Computed and Measured Fuel Vapor Distribution in a Full-Cone Spray at High Chamber Pressure and Temperature

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Abstract

There is limited quantitative experimental data on fuel vapor concentrations in high-pressure vaporizing full-cone sprays injected into a high-pressure high-temperature environment typical of diesel engines. As a result, the accuracy of multidimensional models, which are routinely employed to compute such sprays, has not been quantitatively assessed. In this work, quantitative fuel vapor concentrations obtained from multidimensional computations of a fuel spray with three models are compared with measured concentrations in the spray. The three models employed are a Lagrangian-drop Eulerian-fluid (LDEF) spray model, a gas jet model, and a virtual-liquid source (VLS) model. Comparison of the vapor fraction along the axial centerline during the transient development of the spray shows that the computed values of vapor fraction are generally lower than the measured values, and the leading edge of the computed profiles shows shallower gradients of vapor fraction than in the measured spray. In the case of radial distribution, the peak values of measured and computed vapor fractions agree within 20 % when the profiles are quasi-steady. The three models show similar agreement close to the orifice, but the LDEF model shows the better agreement further downstream at quasi-steady state. During transient development, there is greater disagreement between the computed and measured profiles. As expected, the computed width of the vapor phase of the spray is generally larger than the measured one, though the half-widths show agreement within 10 %. In general, the gas jet and VLS vapor fraction values are within 5% of each other at the centerline during transient development, but differ more at the edge of the spray.

Introduction

Modeling of vaporizing fuel sprays is an important component of multidimensional simulations of in-cylinder phenomena in direct-injection compression-ignition engines, e.g. diesel engines. Accurate quantitative prediction of fuel vapor distribution in the spray is necessary to accurately predict the combustion processes in the engine, and provide useful guidance to engine designers. When the fuel is injected as a liquid, it goes through a series of complex processes before a resultant flammable mixture is created. These include primary and secondary atomization, drop-drop collisions, drop vaporization, and air entrainment [1-3]. Submodels have been developed for the individual processes and they form part of comprehensive spray models [1,4-5]. Lack of understanding of the physics, and inaccuracies in the numerical representation of the sprays can, however, lead to qualitative and quantitative inaccuracies in predictions [6-9]. Simplified approaches to model the essential elements of vaporizing liquid sprays have been proposed [6,10-11] as alternatives to the comprehensive models. These models take advantage of the fact that in high-pressure injection into a high-pressure, high-temperature environment the maximum penetration length of the liquid phase is fairly short relative to the overall spray penetration length, because of rapid entrainment of hot ambient air into the spray which leads to rapid vaporization of the drops [12-14]. In such situations, it has been shown that a gas jet with the same orifice mass and momentum flow rates as the spray has about the same penetration and spreading rate as the spray, beyond the maximum penetration length of the liquid [9,15]. In another approach, Abraham and Magi [10] developed a virtual-liquid source (VLS) model for the liquid phase of the spray. The virtual-liquid serves as a source of mass, momentum, and energy transfer.

While there have been several publications in which spreading and penetration rates are shown with spray models, gas jets and VLS sprays, none of them have *quantitatively* compared the distribution of vapor fuel in the jet. This comparison is the objective of this work. Measured and computed transient and steady-state radial and axial

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profiles of vapor fraction are compared. The next section of the paper briefly describes the experimental approach. This is followed by a description of the computational models, setup, and conditions. Results and discussion follow. The paper ends with summary and conclusions.

Experimental Approach

Quantitative mixing measurements in a vaporizing n-heptane fuel spray were obtained using Rayleigh imaging in an optically accessible constant-volume combustion vessel that simulated the ambient conditions of a diesel engine. Details of the experimental technique and facility are provided in Ref. [16]. The Rayleigh scattering technique provides several benefits towards making the optical mixing measurement quantitative and accurate in a harsh high-temperature, high-pressure environment. These benefits include the lack of a temperature dependency on the Rayleigh cross-section and the ability to correct for laser sheet intensity variations caused by energy variation in the delivery beam as well as beam steering in the high-pressure combustion vessel. Uncertainties for instantaneous mixing images were addressed in [16]. For this paper, the uncertainty of an ensemble-average of 30-40 injections is given to facilitate meaningful comparison to the computational results. The ensemble-average and instantaneous mixing field is also available to download over the internet [17].

Computational Models and Conditions

The three approaches – a liquid spray model, the gas jet model, and the VLS model - employed to model the spray will now be briefly described. Additional details can be found in the cited references. In the spray model, the liquid phase is treated as a dispersed phase in a continuum of gas, employing the Lagrangian-drop Eulerian-fluid (LDEF) approach of Duckowicz [18] and O'Rourke [19]. This approach has been widely employed for over a quarter century [4,18-20]. An important component of the model is the atomization submodel; several submodels have been proposed in the literature within the last twenty-five years [1,5,20]. They are all based on various assumptions, which cannot be assessed under conditions of interest because of the absence of relevant experimental data, e.g. drop sizes and size distribution, within the first 100 diameters of the spray. The challenges are compounded by the fact that the approach is valid only when the liquid volume fraction is fairly small (less than 1%) in computational cells, and when the drops are homogeneously distributed in the computational space, neither of which is satisfied in the near-field of the spray. To keep the liquid volume fraction small, and ensure numerical stability, computational cell sizes which are larger than the orifice diameter are typically employed. These grid sizes are not adequate to resolve the shear layer, and, not surprisingly, lead to results that are often inaccurate. Alternate approaches that are numerically more accurate, but which still require atomization and drop interaction submodels, have been proposed [11,15], but are computationally more intensive.

In using a gas jet model to represent the spray, the assumption is that turbulent jets of the same mass and momentum flow rates have similar structure, i.e. spreading and penetration rates [6,9,21]. In the model, the diameter, injection density, and injection velocity of the gas jet are obtained by equating the mass and momentum flow rates of the liquid spray with the gas jet. It can be shown that when this is done, the injection velocities are identical for the liquid spray and gas jet. The diameter of the orifice can then be estimated knowing the density of the injected vapor fuel.

The VLS model [10] is supported by experimental findings [12,13] which show that vaporizing sprays under high-pressure and high-temperature ambient conditions have short liquid penetration lengths compared to the vapor penetration lengths. In the model, it is assumed that there is a core of liquid originating from the injector orifice which is a source of vapor fuel mass, momentum and energy. Drops are not explicitly modeled. In real physics, such a core, if it exists, would be a source initially of liquid mass in the form of drops which subsequently vaporize, and of momentum and energy. Since the drops vaporize in a relatively short length, and rapidly, it is assumed that this core itself is directly a source of vapor mass. The model permits fairly high grid resolution, with grid sizes smaller than the orifice. Limitations on resolution are imposed primarily by density gradients in the near-field. In both the spray and VLS models, the orifice exit conditions are identical to those in the measurements.

The experimental and computational conditions are given in Table 1. Injection is into an inert environment. Notice that the orifice diameter in the measurements is given to be 0.1 mm, but 0.0927 mm in the LDEF and VLS models. This difference accounts for the area- contraction coefficient of the injector. In the LDEF spray model, the drops were injected from a line source whose length for the conditions of this work is selected to be 4.6 mm [20], half the liquid penetration length. Varying the source length by +/- 25% did not noticeably influence the results. The drops are injected within an included angle of about 14 degrees. Collisions and secondary breakup are modeled [19,22]. The injected drop size has a distribution with a Sauter-mean diameter of 2 microns. In reality, the drop size, its distribution, length of the line source, and the angle, are all parameters whose values are not known. In fact, it is not

even known if a line source really exists, and the evidence is contradictory [23,24]. In the VLS model, the maximum liquid penetration length is an input to the model and obtained from measurements. The time to attain this length is also an input. These have been selected to be 9.5 mm and 0.03 ms, respectively, in this work. Changing the time by a factor of two did not noticeably influence the results.

Table 1. Experimental and computational conditions

	Experiment	LDEF	VLS	Gas jet
Ambient temperature (K)	1000	1000	1000	1000
Ambient density (kg/m^3)	14.8	14.8	14.8	14.8
Injection pressure (MPa)	150			
Injected fluid	n-heptane	n-heptane	n-heptane	n-heptane
Density of injected fuel (kg/m^3)		630	630	136.9
Velocity coefficient	0.93			
Injection velocity (m/s)		632.4	632.4	632.4
Injected fluid temperature (K)	373	373	373	373
Area contraction coefficient	0.86			
Orifice diameter (mm)	0.100	0.0927	0.0927	0.199
Liquid length (mm)	9.5		9.2	

An axisymmetric multidimensional code that has been widely employed in prior work is employed for the simulations [10]. A 1-degree azimuthal slice is considered. For the computations with the spray (LDEF) model, the grid size stretches in the radial direction from 0.3 mm at the injector to 2 mm at the wall. In the axial direction, it stretches from 0.25 mm at the injector to 4.8 mm. The choice of this grid resolution is not dictated by accuracy but by the need to maintain a small liquid volume fraction in the computational cells near the orifice. With this choice of grid, the volume fraction is less than 3%. In the case of the VLS simulations, there are 2 cells within the orifice radius, and outside the orifice the grid stretches from 0.05 mm to 3.0 mm and 0.25 mm to 4.8 mm in the radial and axial directions, respectively. For the gas jet simulations, there are 4 numerical cells within the orifice radius, and outside the orifice the grid stretches from 0.08 mm to 3 mm in the radial direction, and 0.25 mm to 4.8 mm in the axial direction. In the case of the gas jet and VLS simulations, higher resolutions were employed in additional computations to ensure that the results presented here are insensitive to grid resolution. Turbulence is modeled with the standard k-e model and wall functions for boundary layers [10,25]. An RNG k-e model was also employed [25], but the results showed negligible differences relative to the standard k-e model, and they will not be presented here. It is well known that the k-e models overpredict the spreading rate of round jets by about 30 % [26,27].

Results and Discussion

Figure 1 shows a measured image of the spray, and computed images of the spray at 1.13 ms after start of injection (ASI). The measured images show ensemble-averaged two-dimensional Rayleigh-scattering images [16]. The field of view shown for the measured image is determined by optical access. The field of view shown for the computed images is the same as for the measured image. There is no liquid fuel in this field of view since it has fully vaporized. The colors indicate concentrations of mixture fraction. *Note that in the absence of combustion, the mixture fraction and vapor fraction are identical in these images.* Notice that the computed mixture fraction limits in the images are 0.006 and 0.15. The penetration, spreading, and distribution of vapor fuel predicted by the three models are about the same. The computed distributions are also very similar to the measured distribution. Quantitative comparisons of the axial, and radial distributions of vapor fraction at two axial locations, will be shown below to identify the similarities and differences more clearly.

Figure 2 shows the measured and computed axial centerline mixture fraction (vapor fuel fraction) at 0.49, 0.90, 1.13, and 6.0 ms ASI. The shading on the measured trace indicates the uncertainty band. The computed gas jet and VLS results are relatively close. In the case of the spray, fuel exists in both liquid and vapor form near the orifice since it takes a finite amount of time for all the liquid to vaporize. In the computations, by about 1.5 cm from the orifice, all the liquid fuel vaporizes. Beyond 1.5 cm, the differences in computed results are small. It was pointed out above that the injected drop sizes have a distribution with a Sauter-mean diameter (SMD) of 2 microns. The spray results are sensitive to this choice. The results with 2 microns are reported here since they are closest to the measured results, and to the gas jet and VLS model results. This emphasizes the need to improve the spray submodels in

the atomization regime. During the transient (see parts (a) and (b) of Fig. 2), the computed vapor fractions are lower than the measured one. Furthermore, the leading edge of the measured spray shows a steeper slope. Since the three (different) models predict very similar results, the differences at the leading edge and in vapor fraction values along the centerline arise from the basic Reynolds-averaged modeling approach. As pointed out earlier, k-e models are known to overpredict the spreading by about 30%, and the leading edge is smeared by the model [26].

In Fig. 3, the radial profiles of mixture fraction are compared in an axial plane which is 20 mm downstream from the orifice, at 0.49, 0.9, 1.13, and 6.0 ms ASI. The computed peak values are lower than the measured one during the transient, but at 6.0 ms ASI, the quasi-steady profile from the spray model gives the best agreement. It has been pointed out in prior work that differences in model predictions are greatest during transient development [6]. The quasi-steady state behavior is not very relevant in the engine. The radial spread of the computed profiles is greater than that of the measured one. Figure 4 shows the radial results at 0.9, 1.13, and 6.0 ms ASI in a plane that is 40 mm from the orifice. Results are not shown at 0.49 ms since the spray has not penetrated to this distance by then. At 0.9 ms, the peak value of mixture fraction from the spray model is higher, and the radial spread lesser, than those from the gas jet and VLS models. The peak value from the spray model continues to be higher at 1.13 and 6.0 ms, but the radial spread from the three models are about the same at these two later times. At quasi-steady state, the results from the gas jet and VLS models are relatively close, and not very different from the spray model results.

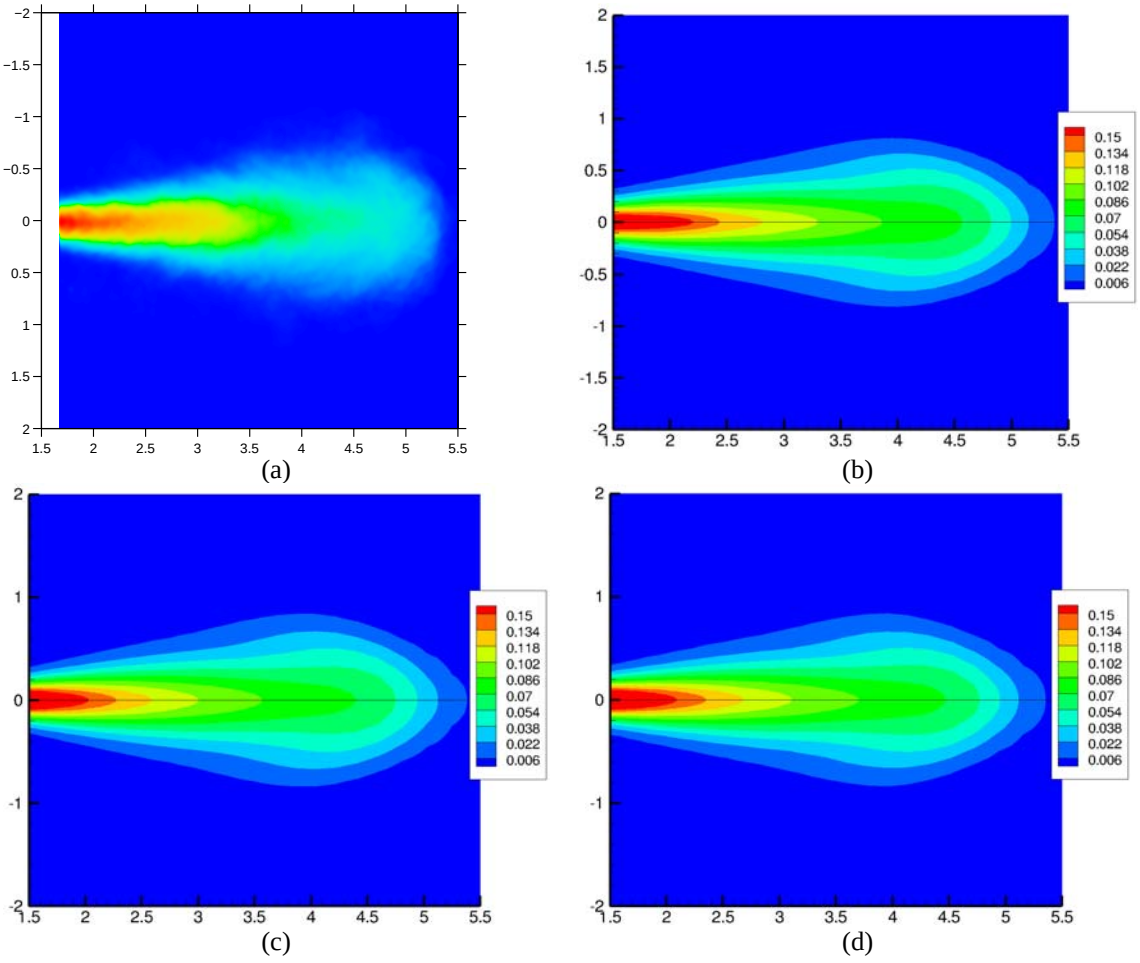

Figure 1. Measured image of the mixture fraction (a), and computed mixture fraction contours at 1.13 ms ASI with the (b) spray, (c) VLS, and (d) gas jet models. Color legend identifies values of mixture fraction.

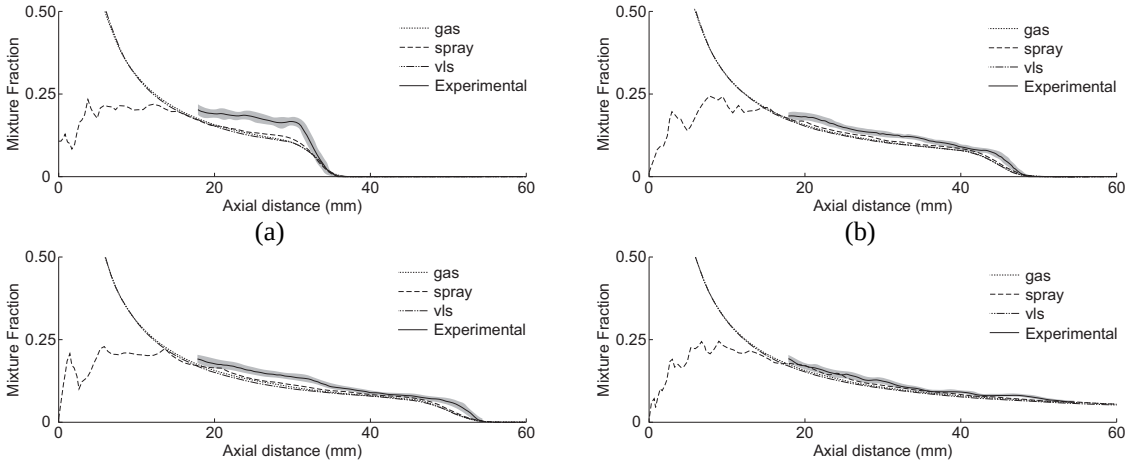

Figure 2. Computed and measured mixture fraction along centerline: (a) 0.49, (b) 0.90, (c) 1.13, and (d) 6.0 ms ASI.

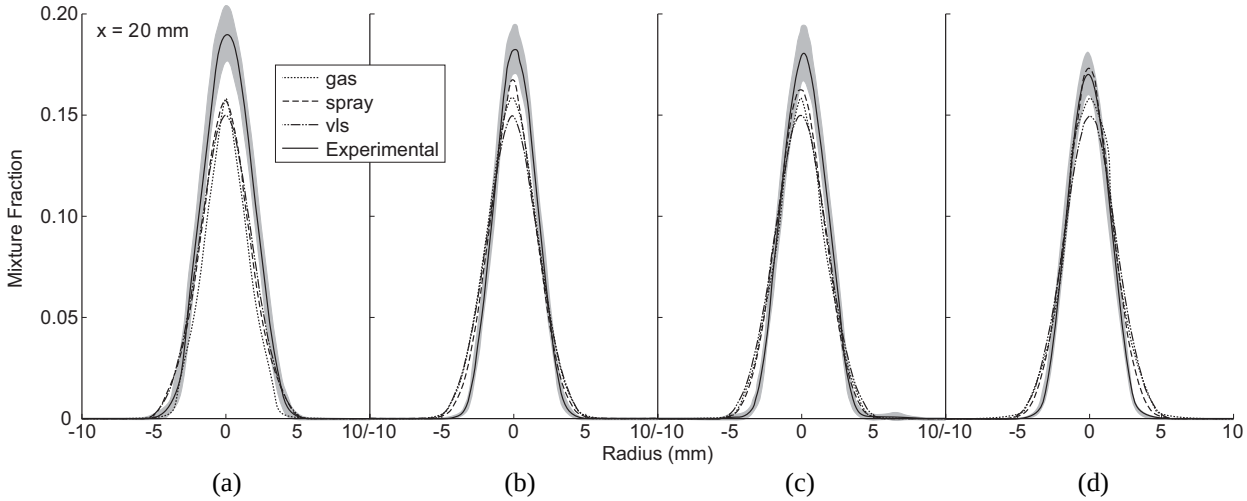

Figure 3. Computed and measured mixture fraction as a function of radius at axial plane 20 mm: (a) 0.49, (b) 0.90, (c) 1.13, (d) 6 ms ASI.

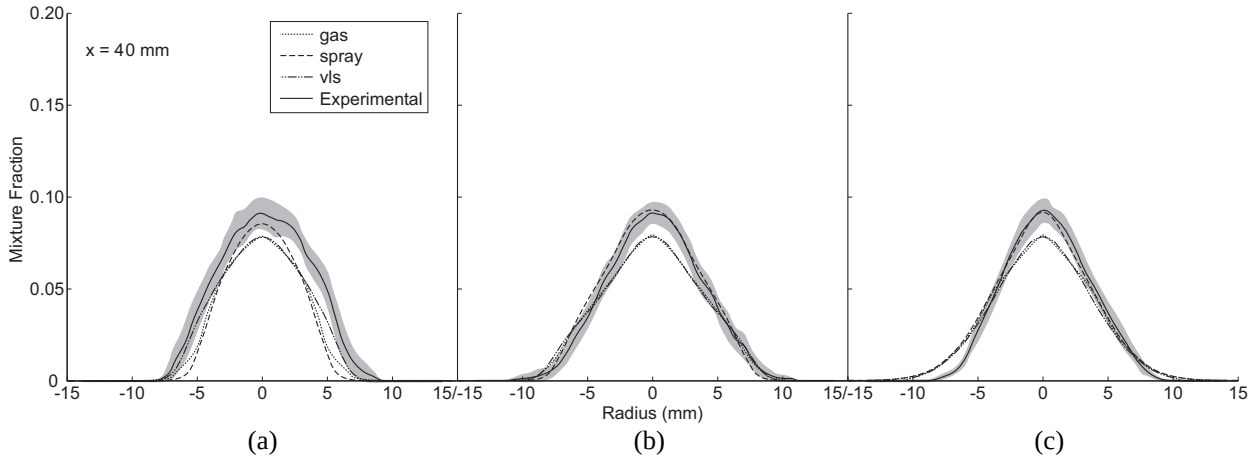

Figure 4. Computed and measured mixture fraction as a function of radius at axial plane 40 mm: (a) 0.90, (b) 1.13, (c) 6 ms ASI.

Summary and Conclusions

Quantitative mixture (vapor) fraction predictions obtained with a spray model, a gas jet model, and a virtual-liquid source (VLS) model for a vaporizing spray under diesel-engine chamber conditions are compared with measured results. It is shown that while the three models are in general agreement, computed and measured results do not agree along the axial centerline during transient penetration. The measured values are higher along the centerline and show a steeper slope at the leading edge. The peak centerline values of measured and computed vapor fractions in two axial planes, where comparisons are presented, agree within 20 % when the profiles are quasi-steady. The computed radial profiles show similar level of agreement close to the orifice, but the spray model shows the better agreement further downstream. During transient development, there is greater disagreement between the computed and measured profiles in both centerline and radial profiles. The computed spreading of the spray is greater than the measured spreading with all three models at quasi-steady state, as expected when using the k-e model. The spray results were obtained with an injected Sauter-mean diameter of 2 microns. The results are dependent on the choice of this size. This dependence does not exist with the gas jet and VLS models.

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References

1. Reitz, R.D., *Atomization and Spray Technology* 3:309-337 (1987).
2. Lefebvre, A.H., *Atomization and Sprays*, Hemisphere Publishing, New York, 1989, pp.43-59.
3. Chigier, N., *Atomization and Sprays* 16:727-736 (2006).
4. O'Rourke, P.J. and Bracco, F.V., *The Institution of Mechanical Engineers Publication* 1980-9, 101-116 (1980).
5. O'Rourke, P.J. and Amsden, A.A., SAE Paper 872089 (1987).
6. Abraham, J., *SAE Transactions* 106(3):141-155 (1997).
7. Aneja, R. and Abraham, J., *Combustion Science and Technology* 138:233-255 (1998).
8. Subramaniam, S. and O'Rourke, P.J., "Numerical Convergence of the KIVA-3 Code for Sprays and its Implications for Modeling," Los Alamos Laboratory Report UR-98-5465, Los Alamos, NM.
9. Iyer, V.A. and Abraham, J., *Combustion Science and Technology* 130:315-335 (1997)
10. Abraham, J., and Magi, V., *SAE Transactions* 108(3):1363-1374 (1999).
11. Iyer, V. and Abraham, J., *ASME Journal of Fluids Engineering* 125:660-669 (2003).
12. Siebers, D.L., SAE Paper 980809 (1998).
13. Siebers, D.L., SAE Paper 1999-01-0528 (1999).
14. Iyer, V. A., Post, S.L, and Abraham, J., *Proceedings of the Combustion Institute*, 28(1):1111-1118 (2000).
15. Iyer, V. and Abraham, J., *Atomization and Sprays* 15(3):249-270 (2005).
16. Idicheria, C.A. and Pickett, L.M., SAE Paper 2007-01-0647 (2007).
17. Engine Combustion Network Experimental Data Archive. http://www.ca.sandia.gov/ECN
18. Dukowicz, J.K., *Journal of Computational Physics* 35(2):229-253 (1980).
19. O'Rourke, P.J., *Collective Drop Effects on Vaporizing Liquid Sprays*, Ph.D. Dissertation, 1981, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, N.J.
20. Bracco, F.V., SAE Paper 850394 (1985).
21. Abraham, J., *Numerical Heat Transfer Part A: Applications* 30(4):347-364 (1996).
22. Reitz, R.D. and Diwaker, R., SAE paper 870598 (1987).
23. Chehroudi, B. and Bracco, F.V., SAE Paper 850126 (1985).
24. Yue, Y., Powell, Yue, Y., Powell, C. F., Poola, R., Wang, J., and Schaller, J., *Atomization Sprays* 11(4): 471–490 (2001).
25. Abraham, J. and Magi, V., *SAE Transactions*, 106(3):1442-1452 (1997).
26. Magi, V., Iyer, V., and Abraham, J., *Numerical Heat Transfer. Part A: Applications* 40(4):317-334 (2001).
27. Wilcox, D.C., *Turbulence Modeling for CFD*, DCW Industries, Inc., La Canada, CA, 2006, ch.4.