Title:

Turbulence-chemistry interactions in a heavy-duty compression-ignition engine

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Figure 1: Computed and measured pressure traces for four operating conditions. Two computed profiles are shown: one for the PDF model, and one for the WSR model. (a) Case 1. (b) Case 2. (c) Case 3. (d) Case 4. = 473 words

Figure 2: Computed apparent-heat-release traces for four operating conditions. Two computed

profiles are shown: one for the PDF model, and one for the WSR model. (a) Case 1. (b) Case 2. (c) Case 3. (d) Case 4. = 473 words

Figure 3: Computed mean temperature contours at 7° aTDC for Case 1 (part-load, lower EGR) for two models. = 77 words

Figure 4: Computed mean OH mass-fraction contours at 7° aTDC for Case 1 (part-load, lower EGR) for two models. = 77 words

Figure 5: Computed in-cylinder soot mass versus crank angle for Case 4 (full-load, higher EGR) for the two models. = 143 words

Figure 6: Computed equivalence ratio versus temperature scatter plots at several instants for Case 4 (full-load, higher EGR). Top: PDF model. Bottom: WSR model. = 370 words

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Abstract

The influences of unresolved turbulent fluctuations in composition and temperature (turbulence-chemistry interactions - TCI) on heat release, flame structure, and emissions are explored in unsteady Reynolds-averaged simulations for a heavy-duty diesel engine at four operating conditions. TCI are isolated and quantified by comparing results from a transported probability density function (PDF) method with those from a model that neglects the influence of fluctuations on local mean reaction rates (a well-stirred-reactor - WSR - model), with all other aspects of the modeling being the same (e.g., spray model, gas-phase chemical mechanism, and soot model). The simulations feature standard fuel-spray and turbulence models, skeletal-level gas-phase chemistry, and a semi-empirical two-equation soot model. Computed pressure and heat-release traces, turbulent flame structure, and emissions from the WSR and PDF models show marked differences, with the PDF-model results being in closer agreement with experiment in most cases. The soot results are especially striking. Computed soot levels from the PDF model are within a factor of five of the measured engine-out particulate matter, and computed soot levels from the WSR and PDF models differ by up to several orders of magnitude, with the PDF-model results being in much closer agreement with experiment. The results show that TCI are important in compression-ignition engines, 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.

Keywords:

Transported probability density function method, turbulence-chemistry interactions, compression-ignition engine, soot emissions

1. Introduction

Energy conversion via turbulent combustion processes is expected to remain an important part of the global energy portfolio for the foreseeable future, and there is continuing pressure to reduce fuel consumption and pollutant emissions from combustion systems. In the United States and elsewhere, compression-ignition reciprocating-piston engines dominate in heavy-duty road vehicle (truck) applications. Recently the U.S. Department of Transportation and the Environmental Protection Agency established the first fuel efficiency and greenhouse-gas emissions standards for heavy-duty trucks in the U.S. [1], and the U.S. Department of Energy launched the “SuperTruck” initiative with the goal of improving the fuel economy of heavy-duty trucks [2].

In conventional diesel combustion, the flame structure is dominated by a lifted nonpremixed turbulent jet flame that is fed by the vaporizing liquid fuel jet [3]. In contrast, several advanced compression-ignition-engine combustion systems have been proposed recently that have the potential to simultaneously lower fuel consumption and engine-out emissions [3, 4]. Compared to conventional diesel combustion, advanced combustion strategies can feature higher pressures, lower temperatures, varying degrees of fuel/air premixing, higher levels of exhaust-gas recirculation (EGR), and/or multiple fuels, and the flame structure can include significant volumetric burning and flame propagation in addition to mixing-controlled burning. Advanced engines are expected to operate closer to the limits of stable operation, where even small local fluctuations in in-cylinder flow or thermochemical state can significantly influence ignition timing and emissions. Under these conditions, highly nonlinear couplings between turbulent fluctuations and reaction-rate chemistry (turbulence-chemistry interactions – TCI) are expected to be more important compared to the relatively robust combustion environment in a conventional diesel engine.

In most computational fluid dynamics (CFD) modeling studies of in-cylinder combustion processes in compression-ignition engines, the influence of unresolved turbulent fluctuations on local mean (in the case of Reynolds-averaged simulations) or spatially filtered (in the case of large-eddy

simulations) reaction rates have been largely ignored, or have been treated using simple models. For example, a locally well-stirred-reactor (WSR) model often has been used, where the local mean/filtered reaction rates are computed directly using the local mean/filtered composition and temperature, thereby neglecting TCI altogether. A few studies have demonstrated the importance of TCI in compression-ignition engines, or under engine-relevant conditions, by comparing results from a WSR model with those from a model that explicitly accounts for effects of unresolved turbulent fluctuations in composition and temperature using a transported composition probability density function (PDF) method [5–10], with all other aspects of the modeling being identical (e.g., fuel-spray model, chemical mechanism, soot model). Here we extend this practice to quantify the influence of unresolved turbulent fluctuations on global combustion system behavior (pressure and heat-release traces, turbulent flame structure, and emissions) in a practical heavy-duty engine. This is done in the context of a particular turbulent combustion model, but that is inevitable for a real engine, and the PDF method is a particularly good turbulent combustion model, as has been amply shown in the references cited above.

Here simulation results are compared with experimental data for four conventional diesel operating conditions (part-load and full-load operation, and different EGR levels). The primary objective is to isolate and quantify the effects of TCI on heat release, turbulent flame structure, and emissions (especially soot), by comparing results from a WSR model with those from a PDF model. A second objective is to validate a high-fidelity turbulent combustion model for conditions that correspond to conventional diesel combustion, as a step toward simulating advanced compression-ignition combustion modes where TCI are expected to be even more important.

2. Engine configuration and operating conditions

The configuration is a single-cylinder research engine that corresponds to one cylinder of a Volvo 13L production six-cylinder heavy-duty truck engine. This is a low-swirl (~ 0.3 swirl ratio), 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. Simulations and experiment are compared for four operating conditions at an engine speed of 1,213 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 at 60° before top dead center (bTDC), and continue until 120° aTDC (before exhaust-valve opening). The assumed initially homogeneous in-cylinder conditions are summarized in Table 1. EGR is modeled by modifying the initial composition to include appropriate mass fractions of CO₂, H₂O, O₂ and N₂.

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. Constant wall temperatures of 400 K are assumed. A deforming/moving grid is used, where layers of cells are periodically added or removed to accommodate the piston motion. The mesh has a maximum of 295,770 cells at bottom dead center and a minimum of 94,770 cells at TDC.

3. Physical models and numerical methods

An unsteady Reynolds-averaged formulation is adopted, and a standard two-equation high-Reynolds-number $k - \varepsilon$ turbulence model is used [11, 12], with wall functions. The liquid fuel spray is modeled using a conventional stochastic Lagrangian parcel method, where the liquid mass is represented using statistical parcels, and each parcel represents a group of droplets having the same properties. Following the usual practice for high-pressure diesel sprays, no explicit primary breakup model has been used. The fuel-injection and spray models are the same as those that were used in an earlier modeling study of high-pressure turbulent spray flames in constant-volume chambers under engine-relevant conditions [10].

The fuel used in the experiments was a standard diesel fuel, while gas-phase chemistry is modeled using a 40-species skeletal n-heptane mechanism [13]. n-Heptane has a cetane number of approximately 56, which is close to that of diesel fuels. Moreover, n-heptane exhibits a two-stage ignition process that is similar to that of real fuels under typical diesel engine conditions. This chemical

mechanism has been used in previous CFD modeling studies of n-heptane spray flames [10] and diesel engines [5]. To account for the differences in heating values between n-heptane (44.93 MJ/kg [14]) and the diesel fuel used in the experiments (42.9 MJ/kg), the mass of n-heptane injected in the simulations was adjusted to maintain the same fuel energy as in the experiments, and the injection-model parameters were adjusted to maintain the same momentum flux of fuel as in the experiments.

Additional models are added for emissions. Carbon monoxide (CO) and unburned hydrocarbons (UHC) are taken directly from the 40-species mechanism, while additional reactions were added for NOx and soot. For the conditions of interest here, thermal NO is expected to be the principal pathway for NOx formation, and this is modeled using the extended Zel'dovich mechanism [15]. This requires two additional transported species beyond those in the 40-species mechanism (N and NO), and the addition of three additional reactions. For soot, a semi-empirical two-equation model from the literature [16] has been implemented. This model accounts for acetylene-based particle inception and surface growth, oxidation by O₂, and particle collisions that result in larger particles. The soot model requires two additional transported variables: soot mass fraction, and soot particle number density.

A modeled transport equation for the joint PDF of the mass fractions of the 42 gas-phase species, the two soot variables, and mixture specific enthalpy is solved to account for turbulent fluctuations in composition and temperature. A consistent hybrid Lagrangian particle/Eulerian mesh algorithm is used [17, 18], where a system of notional particles is introduced whose positions and compositions evolve in time in a manner such that their one-point, one-time Eulerian PDF is the same as that of the real fluid system. Turbulent transport is modeled using a gradient transport model, and molecular transport is modeled using the interaction-by-exchange-with-the-mean (IEM) mixing model, where the value of the mixing model coefficient, C_ϕ , is taken to be $C_\phi = 2.0$, based on previous studies [10]. Compared to the PDF simulations reported in [10], the particle-based solution algorithms have been extended here to deal with deforming meshes, cell-layer addition/removal, and situations where a finite-volume cell face is shared by more than two finite-volume cells.

The models have been implemented in a commercial CFD code, STAR-CD v4.20 [19]. Second-order spatial discretizations are used on the finite-volume side, with a time-implicit PISO-based [20] segregated solver. The PDF method has been implemented via user coding. Simulations are carried out in parallel using up to 30 cores, using domain decomposition. The computational time step corresponds to 0.03125 crank-angle degrees of rotation, and 40 new spray parcels are injected on every computational time step during fuel injection. For the PDF method, the nominal number of particles per finite-volume cell is 30, based on results from previous studies [10, 21].

4. Results and discussion

Results from the PDF and WSR models are compared for four operating conditions, and model results are compared with experimental measurements.

4.1. Pressure, heat release, and flame structure

Figure 1 shows comparisons of mean in-cylinder pressure traces from the two models (PDF and WSR) and experimental data for the four operating conditions. Results from the two models are quite different, with the PDF model being in better agreement with experiment. The differences in the pressure traces are amplified in the apparent-heat-release traces of Fig. 2. The apparent heat release is computed from the pressure using a zero-dimensional model that involves the time derivative of the pressure trace (Eq. [10.6] in [22]). Because the PDF model accounts for a distribution of possible thermochemical states about the local mean state, it tends to broaden the heat release in time. The WSR model burns too fast, resulting in higher peak pressures and higher peak heat-release rates compared to the PDF model and to experiment. This is consistent with the findings for high-pressure constant-volume turbulent spray combustion in [10], and shows that those findings carry over to a real heavy-duty compression-ignition engine.

Significant differences also are evident in the computed flame structures between the two models. Figures 3 and 4 show the computed mean temperature and the mean OH mass fraction contours

at 7° aTDC on a cutting plane that contains the spray axis for the part-load case with lower EGR. The computed peak mean temperatures and OH levels are lower for the PDF model compared to the WSR model, and the PDF model produces a broader turbulent flame brush that is more consistent with what one would expect for a highly turbulent spray flame. This is again consistent with observations that were made in earlier constant-volume work [10].

4.2. Emissions

Computed and measured emissions are compared in Table 2. There the measurements are engine-out values, while the PDF and WSR model values are in-cylinder values immediately before exhaust-valve opening. By that time, the chemistry is essentially “frozen,” and the computed values are no longer changing significantly; that is shown below for soot. The reported UHC values correspond to the sum of all hydrocarbon species in the chemical mechanism. No measurements are available for CO or UHC.

Several observations can be made from Table 2. The relative importance of TCI (differences between results from the PDF and WSR models) is different for each pollutant, and varies with operating condition. For CO, PDF-model values are similar to WSR-model values for the part-load cases but they differ by a factor of two-to-four for the full-load cases. For UHC, differences between the two models are small for the part-load cases, but are large (one-to-two orders of magnitude difference) for the full-load cases. Quenching in the piston top-ring-land crevice (which has been included in the CFD model) is known to contribute to CO and UHC emissions. However, in the absence of experimental measurements, no deeper analysis has been attempted. For NO_x, PDF-model values are consistently lower than WSR-model values, by as much as a factor of 1.7 at part load. Both models follow the measured NO_x trends with variations in operating conditions; WSR-model results tend to be closer to experiment at part-load, while PDF-model results are closer to experiment at full-load. NO_x-formation pathways other than thermal NO may come into play at part load [23], where the overall mixture is leaner compared to full-load conditions.

Particulate emissions from engines are of particular concern, and differences between computed soot levels from the WSR and PDF models are especially striking. For these reasons, we focus on gaining deeper insight into the soot results in the remainder of this section. The PDF-model soot results are within a factor of five of the experimental particulate matter values for all operating conditions. This degree of quantitative agreement with experiment may be somewhat fortuitous, given that the experimental values are for particulate matter (of which soot is one component), the uncertainties in engine particulate measurements are large, and a very simple soot model has been used. The more important observation is that the computed soot levels from the two models differ by as much as several orders of magnitude, with the values from the PDF model being higher and in closer agreement with experiment. The reasons for the differences are explored in Figs. 5 and 6, where results are shown for the highest soot case (full load, higher EGR). In a diesel engine, most of the soot that is formed is oxidized prior to exhaust-valve opening (Fig. 5). The PDF model generates more soot than the WSR model, and a smaller fraction of the soot that is formed oxidizes prior to exhaust-valve opening. Figure 5 also justifies the comparison between pre-exhaust-valve-opening in-cylinder values and exhaust values, since the computed soot mass has leveled out by the end of the simulations. Scatter plots of equivalence ratio versus temperature from the two models (Fig. 6) reveal that a wider range of thermochemical states is accessed by the PDF model. In particular, a larger fraction of the in-cylinder mixture experiences thermochemical states that are conducive to soot formation (high equivalence ratio and high temperature) at a time that corresponds to the maximum rate of soot production ($\sim 367^\circ$) for the PDF model compared to the WSR model. Soot formation ends abruptly after the end of injection ($\sim 377^\circ$) for the WSR model (which burns too fast, as shown earlier) and soot oxidation takes over almost immediately, whereas soot continues to be formed by the PDF model well after the end of injection, and soot oxidation begins later. Similar behavior is found for the other operating conditions. Animations of the equivalence ratio-temperature scatter plots for all four cases are provided in the Supplemental Material.

5. Conclusions

Simulations of auto-ignition, combustion and emissions have been performed for a heavy-duty diesel engine at four operating conditions. A skeletal n-heptane chemical mechanism has been used to represent the gas-phase chemistry, and a semi-empirical two-equation soot model has been implemented. For each operating condition, results from a turbulent combustion model that accounts for turbulence-chemistry interactions using a transported PDF method have been compared with those from a model that neglects TCI (a well-stirred-reactor model) to determine the extent to which turbulent fluctuations in composition and temperature influence heat release, turbulent flame structure, and emissions. No model “tuning” has been performed, and standard values have been used for all model coefficients. There are marked differences in pressure traces, heat-release profiles, turbulent flame structures, and emissions between the two models. Differences in computed pressure and heat-release traces from the WSR and PDF models are more prominent at part load, but the differences in pressure are evident for all four cases (Fig. 1); the PDF-model pressure traces are in uniformly better agreement with experiment, while the WSR model yields overly fast combustion. Computed emissions levels are especially sensitive to the TCI treatment. In particular, the soot levels from the WSR and PDF model differ by several orders of magnitude in some cases, with PDF-model soot levels being within a factor of five of the experimental particulate matter measurements for all four operating conditions.

The results show that turbulent fluctuations in composition and temperature affect heat release and emissions even for conventional diesel combustion; they are expected to be even more important for advanced compression-ignition combustion modes that function close to the limits of stable operation [10]. When turbulence-chemistry interactions are accounted for properly, standard fuel-spray, gas-phase chemistry, and soot models yield good agreement with experiment for the four operating conditions that have been explored here, without model tuning. This does not imply that the simple soot model that has been used here will be sufficient for all engine conditions, but

it does suggest that accurate accounting for turbulent fluctuations in composition and temperature is at least as important as accurate kinetic rate parameters in the soot model.

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Table 1: Initial conditions and fuel-injection parameters corresponding to four operating conditions.

		Case 1	Case 2	Case 3	Case 4
Load		Part-load	Part-load	Full-load	Full-load
EGR		Lower	Higher	Lower	Higher
Pressure (bar)		5.65	5.61	14.28	14.25
Temperature (K)		540.9	547.2	560.9	563.2
Initial composition (% mass)	O ₂	18.68	16.51	18.84	17.89
	N ₂	75.72	75.26	75.75	75.55
	CO ₂	4.06	5.96	3.92	4.75
	H ₂ O	1.54	2.27	1.49	1.81
Start of injection (360°=TDC)		357.2°	357.2°	355.4°	355.3°
End of injection (360°=TDC)		363.5°	363.5°	376.8°	377.8°
Mass of fuel injected (g)		0.013	0.013	0.045	0.047

Table 2: Computed and measured (where available) emissions.

Case	Model or Exp.	NOx [ppm]	Soot [g]	CO [g]	UHC [g]
Part-load, lower EGR	WSR	429.3	3.6e-13	3.7e-06	2.5e-06
	PDF	283.2	1.1e-07	2.7e-06	1.0e-06
	Exp.	365.1	5.8e-07	–	–
Part-load, higher EGR	WSR	122.5	2.0e-10	4.6e-06	3.0e-06
	PDF	71.8	3.0e-06	3.6e-06	1.1e-06
	Exp.	119.5	4.9e-06	–	–
Full-load, lower EGR	WSR	674.5	1.2e-07	6.7e-06	3.8e-07
	PDF	505.6	7.2e-06	2.4e-05	4.0e-08
	Exp.	535.1	1.6e-06	–	–
Full-load, higher EGR	WSR	382.2	4.7e-06	3.1e-04	2.3e-07
	PDF	289.9	9.0e-05	7.2e-04	1.2e-05
	Exp.	255.0	3.4e-05	–	–

Figure 1: Computed and measured pressure traces for four operating conditions. Two computed profiles are shown: one for the PDF model, and one for the WSR model. (a) Case 1. (b) Case 2. (c) Case 3. (d) Case 4.

Figure 2: Computed apparent-heat-release traces for four operating conditions. Two computed profiles are shown: one for the PDF model, and one for the WSR model. (a) Case 1. (b) Case 2. (c) Case 3. (d) Case 4.

Figure 3: Computed mean temperature contours at 7° aTDC for Case 1 (part-load, lower EGR) for two models. Left: WSR model. Right: PDF model.

Figure 4: Computed mean OH mass-fraction contours at 7° aTDC for Case 1 (part-load, lower EGR) for two models. Left: WSR model. Right: PDF model.

Figure 5: Computed in-cylinder soot mass versus crank angle for Case 4 (full-load, higher EGR) for the two models.

Figure 6: Computed equivalence ratio versus temperature scatter plots at several instants for Case 4 (full-load, higher EGR). Top: PDF model. Bottom: WSR model.

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