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Modeling Radiative Heat Transfer and Turbulence-Radiation Interactions in Engines

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Abstract: Detailed radiation modelling in piston engines has received relatively little attention to date. Recently, it is being revisited in light of current trends towards higher operating pressures and higher levels of exhaust-gas recirculation, both of which enhance molecular gas radiation. Advanced high-efficiency engines also are expected to function closer to the limits of stable operation, where even small perturbations to the energy balance can have a large influence on system behavior. Here several different spectral radiation property models and radiative transfer equation (RTE) solvers have been implemented in an OpenFOAM-based engine CFD code, and simulations have been performed for a full-load (peak pressure ~200 bar) heavy-duty diesel engine. Differences in computed temperature fields, NO and soot levels, and wall heat transfer rates are shown for different combinations of spectral models and RTE solvers. The relative importance of molecular gas radiation versus soot radiation is examined. And the influence of turbulence-radiation interactions is determined by comparing results obtained using local mean values of composition and temperature to compute radiative emission and absorption with those obtained using a particle-based transported probability density function method.

Keywords: *Radiation modelling; Turbulence-radiation interactions; Transported probability density function method; Turbulence–chemistry interactions; Compression–ignition engine*

1. Introduction

The importance of accurately accounting for realistic chemical kinetics and turbulence-chemistry interactions in CFD simulations of compression-ignition engines is well established [1]. On the other hand, while it has long been known that radiation can account for a significant fraction of the total heat losses in very large bore, heavy-duty diesel engines [2], conventional wisdom had been that in-cylinder radiation was dominated by soot, and that radiation was of secondary importance in road-vehicle-scale engines (cars and trucks). Few in-cylinder CFD modeling studies have considered radiation heat transfer, and only a subset of those has considered radiatively participating medium effects by solving a radiative transfer equation (RTE) [3-6].

In the meantime, advanced high-efficiency engines that are currently being developed are expected to function close to the limits of stable operation [7], where even small perturbations to the energy balance can have a large influence on global system behavior. The trends toward higher operating pressures and higher levels of exhaust-gas recirculation (EGR) will make molecular gas radiation (absorption coefficient proportional to participating species concentration) more prominent. At the same time, increasing quantitative accuracy is being demanded from CFD-based models for in-cylinder processes, including accurate predictions of heat losses and pollutant emissions. For these reasons, radiative heat transfer under engine-relevant conditions, including the effects of unresolved turbulent fluctuations, has been revisited recently.

Here multiple spectral radiation models and RTE solvers have been implemented to perform coupled simulations (where the radiative source term feeds back to the CFD through the enthalpy equation) for a Volvo truck diesel engine that was the subject of an earlier experimental and modeling study [1]. Preliminary results are presented for a full-load operating condition with EGR, where experimental pressure and heat-release data are available.

2. Physical Models and Numerical Methods

An unsteady Reynolds-averaged formulation has been adopted, with a standard two-equation turbulence model with wall functions, and conventional stochastic-Lagrangian-parcel fuel injection and spray models (using n-heptane liquid fuel properties). A 42-species chemical mechanism (40-species n-heptane [8], plus two additional species for thermal NO) is used to represent the gas-phase chemistry, and a semi-empirical two-equation model is used for soot [9]. Gas-phase chemistry, soot, and radiative emission and absorption are calculated either at the finite-volume cell level using local mean values of composition and temperature (thereby neglecting the influence of turbulent fluctuations: a locally well-stirred-reactor – WSR – model at the finite-volume cell level), or at the notional particle level in a particle-based transported probability density function (PDF) method [10] that accounts for the influences of turbulent fluctuations with respect to local mean values (turbulence-chemistry interactions – TCI – and turbulence-radiation interactions – TRI). With the exception of radiation, the models are essentially the same as those that were used in an earlier modeling study for a heavy-duty diesel engine [1]. There it was shown that the PDF-based model gave better agreement with experimental measurements compared to the WSR model over a range of operating conditions, and that TCI were especially important in the emissions calculations.

An up-to-date review of the theory and applications of radiative heat transfer in turbulent combustion systems can be found in [11]. Here the most recently available spectral radiation properties databases have been used. Radiative properties for molecular gases have been pre-calculated using the HITEMP2010 (CO2, H2O, CO) [12] and HITRAN2008 (CH4, C2H4, etc.) [13] spectral databases for pressures from 0.1 bar to 80 bar, temperatures from 300 K to 3000 K, and for various mole fractions of the participating species. Simple pressure-based scaling is used to extrapolate to higher pressures, where needed. The spectral absorption coefficient for soot is evaluated using the small-particle limit (Rayleigh theory) [14] with the complex index of refraction from [15]; scattering is neglected. Models for participating liquid spray radiation have been developed recently [11], but spray radiation is negligible for the conditions that are of interest here, and the spray radiation models have not been used. From the spectral molecular-gas databases and the presumed soot radiation properties, a hierarchy of spectral models is constructed. These range from full line-by-line (LBL), to narrowband-based and tabulated full-spectrum k-distributions, to gray-gas models with Planck-mean absorption coefficients [14].

Multiple RTE solvers have been implemented to calculate the local radiative intensity in situations where absorption is important. These include the stochastic photon Monte Carlo (PMC) method where no intrinsic assumptions are invoked regarding the directional distribution of radiative intensity, spherical-harmonics methods (SHM), and discrete-ordinates methods (DOM) [11, 14]. In the lowest-order SHM implementation (the P1 method), a single elliptic PDE must be solved. While DOM and variants have probably been used more widely than the others in combustion applications, recent work has shown that SHM methods provide a more favorable tradeoff between computational effort and accuracy as one goes to higher-order implementations [16].

PMC/LBL provides a benchmark against which the performance of simpler RTE solvers and/or spectral models can be compared. When combined with the stochastic Lagrangian particle methods that are used with transported PDF methods for turbulent reacting flows, PMC/LBL has proven to be a powerful approach for computing radiative transfer, including the effects of unresolved turbulent fluctuations in composition and temperature (turbulence-chemistry-soot-radiation interactions) in both Reynolds-averaged [17] and large-eddy simulations [18]. In this paper, preliminary results are presented for a subset of the available combinations of radiation models (Table 1). To separate turbulence-chemistry interaction (TCI) effects from turbulence-radiation interaction (TRI) effects, PDF simulations have been performed using particle-level chemistry and radiation (thereby accounting for both TCI and TRI) and with particle-level chemistry and cell-level radiation (thereby accounting for TCI, while ignoring TRI). Differences between results for WSR/NoRAD and WSR/P1-gray or between PDF/OT/NoTRI and PDF/OT/TRI provide a general impression of the overall importance of radiation. Differences between results for WSR/P1-Gray and WSR/P1-FSK illustrate effects of the spectral radiation model. And differences between PDF/OT/NoTRI and PDF/OT/TRI illustrate effects of TRI.

3. Engine Configuration and Operating Conditions

A simplified model of Volvo 13L production six-cylinder heavy-duty truck engine has been built using OpenFOAM v2.3.x [19], and simulations have been performed for a baseline full-load diesel operating condition with EGR (15.8:1 compression ratio, 1213 r/min, 14.28 bar intake pressure, 561 K intake temperature, 270 mg fuel injected from 4.6° bTDC to 16.8° aTDC, initial O_2, N_2, CO_2 and H_2O mass fraction are 0.1884, 0.7575, 0.392 and 0.149 respectively). A relatively coarse (~45,000 cell) 60-degree sector mesh is centered on one of the six spray plumes, and includes the piston top-ring-land crevice. Simulations begin after intake-valve closure (IVC) with prescribed initial in-cylinder conditions, and end before exhaust-valve opening. A computational time step of 3.4 μs (0.025 CAD) is used, in all cases.

It is important to note that this engine and operating condition were not selected to maximize radiation effects. Previously, the engine was subject of an experimental and modeling study [1], and is thus an appropriate configuration for testing and validating the various radiation models that have been implemented for this investigation. For present purposes, our main interest is to verify that we can match the global engine behavior (e.g., pressure trace) reasonably well for the baseline operating condition, then proceed with systematic parametric studies with the radiation models.

4. Results and Discussion

Computed and measured pressure traces are shown in Fig. 1(a). Computed and measured ignition delays match reasonably well, and as has been noted in earlier modeling studies, the computed burn rate is too fast for the WSR model. Agreement between measured and modeled pressure traces improves with the PDF model, although there is still room for improvement.

Computed total radiative emission and radiative absorption quantities are shown in Table 1 for different combinations of radiation models. At this operating condition the total emission is approximately 50% of boundary-layer heat loss for all radiation models, and total absorption is around 40% of boundary-layer heat loss. On the absorption side, the most significant difference is an approximate 1.5 times increase in computed reabsorption with consideration of a spectral model (FSK) versus a gray model (comparing WSR/P1-Gray and WSR/P1-FSK). The radiative heat loss is on the order of 10% of the boundary-layer heat loss and computed changes in NO and soot emissions with versus without radiation are on the order of 5% (not shown). While global radiation effects are relatively modest for this operating condition, local temperature field changes significantly due to emission and reabsorption. For example, local temperature difference between WSR/NoRad and WSR/P1-gray is as high as 150 K. Hence, similar to diffusion, the net effect of radiative emission and reabsorption is a redistribution of energy.

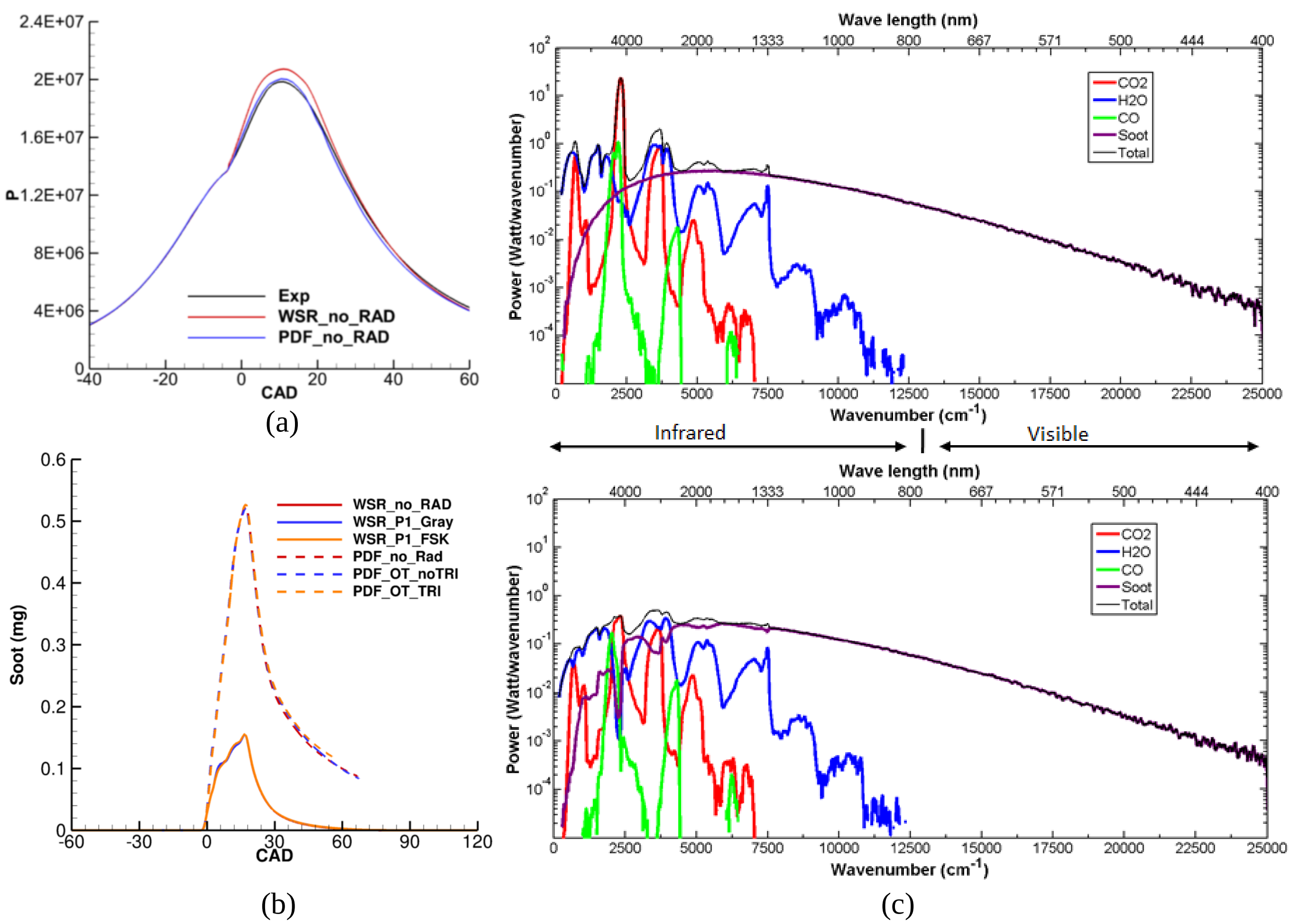

Figure 1: (a) Computed and measured in-cylinder pressure versus crank angle for a baseline operating condition. (b) Computed soot mass variation with crank angle. (c) Spectral analysis of radiation at 10 CAD. Top plot shows energy emitted by CO_2, H_2O, CO and Soot at different wave number. The bottom plot shows energy reached to the wall after absorption for these radiative species and soot.

The top plot of Fig. 1(c) shows spectral emission by radiative species within the domain at 10 CAD. The bottom plot shows the spectral distribution of energy that reaches the wall after reabsorption. The peaks of CO_2, H_2O and CO emission lines (near 2500 cm^{-1} in top plot) disappear due to reabsorption when it reaches the wall (bottom plot). Table 2 and 3 shows emission and reabsorption quantities at 10 CAD with and without considering turbulence-radiation interactions. It is evident from Table 2 that around 5% of CO_2, 40% of H_2O, 17% of CO and 90% of soot emission reaches the wall. These numbers do not vary significantly (~3%) with consideration of turbulence-radiation interactions (Table 3). Soot radiation is more important in terms of radiative heat loss during the initial phase of combustion (5 CAD to 40 CAD in Fig. 1(b)), when a significant amount of soot exists inside the domain. For the rest of the time, radiative heat loss by gas radiation (CO_2, H_2O and CO) dominates over soot.

Table 1: Radiation model combinations and global results for a baseline operating condition with different combinations of radiation models. Boundary-layer wall heat loss, radiative emission, and radiative absorption values are totals from 60° bTDC to 120° aTDC for WSR and 60° bTDC to 60° aTDC for PDF.

WSR or PDF	**RTE solver**	**Spectral model**	**TRI?**	**Model designation**	**BL wall heat loss (J)**	**Radiative emission (J)**	**Re-absorption (J)**	**Radiative heat loss (J)**
WSR	None	None	No	WSR/NoRad	261	0	0	0
WSR	Optically thin	Gray	No	WSR/P1-Gray	258	137	95	42
WSR	P1	FSK	No	WSR/P1-FSK	260	139	121	18
PDF	None	None	No	PDF/NoRad	213	0	0	0
PDF	Optically thin	Gray	No	PDF/OT/NoTRI	212	92	0	92
PDF	Optically thin	Gray	Yes	PDF/OT/TRI	204	84	0	84

Table 2: Species radiation data (Without TRI)

Specie	Emission (Watt)	Reabsorption (Watt)	Reached wall (Watt)
CO_2	4484	4266	218
H_2O	1689	1031	658
CO	245	204	41
Soot	2076	247	1829

Table 3: Species radiation data (With TRI)

Specie	Emission (Watt)	Reabsorption (Watt)	Reached wall (Watt)
CO_2	4605	4384	221
H_2O	1743	1066	687
CO	242	202	40
Soot	2026	254	1772

5. Conclusions

Preliminary coupled-radiation results have been presented for several combinations of radiation models for a heavy-duty compression-ignition engine at a full-load operating condition. Overall, radiation effects are relatively small for this operating condition (in the 5%- 10% range), and the most important influences are from the spectral model that causes notable changes in reabsorption numbers. In terms of radiative heat loss, soot emission dominates over gas radiation during the initial phase of combustion, but in total, heat loss by gas radiation will be more important than soot.

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