7. TOPICS

7.1 Future Research

As discussed above, there are several areas where improvements in spray models would increase the accuracy of spray predictions. A few of these areas are reviewed here.

The thick spray region poses a formidable problem both experimentally and computationally in spray research. Experimental data and theoretical analysis is needed on the mechanisms of breakup of liquid sheets and jets in the "thick" spray regime. Mathematical models are available that describe the breakup of jets and drops by following the unstable growth of waves on the liquid surface. This theory provides qualitative descriptions of breakup phenomena and various breakup regimes. However, the influence of nozzle internal flow effects is only included empirically in the theory, and these effects are known to be important, particularly for high speed breakup. A useful area for future research would be the development of fundamentally based models that describe the effect of nozzle internal flows on the atomization process. Boundary element models and direct numerical simulations may be appropriate approaches.

Current breakup models need to be extended to further study the effects of liquid distortion, ligament formation and stretching on the atomization process. In addition, there is uncertainty about the role that shear stresses (due to viscous effects in the gas) play in the liquid breakup process. Experiments and analysis are needed to be able to resolve the importance of tangential stresses on the liquid breakup process. A notable shortcoming of current atomization and drop breakup models is that they do not predict the size distribution of drops at the moment of breakup, and also the time between successive ruptures of liquid surfaces. The size distribution may be influenced by events that occur within the nozzle (e.g., cavitation and nozzle turbulence), or by prior breakups and collisions that perturb liquid surfaces. The importance of these effects needs to be established.

Drop collision and coalescence models need to be extended to account for satellite drop formation and for drop shattering. For engine applications, the correlations used in the collision and coalescence models need to be tested against fundamental experiments at high pressures since they come from sprays in entirely different regimes (rain drops and cloud physics).

The relationship between drop breakup and drop shattering, and turbulence production and dissipation in sprays needs to be established. Turbulence dispersion models applicable to thick sprays need to be formulated. The effect of drop distortion on drop drag and vaporization needs to be analyzed further. In particular, the validity of the assumed relationship between drop drag and drop distortion (Eq. 4.23) needs to be assessed. The effects of drop internal circulation, realistic liquid properties and multicomponent fuels on vaporization needs to be assessed for distorting drops.

More experimental data is needed in order to improve wall impingement models. In particular, data on the secondary breakup of impinged drops is needed under high wall temperature and high gas temperature and density conditions. More accurate models for the thickness of the wall film also need to be developed. Improved models should be able to model the spreading of a liquid film, and should account for the phenomena of wall wetting and liquid splashing. Wall interaction models are needed for films outside of the evaporative-wetting regime with Leidenfrost effects.

The Shell model gives reasonable predictions of diesel ignition, but there is uncertainty about the values of the model constants for different fuels. A more fundamentally based chemical kinetics model is needed to allow consideration of multicomponent fuels, and the effect of additives on ignition. Fundamental information is needed about the mechanisms of turbulent combustion. The laminar-and turbulent-characteristic time combustion model used for the diesel combustion studies described above has the advantage of simplicity. However, details of the structure of turbulent flames are not well represented in the model, and it is likely that soot and NOx predictions depend on these details.

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Appendix A - Available Computer Codes

A.1 Multidimensional CFD Codes

The sources listed below provide multidimensional CFD codes with spray models:

KIVA-2 and KIVA-3 Attn: Ed Kidd Energy Science and Technology Software Center, P.O. Box 1020, Oak Ridge, TN 37831-1020 (615) 576-2606	Turbo-KIVA Attn: Reza Taghavi Manager, Combustion Engineering Applications Department Cray Research, Inc. 655E Lone Oak Drive Eagan, MN 55121 (612) 683-3643
SPEED/STAR-CD Attn: Peter Epstein Adapco 60 Broadhollow Road Melville, NY 11747 (516) 549-2300	FIRE KIT Corporation 1355 Mendota Heights Road St. Paul, MN 55120 (612) 688-0620
CFD-ACE Attn: Ashok Singal CFD Research Corp. 3325 Triana Blvd. Huntsville, AL. 35805 (205) 536-6576	PHOENICS-2 Attn: Pedro Marcal Concentrated Heat & Momentum (CHAM) P.O. Box 77574 Atlanta, GA 30357-7574 (404) 351-3709
FLUENT Fluent, Inc. Centerra Resource Park 10 Cavendish Court Lebanon, NH 03766 (603) 643-2600	CFDS-FLOW3D Computational Fluid Dynamics Services, Inc. 1700 North Highland Road Pittsburgh, PA 15241

A.2 Dilute Spray Models

Simpler PC-based dilute spray models are also available:

TESS™
L.G. Dodge
P.O. Drawer 28510
San Antonio, TX 78228-0510
(210) 522-3251

The TESS™ computer code (Trajectory and Evaporation of Spray Systems) is a fast PC-based code for estimating transient drop sizes, drop evaporation and drop trajectories for pressure atomized or air-assist atomized "dilute" sprays in simple one-dimensional air flows, with or without swirl. Fluid properties for water, methanol, ethanol, and hydrocarbons from propane (C_3H_8) to heavy oil ($C_{30}H_{62}$) are built in to the program. The code is also useful for evaluating the difference between drops sizes obtained using number-flux (temporal) weighting sampling, and those obtained using number density (spatial) sampling.

The TESS™ model assumes that the spray is in the "very dilute" spray regime (see Section 2.1). In this case the mass flow of liquid is assumed to be small compared to the mass flow of air, and drop drag forces affect drop velocities, but drops do not affect the air velocity (see Section 2.5). Similarly, although liquid vapor effects on transport properties of the gases surrounding the drops are accounted for (using a 1/3 averaging rule), the free stream gas flow is assumed to not build up vapors from the evaporating liquid. Because of these assumptions the code should not be used for analyzing dense sprays such as diesel sprays or other sprays close to the atomizer source.

The TESS™ drop injection model uses up to 20 drop size classes to represent the spray at the injector exit which is assumed to have a Rosin-Rammler distribution. The drop size distribution changes as the drops move away from the injector due evaporation and drag effects. Drop evaporation is modeled using the methods described in Section 4.5 and summarized by Lefebvre (1989). Drop trajectories are computed assuming spherical drop drag coefficients that are a function of Reynolds number, similar to those in Eqs. 4.22.