

Numerical Study of Multi-Component Spray Combustion with a Discrete Multi-Component Fuel Model

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Abstract

A numerical investigation of fuel composition effects on spray combustions is presented. A new discrete multi-component (DMC) fuel model was used to represent the properties and composition of multi-component fuels. A multi-dimensional CFD code, KIVA-ERC-Chemkin, that is coupled with improved sub-models and the Chemkin library, was employed for the simulations. A large-bore, optically accessible, DI diesel engine operating in a low temperature combustion (LTC) regime was simulated with primary reference fuels for validation of the fuel models. Then, a small-bore, high-speed DI diesel engine operating in a low temperature combustion (LTC) regime was simulated with two different diesel fuels using a 6-component fuel model. The oxidation chemistry was calculated using a reduced mechanism for primary reference fuel, with the reaction rate coefficients adjusted to account for the Cetane number (CN) variation of the fuels of interest. The major property differences of the fuels include volatility, viscosity, and autoignitability. The predicted pressure and heat release rate are compared with experimental data available in the literature. The results show that the present multi-component fuel model performs reliably, and captures the effects of fuel composition differences on combustion.

Introduction

In most multi-dimensional models of internal combustion engines the fuel is represented for simplicity as a single-component fuel. However, single-component fuel models are not able to predict the complex behavior of the vaporization of practical fuels, such as gasoline and diesel. The preferential vaporization of light-end components in these multi-component fuels affects greatly the fuel distribution near the spray and cannot be represented adequately with a single-component [1-3].

Studies have been performed on the vaporization of multi-component fuels [1-6]. Multi-component fuel models are classified into two types, i.e., discrete multi-component (DMC) models and continuous multi-component (CMC) models. The continuous multi-component model, which is based on the continuous thermodynamics method [4], represents the fuel composition as a continuous distribution function with respect to an appropriate parameter such as molecular weight. This enables a reduction of computational load while maintaining the predictability of the complex behavior of the vaporization of multi-component fuels. However, when this model is applied to combustion simulations, especially with detailed chemistry, describing the multi-component features of the fuel is inevitably limited, making it difficult to model the consumption of individual components appropriately.

On the contrary, the DMC approach tracks the individual components of the fuel during the evaporation process and allows coupling with the reaction kinetics of the individual fuel components. Although the DMC approach can have a high computational overhead due to the additional transport equations that must be solved when it is used for fuels with a large number of components, it is becoming more affordable as computational capacity and numerical solution techniques have improved substantially.

In order to simulate spray vaporization in engine combustion, a robust model that is applicable in a wide range of operating temperatures and pressures, including normal, boiling and trans-critical evaporation regimes, is desirable. Ra and Reitz [3] developed a robust multi-component evaporation model that is applicable to both normal and boiling vaporization modes using a discrete composition distribution of the fuel. The model was applied to simulate evaporation under various drop interior, surface and surrounding gas temperature scenarios. In the model, the physical mechanism of droplet heating/cooling was treated as heat transfer from the surface/interior to the interior/surface of the droplet that is at different temperatures.

One of the crucial characteristics of fuels considered in diesel engines is autoignitability, which depends on the detailed chemical composition of the fuel, as well as the evolution of the thermal and compositional state of the

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charge mixture. Risberg et al. [7] tested diesel fuels of different Cetane number (CN) and volatility characteristics in an engine and showed that the CN describes the autoignition quality of diesel-like fuels in homogeneous charge compression ignition (HCCI) combustion. Kalghatgi et al. [8,9] and Weall and Collings [10] also reported that change of CN and the volatility of fuels via composition variation can significantly reduce smoke emissions at higher operating loads with no detriment to NO_x, CO, HC and fuel consumption.

In the present study a numerical investigation of fuel composition effects on diesel engine combustion is presented. A discrete multi-component (DMC) fuel model is applied to represent the properties and composition of multi-component diesel fuels that are directly injected into the combustion chamber under low temperature combustion (LTC) conditions. A multi-dimensional CFD code, KIVA-ERC-Chemkin, that is coupled with improved sub-models and the Chemkin library [11], was employed for the simulations.

A large-bore, optically accessible, DI diesel engine operating in a low temperature combustion (LTC) regime was simulated with primary reference fuels for validation of the fuel models. Then a small-bore, high-speed DI diesel engine operating in the LTC regime was simulated with two different diesel fuels using a 6-component fuel model. The oxidation chemistry was calculated using a reduced mechanism for primary reference fuel, with the reaction rate coefficients adjusted to account for the CN variation of the fuels of interest. The major property differences of the fuels include volatility, viscosity, and autoignitability. The predicted pressures and heat release rates are compared with experimental data available in the literature.

Numerical Approach

Physical sub-models

For simulating the spray processes and the mixing and combustion of fuel/air mixtures in the cylinder, various physical sub-models were employed in the KIVA-ERC-CHEMKIN code, which is based on KIVA3V Release 2 [12] coupled with the CHEMKIN II library [11]. The sub models include those related to drop breakup [13], collision and coalescence [12], drop deformation [14], drop evaporation [3], wall impingement and vaporization [15, 3], etc.

The droplet vaporization model considers the evaporation of spray droplets using the Discrete Multi-Component (DMC) approach under temperatures ranging from flash-boiling conditions to normal evaporation. The improved model accounts for variable internal droplet temperatures, and considers an unsteady internal heat flux with internal circulation, and a model for the determination of the droplet surface temperature. For a detailed description of the model, refer to Ref. [3]. For the turbulence calculation, the RNG k- ϵ model [16] was used.

Combustion models

In the present study the reaction mechanism developed by Ra and Reitz [17] was used to calculate ignition/combustion of the fuels. To account for the variation of CN of the diesel fuels of interest, the reaction rate constants of the n-heptane oxidation branch of the PRF mechanism were adjusted, since the CN range of the fuels considered in this study is greater than that of pure n-heptane. For the calculation of NO_x formation, a 4 species (N, NO, N₂O and NO₂) and 12 reaction NO_x mechanism was used that was reduced from the GRI NO_x mechanism [18] and added to the PRF reaction mechanism. A phenomenological soot model [19] was employed to predict soot emissions.

Surrogate fuel composition model

In order to investigate the effects of fuel properties, two different diesel fuels were considered, featuring differences in volatility, and CN [20], as shown in **Table 1**. Of the two fuels, Fuel-A has the higher volatility, and Fuel-B has the higher CN.

To model the fuel composition 6 hydrocarbon species (C₇H₈ (toluene), C₁₀H₂₂, C₁₂H₂₆, C₁₄H₃₀, C₁₆H₃₂, C₁₈H₃₄) were considered whose molecular weights range from 92 to 254 g/mol. By altering the proportion of the components, the physical properties and vaporization characteristics were adjusted to match those of the target fuels. The composition of each modeled fuel was determined to match the measured distillation curves of Butts [20]. The measured and predicted distillation curves of the four diesel fuels are shown in Fig. 1. The predicted distillation characteristics of fuels A and B are in good agreement with the measured data, except for the late phase of evaporation of Fuel-B, where the vaporization is over-predicted. This indicates that more heavy-end, lower volatility components could be considered in the Fuel-B model for better agreement. It is clearly seen that the volatility of Fuel-B is much higher than Fuel-A.

In addition to the vaporization characteristics, the density, viscosity and lower heating value (LHV) of the modeled fuels were also matched with the measured data of Butts [20]. The selection of density and viscosity as matching properties was based on the findings of Ra et al. [21] that numerical simulations of spray combustion are most

sensitive to those two properties. Other thermal and transport properties of the liquid phase, and the properties of the fuel vapor-air mixtures were calculated based on the gas phase properties of the individual fuel components. The compositions and average molecular weight of the two model fuels are listed in **Table 2**.

Adjustment of reaction rate constants for CN variation

The combustion processes were modeled using a single surrogate fuel chemistry model (n-heptane oxidation). Therefore, the reaction rate constants of a selected reaction were adjusted to account for the different CN fuels. The ignition times of a reference case (injection timing -33° after top dead center (ATDC)) were compared with experimental data and the reaction rate constants were adjusted, using the methodology of Ra and Reitz [17]. The reaction and its rate constants that were adjusted are listed in **Table 3**, along with the rate constant of the original mechanism.

Computational conditions

In order to validate the performance of the present multi-component spray combustion model, well-defined late-injection compression-ignition experimental results measured in a single-cylinder, direct-injection, optically accessible heavy-duty diesel engine were used [22]. In the experiments, the equivalence ratio distributions as well as the profiles of the cylinder gas pressure and heat release rate of PRF29 fuel (29% iso-octane and 71% n-heptane) combustion were compared for an injector with a spray included angle of 152° . Detailed specifications of the engine are given in Ref. [22]. Then, a small-bore light-duty diesel engine with a compression ratio of 16.5 [23] was used for the combustion simulations of the two diesel fuels. A 7-hole injector with an included spray angle of 155° was modeled. Injection timings were set to -33° atdc for single injections to simulate early injection PCCI, and the initial conditions were obtained from the measured data of Butts [20] who provides detailed specifications of the engine, injector and operating conditions.

Three dimensional computational grids with the piston-liner crevice volume resolved as an elongated top land region were employed. To save computation load, a $1/8^{\text{th}}$ ($1/7^{\text{th}}$) sector of the full 360 degree mesh with periodic boundaries (corresponding to one plume from the eight (seven)-hole injector nozzle) was used for the large (small)-bore engine, respectively. The average cell dimensions were 1.2 to 1.8 mm and 0.6 to 4.1 mm in the radial and vertical directions, respectively, with twenty cells azimuthally.

Results and Discussion

Figure 2a shows a comparison of the equivalence ratio distributions of PRF29 spray injections between the predictions and measurements at a crank angle of 12 degrees after top dead center. The measurements were made in horizontal planes at three different distances (7, 12, and 18 mm) below the fire deck. The simulated fuel distributions agree well with the measured distributions, which indicates that the performance of the present spray model is well validated.

Profiles of pressure and heat release rate of the PRF29 fuel combustion are plotted in Fig. 2b along with the experimental measurements. The simulation successfully predicts both the pressure and heat release rate profiles of the experiments. The heat release during the cool flame period is overpredicted slightly. This may be due, in part, to minor differences between the predicted and measured mixture distributions seen in Fig. 2a.

The combustion predictions of the two diesel fuels were also compared with the experimental results of Butts [20] in Fig. 3. The SOIC was -33° atdc for all cases, which corresponds to the minimum UHC/CO emissions injection timing reported by Opat et al. [23]. The predicted pressure profiles are in good agreement with the experimental results in both cases. As can be expected from the difference in the CN of the fuels, Fuel-B (CN=59) has an earlier main ignition time (or 50% accumulated heat release point) than Fuel-A (CN=45). The start of cool flame timing was predicted to be earlier than the experiments for both cases, which indicates that further improvement of the reaction kinetics considering the components of the fuel would be desirable.

Since Fuel-A is more volatile (see Fig. 1), the vaporized fuel amount before the start of cool flame stage ($\sim 16^\circ$ atdc), is higher. The effects of differences in physical properties and CN is reflected in the in-cylinder mixture conditions. Figure 4 compares the predicted distributions of spray droplets, local average molecular weight of fuel vapor, local equivalence ratio and gas temperature in the combustion chamber for the two model fuels. The local average molecular weight was calculated from the fuel vapor components. The equivalence ratio was calculated considering all species that contain both hydrogen and carbon atoms, including carbon-monoxide, hydrogen and hydrogen peroxide.

It is seen in Fig. 4 (a) that the spray droplets impinge on the cylinder bowl-lip wall and are re-directed into the cylinder bowl and squish regions. Slight differences of size and location of the spray droplets between the two fuel cases are seen, especially in the middle of the spray plumes. Due to preferential vaporization of the spray droplets, in particular, near the upstream region of the spray plumes, the average molecular weight of the fuel vapor is signifi-

cantly lower than that in the cylinder bowl bottom and squish regions where the heavy-end components are found predominantly.

Note that a significant portion of the fuel vapor is vaporized from wall film fuel, which consists of more heavy-end components than in the initial injected fuel since the light-end components are mostly vaporized before wall impingement. The local composition of the fuel vapor influences the oxidation reaction kinetics of the local charge. It is also interesting that the extent of stratification is dependent on the volatility of the fuel. It is clearly seen from Fig. 4 (b) that Fuel-A has larger stratification in the average molecular weight distribution than Fuel-B.

The distribution of local equivalence ratios of the gas mixtures are similar, as shown in Fig. 4 (c). However, oxidation reactions occur faster in Fuel-B than in Fuel-A, according to the order of the CN of the fuels, and this can be seen by comparing the areas of the high temperature regions shown in Fig. 4 (d).

Conclusions

A discrete multi-component (DMC) fuel model was used to represent the properties and composition of multi-component diesel fuels with specially designed compositions to study the effects of fuel properties on low temperature diesel combustion. The two different diesel fuels were modeled using a 6-component fuel model. Based on the results, the following conclusions are drawn.

1. The results show that the present discrete multi-component fuel model performs reliably, and can describe the effects of fuel composition differences on combustion.
2. Using the present multi-component model, information about the local in-cylinder distributions of fuel vapor composition were successfully obtained.
3. The effect of differences in the CN of the fuels on ignition timing was modeled well by adjustment of the reaction rate constants of a selected (low temperature ketoperoxide formation) reaction step.

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References

1. Ra, Y., and Reitz, R.D., *Int. J. of Engine Research* 4:193-218 (2003).
2. Ra, Y., and Reitz, R.D., *Journal of Engineering for Gas Turbines & Power* 126:422-428 (2004).
3. Ra, Y. and Reitz, R.D., *Int. J. Multiphase Flow* 35:101-117 (2008).
4. Tamim, J., and Hallett, W.L.H., *Chem. Engr Sci.* 50:2933- 2942 (1995).
5. Lippert, A.M., and Reitz, R.D., SAE Paper 972882, 1997.
6. Zhu, G.-S., and Reitz, R.D., *Int. J. Heat Mass Transfer* 45:495- 507 (2002).
7. Risberg, P., Kalghatgi, G., Ångström H-E, and Wåhlin, F., SAE 2005-01-2127, 2005.
8. Kalghatgi, G. T., Risberg, P., and Ångström, H-E., SAE Paper 2006-01-3385, 2006.
9. Kalghatgi, G. T., Risberg, P., and Ångström, H-E., SAE Paper 2007-01-0006, 2007.
10. Weall, A.J. and Collings, N., SAE Paper 2007-01-4058, 2007.
11. Kee, R.J., Rupley, F.M., and Miller, J.A., "CHEMKIN-II: A FORTRAN Chemical Kinetics Package for the Analysis of Gas Phase Chemical Kinetics," Sandia Report SAND 89-8009, 1989.
12. Amsden, A.A., KIVA-3V, Release 2, improvements to KIVA-3V. LA-UR-99-915, 1999.
13. Beale, J.C., and Reitz, R.D., *Atomization and Sprays* 9:623-650 (1999).
14. Liu, A.B., Mather, D., Reitz, R.D., SAE 930072, 1993.
15. O'Rourke, P.J., and Amsden, A.A., SAE Paper 961961, 1996.
16. Han, Z., and Reitz, R.D., *Combustion Science and Technology* 106:267-295 (1995).
17. Ra, Y. and Reitz, R.D., *Combustion and Flame* 155:713-738 (2008).
18. GRI-Mechanism, http://www.me.berkeley.edu/gri_mech/
19. Kong, S.C., Sun, Y., and Reitz, R.D., *Journal of Gas Turbines and Power* 129:245-251 (2007).
20. Butts, R., MS Thesis, University of Wisconsin-Madison, 2008.
21. Ra, Y., Reitz, R.D., McFarlane, J., and Daw, C.S., SAE Paper 2008-01-1379, 2008.
22. Genzale, C.L., Reitz, R.D., and Musculus, M.P.B., *Proceedings of the Combustion Institute* 32:2767-2774 (2009).
23. Opat, R., Ra, Y., Gonzalez, M.A., Krieger, R.B., Reitz, R.D., Foster, D.E., Durrett, R.P., and Siewert, R.M., SAE 2007-01-0193, 2007.

Table 1. Specification of diesel fuels modeled in the present study [20].

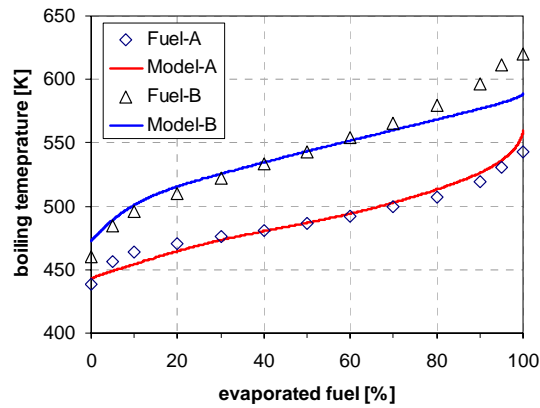
	Fuel-A	Fuel-B
Specific gravity	0.8132	0.8229
Viscosity [cSt]	1.503	2.704
LHV [MJ/kg]	46.2316	45.8780
Non-aromatics	79.88	82.22
Mono-aromatics	19.16	14.95
PAH	0.96	2.83
Cetane number	45	58.9

Table 2. Composition of the model diesel fuels.

	Fuel-A	Fuel-B
C_7H_8	0.07953	0.03473
$C_{10}H_{22}$	0.32660	0.09583
$C_{12}H_{26}$	0.32381	0.19372
$C_{14}H_{30}$	0.20244	0.22168
$C_{16}H_{34}$	0.06762	0.21824
$C_{18}H_{38}$	0.00000	0.23580
Molecular weight [g/mol]	156.47	192.11

Table 3. Reactions and rate constants used to model CN variation.

Reaction	$C_7H_{15}O_2 + O_2 = C_7ket12 + OH$		
	Original value	Fuel-A	Fuel-B
Pre-exponential factor	3.948E14	4.738E14	7.786E14

**Figure 1.** Comparison of distillation curves of diesel fuels between the measured data [20] and model predictions.

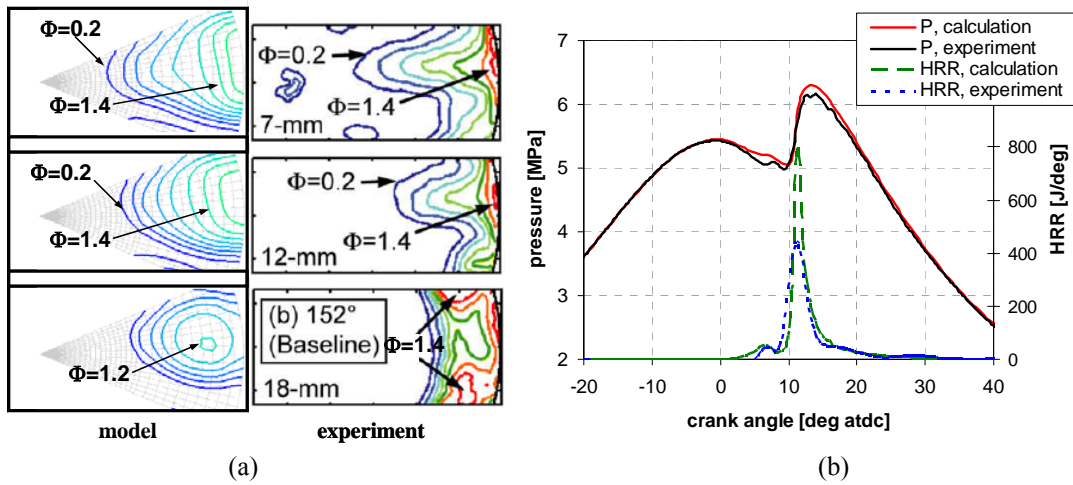


Figure 2. Comparison of equivalence ratio distributions (a), pressure and heat release rate profiles (b) between predictions and experiments of Genzele et al. [22]

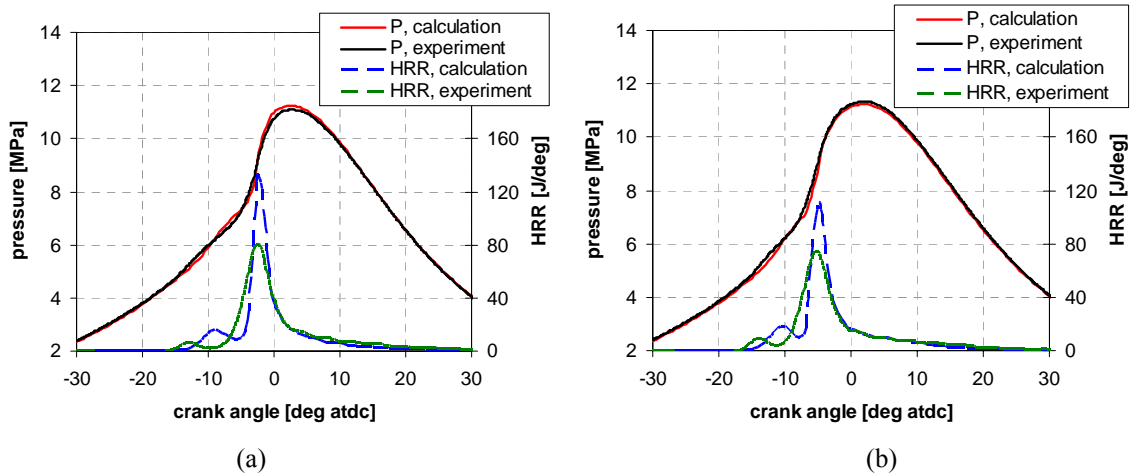


Figure 3. Comparison of predicted and measured [20] pressure and HRR. (a) Fuel-A, (b) Fuel-B.

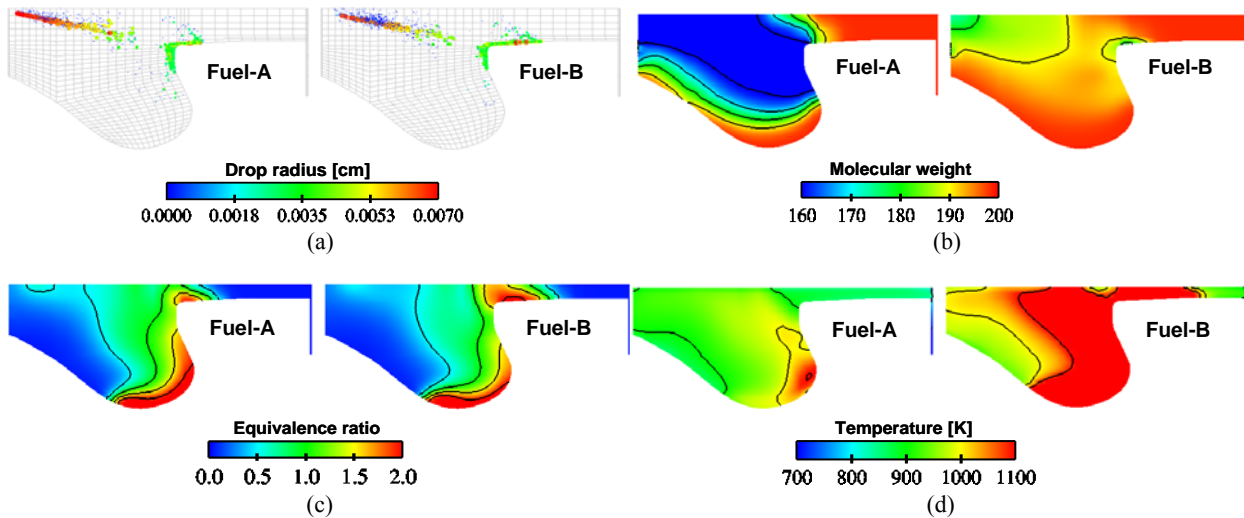


Figure 4. In-cylinder distributions of (a) spray droplets at CA = -19° atdc, (b) average molecular weight at CA = -16° atdc, (c) equivalence ratio CA = -8° atdc, and (d) gas temperature at CA = -4° atdc.