]. Radiation in luminous flames was observed to decrease the flame temperature by more than 100 K [13]. Also, the importance of turbulence-radiation interaction (TRI) - arising from highly nonlinear coupling between the fluctuations of the radiation intensity, temperature and species concentration - has been explored and assessed [10, 12, 14]. The effects of temperature and radiation fluctuations can increase the radiative fluxes up to 2-3 times based on the mean properties [11, 15].

In the diesel engines, the influence of radiative heat losses is expected to increase for larger engines. In very large bore, heavy duty diesel engines, radiation accounts for more than 40% of the total heat losses [16, 17]. For example, radiation in a heavy-duty diesel engine can affect the peak temperature by the amount of 20-30 K having an impact on the formation of nitric oxide (NO_x) by

12-25% [18]. Quite a few studies are reported for the radiation heat transfer modeling in the context of diesel engines, e.g. [19,20,21,22,23,24,25,26]. All of them have neglected the effect of TRI and focused on the influence of radiation on NO_x production and soot deposition. Few studies illustrated that soot radiation is more important in the diesel engine, however, during the combustion, many intermediate species are formed which emits radiation but their effects are assumed to be even less important [17, 27, 28]. Recently, it has been proposed that radiation from the gas phase species are more dominant than the soot radiation, and the significant fraction of emitted radiation can be reabsorbed before reaching the walls [26].

The aim of this study is to evaluate the role of radiation heat transfer under ECN Spray A conditions. The TPDF method - which accounts for unresolved turbulent fluctuations in composition and temperature - is used in conjunction with three different radiation models and the influences of TRI and TCI are explored. Furthermore, the impact of radiation for different ambient temperatures and oxygen mole fractions is presented.

METHODOLOGY

Numerical Setup

The ANSYS FLUENT 14.5 finite volume based CFD commercial code was used in this study. Numerical simulations were carried out on a 2D axis-symmetric mesh using the unsteady Reynolds Averaged Navier Stokes (RANS) $k-\epsilon$ realizable turbulence model. The liquid *n*-dodecane fuel is injected at high pressure of 1500 bar and the injection parameters and reacting ambient conditions are listed in Table 1 and 2, respectively. The spray is modeled using the Lagrangian discrete phase approach and similar case setup has been employed which has been used in our previous studies [29,30,31].

The composition transported probability density function (TPDF) method [4] is employed for accounting turbulence-chemistry interactions due to its several advantages over other TCI approaches [11, 30, 32]. The convergence studies of mesh, time step size, number of particles per cell and ISAT error tolerance have been conducted in our previous studies [33]. A relatively compact reduced 53 species *n*-dodecane chemical mechanism [34] has been employed in conjunction with the two-equation soot model by Leung et al. [35]. The transport equations are solved for the soot mass fraction (Y_s) and particle number density (N_s) and acetylene is used as the soot precursor. This soot model has been successfully applied for Spray A by the same authors in Ref. [30, 31] and more information can be found in Ref. [36]. The focus here is to assess the importance of radiation heat transfer rather than evaluating the performance of the combustion and soot models. In a second step, the results are compared with the well-mixed model to examine the effect of TCI. The well-mixed model is further used to explore the impact of radiation heat transfer for different ambient temperature and oxygen mole fractions as listed in Table 2. It is worth noting that the TRI effects are considered for all the TPDF cases.

Table 1. Injection parameters

Fuel temperature	363 K
Fuel density	713 kg/m ³
Ambient density	22.8 kg/m ³
Injection velocity	650.77 m/s
Injection duration	6 ms
Orifice diameter	0.09 mm

Table 2. Ambient conditions at 1500 bar and 22.8 kg/m³ of pressure and ambient density, respectively.

Case	O ₂ (%)	T _{amb} (K)	P _{amb} (MPa)
1	15	900	5.98
2	15	850	5.63
3	15	1000	6.62
4	13	900	6.04
5	21	900	5.91

Radiation Modeling

Radiative Properties and RTE Solution Methods

The RTE is solved with three different methods: the discrete ordinate method (DOM), the spherical-harmonics method (P1 method) and the optically thin method (no absorption). The effect of radiation is included in the energy conservation equation through a heat source term, S_{grad} , expressed as:

$$S_{grad} = (4\sigma\alpha_{total}T^4 - G\alpha_{total}) \quad (1)$$

where the first and second term on right hand side of Eq. (1) represents the radiation emission and absorption, respectively. σ , α_{total} and G are the Stefan-Boltzmann constant, the total mean absorption coefficient and the incident irradiation. In this study, grey gas radiative properties have been assumed, neglecting the spectral dependence of the absorption coefficient. The effect of soot particles as $\alpha_{soot} = 2370 \times f_{v_{soot}} \times T$ [37] as well as the major gas-phase species as function of temperature and their respective partial pressure and mass fractions [38], are included in the total Plank mean absorption coefficient. The radiative properties of liquid fuel droplets in the vicinity of the nozzle (the liquid length is approximately 10 mm but clearly upstream from the high-temperature reactions) have been neglected for simplicity.

For the optically thin method, the radiation absorption is neglected and there is no need to solve the RTE. For the P1 method [39], a transport equation of incident radiation, G , is solved, which is based on the expansion of the radiation intensity into an orthogonal series of spherical harmonics. In the DOM [40, 41], a finite number of solid angles are solved for the RTE with an angular discretization of 4×4 , resulting into 64 directions for the 2D case considered here. Further details of the radiation models can be found in the Fluent theory guide [42].

Turbulence-Radiation Interactions

The RTE is solved at the CFD resolution. With the WM model the radiation emission is directly computed using the cell mean temperature and composition. Here, both effects of TCI and TRI are not considered.

For the TPDF method, the mean radiation emission in a CFD cell is computed as the sum of the radiation emitted by every notional particle present in the CFD cell. In this way, the effect of emission TRI has been included, which is described as a correlation between the Plank-mean absorption coefficient and the fourth power of temperature, i.e. $\langle \alpha_{total} T^4 \rangle = \langle \alpha_{total} \rangle \langle T^4 \rangle + \langle \alpha_{total}' (T^4)' \rangle$. Emission TRI is further decomposed into the temperature and the absorption coefficient self-correlations, which are examined in the next section in Figure 4.

On the other hand, the influence of absorption TRI has been neglected. Absorption TRI appears as a correlation between the incident radiation and the absorption coefficient as, $\langle G \alpha_{total} \rangle = \langle G \rangle \langle \alpha_{total} \rangle + \langle G' \alpha_{total}' \rangle$. For optically thin flames, the fluctuations in the incident radiation and the absorption coefficient (locally) are uncorrelated. At the other extreme, for the optically thick flames, fluctuations in the intensity are large and would be expected to be strongly correlated with the absorption coefficient [11, 12, 15]. For the intermediate optical thickness of the Spray A case, absorption TRI is expected to play a subordinate role.

RESULTS AND DISCUSSION

The results are divided into two parts: first, the effect of turbulence-chemistry interaction is studied by comparing simulation results from the TPDF and the WM model, also the relevance of turbulence-radiation interaction is evaluated by considering the TPDF results. Second, the influence of ambient temperature and oxygen mole fraction on the radiative effect is presented for the WM model. One important note is that the flame reaches a quasi-steady condition in terms of mixing after approximately 3 ms but radiation heat transfer need more time to achieve equilibrium. Therefore, simulations have been run until 4 ms due to the higher response time of radiation for Spray A.

Sensitivity Analysis for the Turbulence-Chemistry Interactions and Turbulence-Radiation Interactions

As the focus of this paper lays on the effect of radiation under Spray A conditions, here only radiation relevant results are presented. For a more comprehensive validation and analysis of current modeling results such as inert and reactive spray tip penetration, ignition delay, flame lift-off length and soot formation, the reader is referred to [30].

Figure 1 depicts the spatial distribution of the three most radiative species (soot, CO₂ and H₂O) in conjunction with their respective Plank mean absorption coefficient obtained using the TPDF model at 4 ms after start of injection. Note that these spatial distributions with the WM model are comparable and minor differences are observed. The black lines represent the stoichiometric mixture fraction. Numbers drawn at the colorbars are the minima and maxima values of the respective quantity. The same approach is used for all other iso-contour figures in this paper.

Concerning the radiative species, soot is present in the fuel rich region downstream from the lift-off location (here 16 mm), as expected. The maximal reported value for the soot volume fraction is 7 ppm and the maximal mean absorption coefficient is 35.5 m⁻¹.

In the ambient gas before start of injection there is a considerable amount of CO₂ ($Y_{CO_2} \sim 0.09$) and H₂O ($Y_{H_2O} \sim 0.03$), which arise from the premixed pre-burn of a C₂H₂-H₂-O₂-N₂ mixture to enable the generation of the targeted ambient pressure, temperature and oxygen mole fraction at the start of injection. The CO₂ mass fraction peaks along the stoichiometric region. In the fuel region, there is a considerable amount of CO, which has not been converted to CO₂ yet. On the other hand, a high concentration of H₂O mass fraction is homogeneously distributed within the entire fuel-rich cross-section. It is observed that the CO₂ mean absorption coefficient is much higher than the one of H₂O and soot, in particular in the fuel lean region. This is due to the increase of the absorption coefficient for lower temperatures. The peak magnitude of α_{CO_2} is 3.7 times higher and 1.4 times lower for α_{H_2O} in comparison with α_{soot} . At Spray A conditions, the radiation effects of gas-phase species are more dominant than the soot radiation.

Figure 2 shows spatial distributions of various quantities related to radiation obtained using the DOM approach in conjunction with two different combustion models: the well-mixed (upper) and the TPDF model (lower). From left to right: temperature, total absorption coefficient (i.e. $\alpha_{soot} + \alpha_{gas-phase}$), radiative absorption and emission rate, net radiation source term (defined as positive for a heat loss) and rate of temperature change induced by radiation ($T_{rate} = S_{grad}/(\rho C_p)$).

Note that results with the P1 radiation model are similar and have been omitted here for brevity.

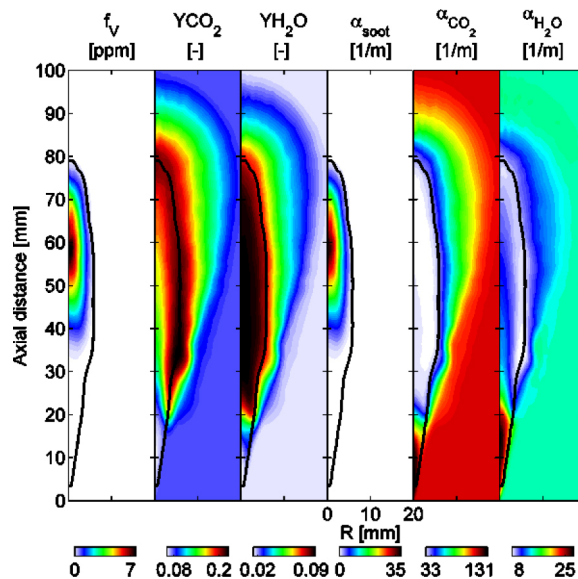


Figure 1. Spatial distribution of flame structure quantities using the TPDF model at 4 ms. From left to right: soot volume fraction (ppm), mass fraction of CO₂, H₂O and their respective mean absorption coefficients, respectively.

The temperature contour shows the overall spread of the flame. The major difference between the two combustion models is the thickness of the reaction zone. A comparatively thin layer has been observed for the WM model in comparison with the TPDF model where the reaction zone is more distributed due to the consideration of turbulent fluctuations within a cell. These observations are consistent with