International Multidimensional Engine Modeling User's Group Meeting at the SAE Congress
Detroit, MI, 3 April 2017

Soot and Spectral Radiation Modeling in ECN Spray A and in Engines

D.C. Haworth[1], S. Ferreryo-Fernandez[1], C. Paul[1], A. Sircar[1], A. Imren[1], S.P Roy[2], W. Ge[3], M.F. Modest[3]

[1]Department of Mechanical & Nuclear Engineering, The Pennsylvania State University, University Park, PA, USA
[2]Department of Mechanical Engineering, Marquette University, Milwaukee, WI, USA
[3]School of Engineering, University of California, Merced, CA, USA

Abstract: The amount of soot formed in a turbulent combustion system is determined by a complex system of coupled nonlinear chemical and physical processes. Different physical subprocesses can dominate, depending on the hydrodynamic and thermochemical environments. Similarly, the relative importance of reabsorption, spectral radiation properties, and molecular gas radiation versus soot radiation varies with thermochemical conditions, and in ways that are difficult to predict for the highly nonhomogeneous in-cylinder mixtures in engines. Here it is shown that transport and mixing play relatively more important roles as rate-determining processes in soot formation at engine-relevant conditions. It is also shown that molecular gas radiation and spectral radiation properties are important for engine-relevant conditions.

Introduction

Soot modeling for engine-relevant conditions has received considerable attention, because of the importance of soot as a component of particulate matter, a regulated pollutant. However, most soot models are based largely on physical understanding of soot formation derived from experiments at atmospheric pressure or at moderately elevated pressures (usually less than 10 atm) compared to engine-relevant conditions. On the other hand, radiative heat transfer modeling in engines has received relatively little attention, although it is increasingly recognized that it can be important both for energy redistribution within the combustion chamber and as a contributor to heat losses to combustion chamber walls. Conventional wisdom has been that radiation in engines is dominated by soot radiation. However, as operating pressures and exhaust-gas recirculation (EGR) levels in engines increase, molecular gas radiation (primarily from CO_2 and H_2O) and spectral radiation properties become more important. In this paper, it is shown that the relative importance of various physical subprocesses in soot formation and radiative heat transfer can be different at engine-relevant pressures compared to atmospheric pressure. By properly accounting for these differences, more predictive CFD-based models for in-cylinder processes can be developed.

Physical Models and Numerical Methods

Unsteady Reynolds-averaged simulations (URANS) are performed using OpenFOAM-based solvers [1]. The liquid fuel injection and spray evolution are modeled using a stochastic Lagrangian parcel method, turbulence is modeled using a two-equation *k*-ε model with wall functions, skeletal chemical mechanisms are used for gas-phase chemistry, and a semi-empirical two-equation model [2] is used for soot. A new stiff ODE solver [3] has been used to reduce the high computational overhead of the chemistry calculations.

The effects of turbulent fluctuations in species composition, soot quantities, and temperature or enthalpy (turbulence-chemistry interactions – TCI) are accounted for using a Lagrangian-particle-based transported probability density function (tPDF) method [4]. The composition variables are taken to be the mass fractions of the N_S species in the chemical mechanism, the soot model variables (here two), and the mixture-specific absolute enthalpy. Turbulent transport is modeled using a gradient-diffusion assumption, and molecular mixing is modeled using either the interaction-by-exchange-with-the-mean (IEM) or the Euclidean-minimum-spanning-tree (EMST) model. In contrast to IEM, EMST enforces locality of mixing in composition space. To isolate and quantify the importance of TCI, results from the tPDF model are compared with those from a locally well-stirred reactor (WSR) model that neglects the effects of turbulent fluctuations.

Radiative properties for participating molecular gases (primarily (CO_2, H_2O and CO) have been calculated using the HITEMP2010 spectral database [5] for temperatures from 300 K to 3000 K and pressures from 0.1 bar to 80 bar; pressure-based scaling is used to extrapolate to higher pressures. The spectral absorption coefficient for soot is evaluated using the small-particle limit (Rayleigh theory) with the complex index of refraction from [6]; scattering is neglected. From these underlying 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 [7,8]. Multiple RTE solvers have been implemented to calculate the local radiative intensity for conditions where absorption is considered. 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, and discrete-ordinates methods [7,8].

Target Configurations

Examples of soot and radiation modeling results are shown for two configurations: a transient high-pressure turbulent spray flame (ECN Spray A [9]), and a heavy-duty diesel engine [10].

The ECN Spray A experimental configuration is a constant-volume optically accessible cubic combustion vessel. Sprays of n-dodecane are injected using a common-rail diesel fuel injector with a single orifice of nominal diameter 90 μm located at the center of one vessel wall. The initial temperature, pressure, density and O_2 molar concentration in the vessel are 900 K, 60 bar, 22.8 kg/m^3, and 15%. The nominal fuel injection pressure is 150 MPa and the total injection duration is 6 ms. The computational domain is a 2D axisymmetric mesh that represents a 5° section of the vessel. A 54-species n-dodecane mechanism is used for gas-phase chemistry [11].

The engine is a single-cylinder research engine that corresponds to one cylinder of a Volvo13L production six-cylinder heavy-duty truck engine. This is a low-swirl, four-valve, flat-head, bowl-in-piston, direct-injection diesel engine with a compression ratio of 15.8:1 and a six-hole, centrally located high-pressure fuel injector. Experimental data are available for four operating conditions at an engine speed of 1213 r/min. There are two full-load conditions and two part-load conditions, each with two levels of EGR. The gas-exchange processes are not simulated. Simulations begin after intake-valve closure and continue until shortly before exhaust-valve opening. A 60-degree sector mesh is used, centered around one of the six fuel-injector nozzle holes, with cyclic symmetry conditions on the lateral faces. A 42-species chemical mechanism (40-species n-heptane [12] plus two additional species for thermal NO) has been used for the engine simulations.

Results and Discussion

The emphasis is on aspects of soot and radiative heat transfer modeling that are of particular importance at engine-relevant pressures. Examples of soot results are shown first, followed by an example of radiation results.

Soot modeling

An important finding pertains to the differences in the relative importance of different physical processes in soot formation between atmospheric-pressure versus high-pressure turbulent combustion. Compared to atmospheric-pressure flames (where most soot modeling and experimental studies have been done), it has been found that at engine-relevant pressures, computed soot volume fractions are relatively less sensitive to the kinetic rates in the soot models (because the rates are so fast [13]) and are relatively more sensitive to the details of the turbulent combustion modeling (accurate accounting for unresolved turbulent fluctuations in composition and temperature) and turbulent mixing. This does not mean that soot kinetics are unimportant at high pressures. Rather, it means that transport and mixing become relatively more important as rate-controlling process. One must exercise caution to avoid tuning rate coefficients to account for deficiencies in the turbulent combustion modeling. The tPDF method provides a framework that allows these different physical processes to be separated cleanly.

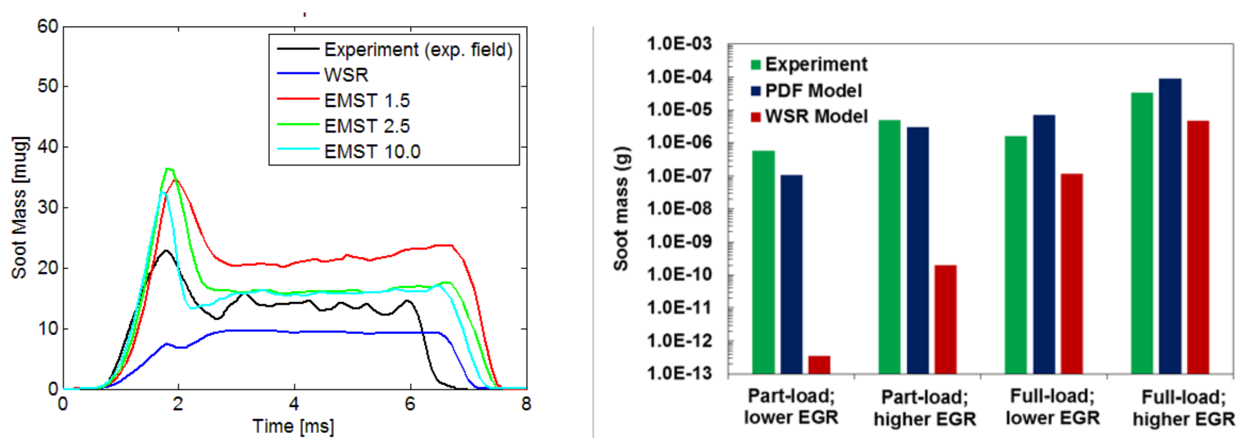

Figure 1: Left: Computed and measured total soot mass in the experimental field of view for ECN Spray A; computed results for WSR and tPDF models are shown, with variations in the EMST mixing model coefficient C_ϕ for the tPDF model. Right: Computed soot and measured PM for a Volvo heavy-duty engine at four different operating conditions [10].

Two examples are shown in Figure 1. The left-hand figure shows the computed and measured total soot mass in the experimental field of view as functions of time for ECN Spray A. Results from a well-stirred reactor (WSR) model that neglects unresolved turbulent fluctuations in composition and temperature are compared with those from a tPDF model that accounts for unresolved turbulent fluctuations, both using the same chemical mechanism and soot model. The tPDF model shows better agreement with experiment, especially in capturing the rapid initial transient rise and drop off in soot before a quasi-stationary state is reached. The computed soot levels are sensitive to the mixing model used (IEM versus EMST – only the latter is shown in the left-hand-side of Figure 1), to the value of the mixing model coefficient C_ϕ that is used, and to whether or not the transported soot variables are mixed at the same rate as the gas-phase species and enthalpy. The effective Schmidt number for soot particles is orders of magnitude higher than for gas-phase species, and this effect can be approximated by not mixing the transported soot variables; that is what has been done in the simulations shown on the left-hand-side of Figure 1. Computed spatial distributions of soot volume fraction are also in much better agreement with experiment for the tPDF model (not shown). This suggests that it is important to account for unresolved turbulent fluctuations, but that the specific spatial/temporal coherence of the fluctuations is not as important (these are unsteady RANS results, not LES).

Similar results have been found in a modeling study of a heavy-duty diesel engine over a range of operating conditions [10]. In that study, with all other aspects of the models being the same, computed engine-out soot levels from a tPDF model were higher (by orders of magnitude, in some cases) than those from a WSR model, and the tPDF results were in much closer agreement with experiment (right-hand-side of Figure 1). The reasons for this extreme sensitivity were elucidated by comparing the WSR-model and tPDF-model flame structures in equivalence-ratio/temperature space [10]. The results demonstrated that turbulence-chemistry interactions are important in compression-ignition engines (especially for soot formation), and that accurate accounting for turbulent fluctuations is at least as important as accurate kinetic rate parameters in the gas-phase chemistry and soot models.

Radiation modeling

Computed power spectra of emitted radiation and radiation reaching the wall are shown at one instant in time during the quasi-stationary flame for ECN Spray A in Figure 2. These spectra are computed by post-processing computed instantaneous fields of gas-phase concentrations, soot and temperature using PMC/LBL. The individual contributions from three molecular gases (CO_2, H_2O and CO) and from soot particles are shown, in addition to the total radiation. Approximately 94% of the radiation that is emitted is reabsorbed before reaching the wall. Radiative emission is dominated by CO_2 (~87% of total emission). However, the system is optically very thick at wavenumbers corresponding to CO_2 emission (especially in the 4 μm band), such that the radiation reaching the wall is dominated by H_2O radiation (~58% of radiation reaching the wall). The contribution of soot radiation to the total radiation reaching the wall is approximately 7%. Experimental measurements of radiation for this flame have been reported in [14]. There the measurements were limited to visible wavelengths of 400-700 nm. As can be seen in Figure 2, this corresponds to a small fraction of the radiation that reaches the wall. The experimentally reported radiant fraction for this flame (percentage of fuel energy reaching the wall as thermal radiation) was 0.068% [14]. The computed total radiant fraction is much higher (approximately 1%), but the computed radiant fraction considering soot radiation alone is less than 0.1%, close to the measured value. This provides some confidence that the model can be used to extrapolate to wavenumbers for which experimental measurements are not available. It also shows that molecular gas radiation is more important than soot radiation for this configuration, and the importance of accounting for spectral radiation properties at engine-relevant conditions.

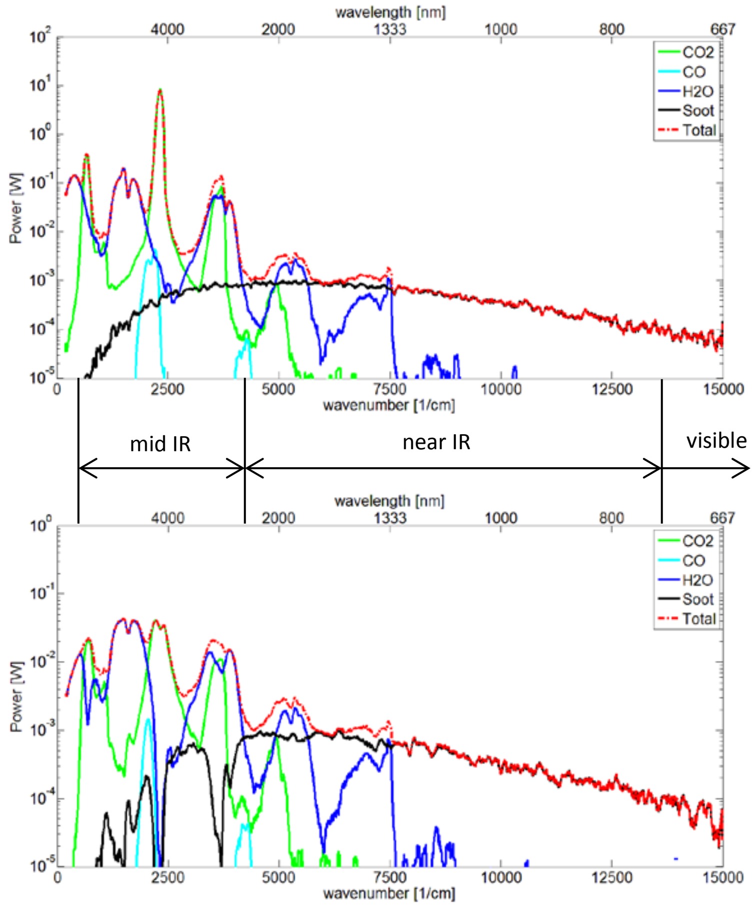

Figure 2: Computed power spectra of emitted radiation (top) and radiation reaching the walls (bottom) for ECN Spray A.

Analyses similar to that shown in Figure 2 have been performed for engines, leading to similar conclusions regarding the importance of spectral radiation properties and molecular gas radiation.

Conclusions

Soot modeling

- As was observed in earlier simulations of laminar flames [13], computed soot volume fractions are less sensitive to variations in the assumed soot kinetics rates at elevated pressures compared to atmospheric pressure. Transport and mixing become relatively more important for soot formation at engine-relevant conditions.
- Comparisons of computed total soot mass and soot spatial distributions from a WSR model and a tPDF model show significant differences, with results from the tPDF model being in

better agreement with experiment. This demonstrates the importance of accurately accounting for the effects of unresolved turbulent fluctuations in soot modeling. At the same time, the fact that an unsteady RANS model captures the observed transient behavior of total soot mass in ECN Spray A suggests that capturing the spatial and temporal coherence of the fluctuations may be less important.

- The tPDF computed soot results are especially sensitive to the modeling of molecular transport (mixing model and mixing rate). A model that enforces locality in composition space (EMST) gives better results that a model that does not (IEM). Accounting for the high effective Schmidt number of soot particles (by not mixing soot variables) also gives better results, compared to mixing all gas-phase species and soot variables at the same rate.

Radiation modeling

- Molecular gas radiation can be at least as important as soot radiation, especially for high operating pressures and/or with EGR.
- It is essential to account for spectral radiation properties when considering radiative transfer at engine-relevant conditions.

Acknowledgements

This research has been funded by the U.S. National Science Foundation through grants CBET-1258613 and CBET-1604446 (Haworth) and CBET-1258635 (Modest). This material also is based upon work supported by the Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE) and the Department of Defense, Tank and Automotive Research, Development, and Engineering Center (TARDEC), under Award Number DE-EE0007278.

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