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Developments in Spray Modeling in Diesel and Direct-Injection Gasoline Engines

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Résumé — Progrès de la modélisation des sprays dans les moteurs Diesel et à essence — Dans les moteurs à injection directe, les caractéristiques du spray de carburant influent directement sur le rendement et les émissions. Les performances des modèles de spray existants et leur influence sur la combustion pour les moteurs Diesel et essence à injection directe sont analysées.

Un modèle phénoménologique d'écoulement dans les injecteurs indiquant les effets de la géométrie sur les processus d'injection est présenté. Ce modèle donne les conditions initiales d'un modèle d'atomisation prenant en compte les instabilités de Kelvin-Helmholtz (KH) et Rayleigh-Taylor (RT). Une analyse de stabilité linéaire a aussi été menée pour prendre en compte l'atomisation des nappes liquides caractéristiques des injecteurs à swirl des moteurs à essence.

Des résultats de simulations Diesel ont été comparés aux données obtenues avec des diagnostics laser sur des moteurs à accès optique Diesel ID de fort alésage pour une large gamme de conditions opératoires. Les résultats montrent que le modèle d'injecteur utilisé en combinaison avec le modèle d'atomisation (KH + RT) donne des résultats réalistes. En particulier, la courte pénétration liquide et les détails de forme des flammes sont bien reproduits.

Le modèle d'atomisation de nappe a aussi été comparé avec succès à des pénétrations expérimentales et des données de taille de gouttes pour des injecteurs en cône creux. Ce modèle est en cours d'utilisation pour l'étude de la combustion en mode stratifié dans les moteurs GDI.

Mots-clés : sprays, Diesel, modélisation, Kelvin-Helmholtz, Rayleigh-Taylor, injection directe.

***Abstract* — *Developments in Spray Modeling in Diesel and Direct-Injection Gasoline Engines* —** *In direct-injection engines the fuel spray characteristics influence the combustion efficiency and exhaust emissions. The performance of available spray models for predicting liquid and vapor fuel distributions, and their influence on combustion is reviewed for both diesel and gasoline direct injection engines.*

A phenomenological nozzle flow model is described for simulating the effects of diesel injector nozzle internal geometry on the fuel injection and spray processes. The flow model provides initial conditions for the liquid jet breakup model that considers wave instabilities due to Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) mechanisms. A linearized instability analysis has also been extended to consider the breakup of liquid sheets for modeling pressure-swirl gasoline injectors.

Diesel engine predictions have been compared with extensive data from in-cylinder laser diagnostics carried out in optically accessible heavy-duty, DI Diesel engines over a wide range of operating conditions. The results show that the nozzle flow model used in combination with the KH and RT models gives realistic spray predictions. In particular, the limited liquid fuel penetration length observed experimentally and the flame shape details are captured accurately.

The liquid sheet breakup model has also been compared favorably with experimental spray penetration and drop size data for gasoline hollow-cone sprays. This model is currently being applied to study stratified charge combustion in GDI engines.

Keywords: sprays, Diesel, modeling, Kelvin-Helmholtz, Rayleigh-Taylor, direct injection.

INTRODUCTION

Accurate modeling of fuel spray dynamics is essential for combustion and emission predictions in internal combustion engines. A comprehensive spray model needs to address the fuel injection process, the spray atomization and drop breakup, drop collision and coalescence, drop/wall interactions, and vaporization. Many of these processes occur on time and length scales that are below the scale of resolution of the numerical grids used in practical computations. The complexity of the processes makes it necessary to introduce models that must be validated using detailed experimental data. Several current spray models are briefly described in this paper, together with example applications for diesel and gasoline direct-injection (GDI) engine simulations.

1 MODEL FORMULATION

1.1 Nozzle Flow Models

To avoid the need to resolve the dense spray/liquid interface at the injector nozzle exit, in most models the liquid fuel is injected as computational parcels which contain drops or “blobs” (Reitz, 1987) with sizes equal to the nozzle effective diameter. Fuel injection system (FIS) codes are available to simulate the injection process from the injection pump to the nozzle (e.g., Arcoumanis *et al.*, 1997, Hountalas and Kouremenos, 1998). These models supply the injection sac-pressure history. Alternatively, the injection characteristics can be measured experimentally using a Bosch rate-of-injection apparatus.

The injector nozzle geometry influences the fuel atomization and subsequent combustion. A nozzle flow model is needed to describe the flow inside the injector nozzle holes and to provide initial spray conditions for multi-dimensional modeling. Several possible flow regimes occur in the injector nozzles including laminar, turbulent, cavitating and hydraulic flip regimes (Sarre *et al.*, 1999). Due to the high injection pressure in modern diesel injectors, cavitating flows are very likely to occur within injector nozzle passages.

The instantaneous flow conditions inside the nozzle can be calculated from the input parameters including the fuel mass flow rate, combustion chamber pressure, nozzle hole diameter and L/D and R/D ratios. The output parameters are the instantaneous discharge coefficient, spray angle, effective injection velocity and flow exit area. In the model, the discharge coefficient is first estimated from the “nominal” mean velocity U_{mean}, wall friction (f) and inlet loss coefficient (K_{inlet}), which is a function of inlet R/D (Benedict, 1980). The inlet pressure is also estimated accordingly:

$$C_d = \frac{1}{\sqrt{K_{inlet} + f \cdot L/D + 1}}$$

$$\text{and} \quad p_1 = p_2 + \frac{\rho}{2} \cdot \left(\frac{U_{mean}}{C_d} \right)^2$$

The static pressure at the vena contracta is calculated following Nurick (1976) and is used to check whether the flow is already cavitating using:

$$U_{vena} = \frac{U_{mean}}{C_c} \quad \text{and} \quad p_{vena} = p_1 - \frac{\rho}{2} \cdot U^2_{vena}$$

If p_{vena} is higher than p_{vapor}, the flow remains in the liquid phase, the exit velocity is set equal to U_{mean} and the initial drop size (SMD) is equal to the nozzle diameter. However, if p_{vena} is lower than p_{vapor}, it is assumed that the flow must be fully cavitating and a new inlet (nozzle sac) pressure and discharge coefficient are obtained. The effective exit velocity and area are calculated by applying corresponding continuity and momentum equations between the vena contracta and the nozzle exit, i.e.:

$$p_1 = p_{vapor} + \frac{\rho}{2} \cdot U^2_{vena}$$

$$C_d = C_c \cdot \sqrt{\frac{p_1 - p_{vapor}}{p_1 - p_2}}$$

$$\text{and } U_{eff} = U_{vena} - \frac{p_2 - p_{vapor}}{\rho_1 \cdot U_{mean}}$$

The nozzle flow model gives the typical variation of the discharge coefficient shown in Figure 1 as the flow Reynolds number is changed. The model has been used to simulate the experiments of Ohrn *et al.* (1991) that investigated effects of the nozzle inlet R/D ratio. Figure 2 shows that the agreement in discharge coefficients is good, especially for small R/D ratio in the range of practical diesel injector nozzles. Other model validation results can be found in Sarre *et al.* (1999).

1.2 Initial Spray Angle

The initial spray angle is also needed for the injected liquid parcels. The spray angle is estimated using the Wave model (Reitz, 1987) as:

$$\tan\left(\frac{\theta}{2}\right) = \frac{4 \cdot \pi}{A} \cdot \sqrt{\frac{\rho_g}{\rho_l}} \cdot f(T)$$

where $f(T)$ is a function of We, Re and liquid and gas conditions (Dan *et al.*, 1997).

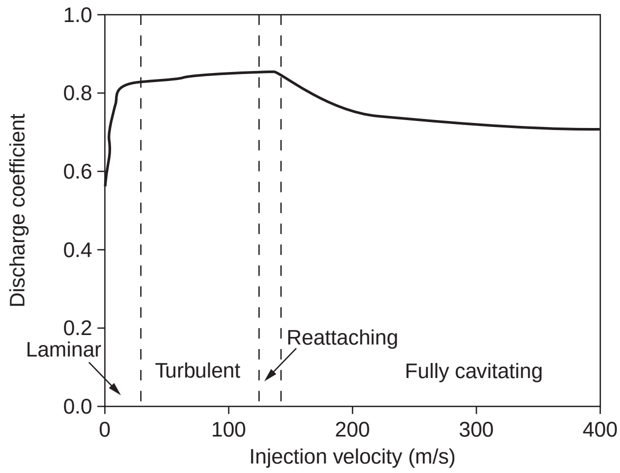

Figure 1

Discharge coefficient variation in different flow regimes.

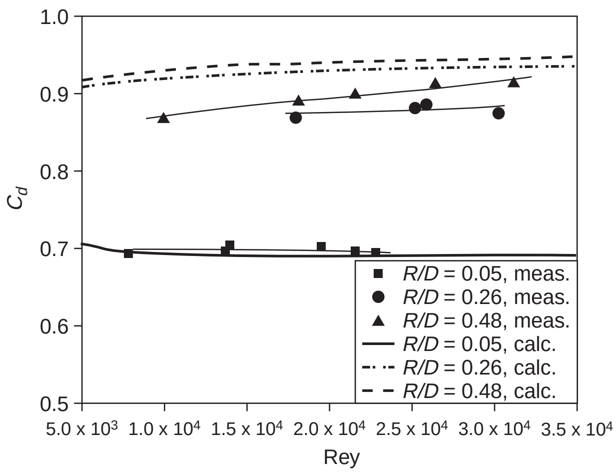

Figure 2

Comparisons of experimental and model results for the influence of *R*/*D* on *Cd*.

1.3 Liquid Jet Breakup

Classical spray breakup models are reviewed by Pelloni and Bianchi (1999). Among the available models are "wave" models (e.g., Reitz, 1987; Habchi, 1997) and models that ascribe liquid breakup to nozzle flow turbulence (e.g., Huh *et al.*, 1991 and Arcoumanis *et al.*, 1997). The wave models assume that aerodynamic forces at a liquid gas interface and the resulting surface waves are responsible for the atomization. Nozzle cavitation and flow turbulence effects are introduced through an initial disturbance level that is accounted for in model constants. The so-called "wave breakup model" (Reitz, 1987) considers the breakup of the injected liquid to be due to the relative velocity between the gas and liquid phases. The growth of Kelvin-Helmholtz (KH) instabilities induces the shearing-off of droplets from the liquid surface, as shown schematically in Figure 3. The rate-of-change of the drop radius and the resulting child droplet size are related to the frequency (Ω) and wavelength (Λ) of the fastest growing surface wave, with (Reitz, 1987):

$$\frac{\Lambda}{a} = 9.02\frac{\left(1 + 0.45\ Z^{0.5}\right)\left(1 + 0.4\ T^{0.7}\right)}{\left(1 + 0.87\ We_2^{1.67}\right)^{0.6}}$$

$$\Omega\left(\frac{\rho_1 a^3}{\sigma}\right)^{0.5} = \frac{0.34 + 0.38\ We_2^{1.5}}{(1 + Z)\left(1 + 1.4\ T^{0.6}\right)}$$

where We, Z and T are the Weber, Ohnesorge and Taylor number, respectively.

Jet breakup models that ascribe breakup to nozzle turbulence are under development (e.g., Polloni and Bianchi, 1999). These models assume that breakup is controlled by a characteristic turbulence timescale, usually obtained from the k-ε model applied to the nozzle flow, and initial drop sizes are related to turbulent length scales.

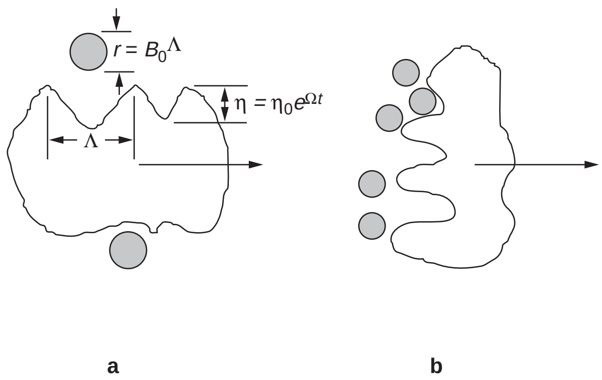

Figure 3

Schematic diagram of drop breakup mechanisms
a: KH-type; b: RT-type.

1.4 Liquid Sheet Breakup

Liquid sheet breakup is influenced by the surrounding gas, surface tension and liquid viscosity and is thought to be due to the growth of unstable waves (Squire, 1953; Hagerty and Shea, 1955; Li and Tankin, 1991). Senecal *et al.* (1998) and Schmidt *et al.* (1998) have shown that short waves dominate the wave growth process for high-speed sheets where the surrounding gas density is much less than the liquid sheet density. In this case, the maximum growth rate Ω_s is obtained from a dispersion relation that relates the growth rate ω to the wave number k for sinuous wave growth. The equation shows that a transitional gas Weber number $We_2 = \rho_2 U^2 h/\sigma = 27/16$ exists, below which long waves dominate and above which short waves dominate. This is shown graphically in Figure 4. Here the dimensionless breakup length is L/h where $L = CU/\Omega_s$ is the breakup length, C is a constant and h is the sheet half-thickness.

Injection velocities and the sheet thickness for pressure-swirl injectors are typically such that We_2 is well above 27/16. As a result, the short wave assumption is appropriate. In addition, the density ratio $Q = \rho_2/\rho_1 << 1$. With these simplifications, the dispersion relation becomes:

$$\omega_r = -2\nu_1 k^2 + \sqrt{4\nu_1^2 k^4 + QU^2k^2 - \frac{\sigma k^3}{\rho_1}}$$

where ω_r is the real part of the complex growth rate ω.

Drop formation from the primary breakup process is assumed to follow the physical mechanism of Dombrowski and Johns (1963). This mechanism assumes that tears in the thinning sheet contract to form ligaments which subsequently breakup to form drops. Conservation of mass and Weber's theory (1931) are used to predict the size of the initial droplets.

1.5 Drop Breakup

The Taylor analogy breakup (TAB) model of O'Rourke and Amsden (1987) has been used to predict both primary and secondary droplet breakup for both Diesel (e.g., Tanner, 1997) and gasoline sprays (e.g., Han *et al.*, 1997). Drop breakup models have also been proposed based on the wave breakup mechanism (Reitz, 1987, Habchi *et al.* 1997). Recent improvements account for Rayleigh-Taylor (RT) instabilities resulting from the deceleration of the drops (Patterson and Reitz, 1998). The deceleration normal to the interface between two fluids of different densities causes the instabilities. In the case of liquid drops moving at a high velocity, the leeward surface of the drop is unstable as it is deformed and this can lead to breakup into small droplets, as shown in Figure 3b.

Drop breakup has also been modeled by considering the different secondary breakup regimes described by Pilch and Erdman (1987) in several studies (e.g., Arcoumanis *et al.*, 1997). The models account for the regimes indicated in Figure 5. Notice, however, that the correlations predict non-dimensional breakup times that are essentially constant (varying between 4 and about 6). This agrees with the wave model that also predicts a constant breakup time with the same non-dimensionalization.

1.6 Drop Collision, Coalescence, Drag and Wall Interaction

The collision frequency and probability of coalescence between drops in two parcels control the outcome of collisional interactions. When drops collide they experience coalescence or maintain their sizes and temperatures but undergo velocity changes (grazing collision—Amsden *et al.*, 1989). Recent improvements to the collision model include consideration of reflexive collisions (Tennison *et al.*, 1997) and drop shattering collision (Georjon and Reitz, 1998). Shattering occurs at high Weber numbers when coalesced drops form a stretched liquid ligament that breaks into droplets due to wave instabilities.

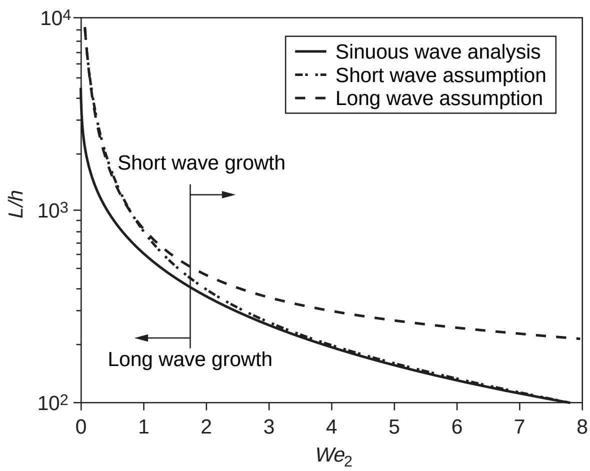

Figure 4

Dimensionless breakup length as a function of sheet Weber number, We_2.

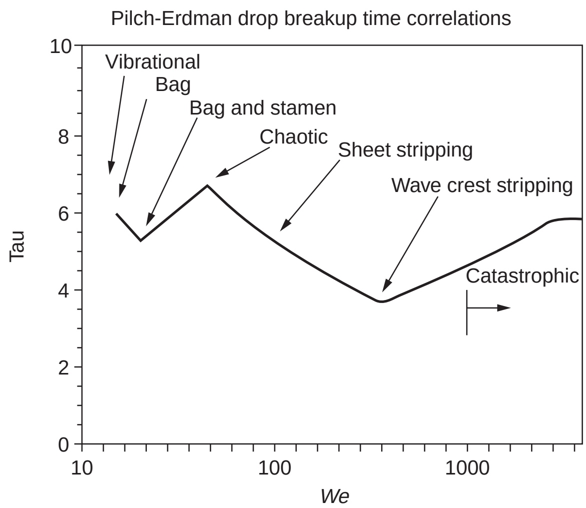

Figure 5

Drop secondary breakup timescales.

In engine sprays the fuel drops undergo high distortion due to the ultra-high injection velocity. The drop drag coefficient changes and is increased as the drop departs from the spherical shape. Liu and Reitz (1993) calculated the drop distortion using the TAB model and evaluated the drag coefficient dynamically during the injection.

The impact of a drop on a heated surface may lead to instantaneous breakup, sudden vaporization, formation of a liquid film on the surface, or sliding or bouncing back with a highly distorted drop. The above phenomena depend on the drop Weber number (e.g., Naber and Reitz, 1989). Recent improvements account for the formation and breakup of liquid films (Bai and Gosman, 1995; Stanton, *et al.* 1998).

2 MODEL VALIDATION – DIESEL SPRAYS

The present spray models have been implemented in Kiva to simulate non-vaporizing diesel spray experiments of Su *et al.* (1995). Hydraulic electronic unit injectors (HEUI) were used with two different inlet configurations, namely, a rounded inlet (RI) and a sharp-edge inlet (SEI). Both injectors had the same diameters (0.259 mm) and L/D ratios (2.915). Two cases, 72 MPa injection using RI nozzle and 90 MPa injection using SEI nozzle, were considered. Both cases have the same measured rate-of-injection profiles and the only difference is the nozzle inlet geometry.

The computed discharge coefficients are shown in Figure 6. The sudden drop of C_d at early times indicates the onset of cavitation. Note that the small change in the inlet R/D ratios (0.03 for SEI and 0.07 for RI) causes a big difference in the discharge coefficient. The results show that the flow is cavitating for most of the time due to the high injection pressures. Figure 7 shows the computed overall spray drop-size SMD is in good agreement with the measurements. Other results of liquid penetration, spray angles and SMD for different cases are documented by Sarre *et al.* (1999).

The present spray model was also applied with a characteristic-time combustion model (Kong *et al.*, 1995) to simulate combustion in a Cummins optical-access engine (Dec, 1997). The nozzle geometry data and injection profile are needed for inputs without the need to estimate the injector discharge coefficient. Figure 8 shows that the computed cylinder pressure and apparent heat-release rate are improved by using the nozzle flow model. The early part of combustion is not affected since the effective injection pressure is still relatively low. As the injection pressure continues to rise, cavitation takes place in the nozzle resulting in a lower effective flow area and thus a high injection velocity. In the baseline case without using the nozzle model, an average nozzle discharge coefficient and initial SMD were used. However, if the nozzle flow model is used, variations of the effective injection velocity and injected drop SMD are better described during the injection process. A longer penetration of the fuel vapor plume and the combustion flame is observed inside the cylinder (Fig. 9) which agrees better with experimental images of Dec *et al.* (1997). The use of the nozzle model thus improves simulations of combustion process in the engine.

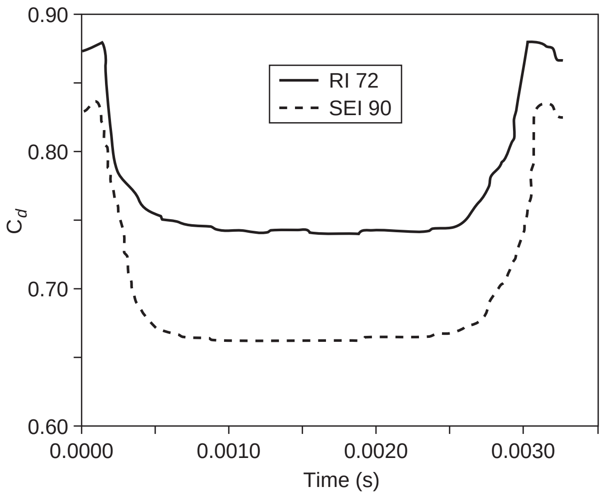

Figure 6

Computed discharge coefficient during the injection process.

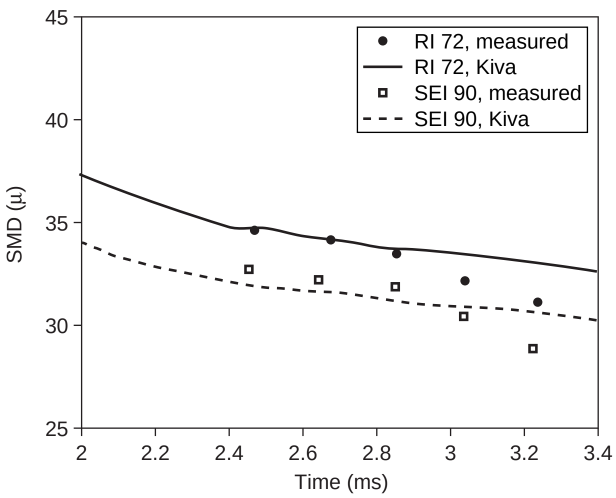

Figure 7

Comparison of measured and computed SMD.

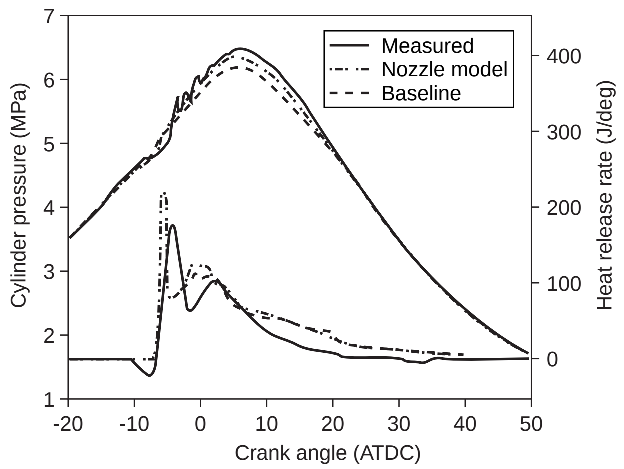

Figure 8

Effects of nozzle flow details on engine combustion simulations.

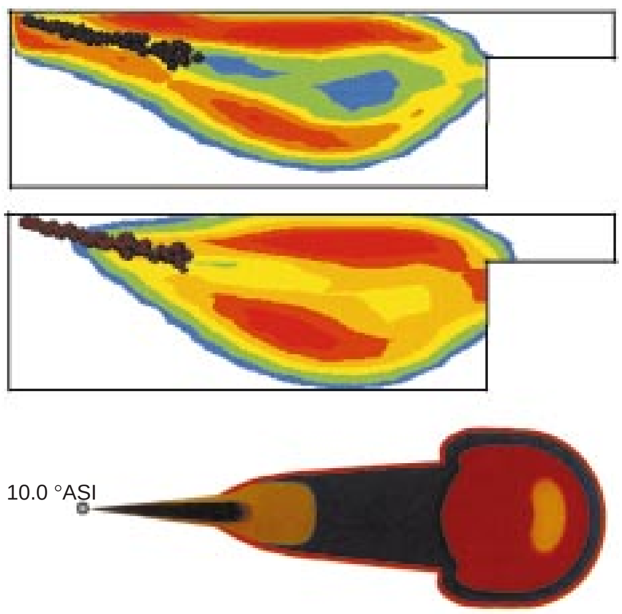

Figure 9

Temperature distribution for the baseline case (top), with nozzle flow model (middle), experimental soot image (bottom – Dec, 1997) at 10 ASI.

3 MODEL VALIDATION – GASOLINE SPRAYS

Schmidt *et al.* (1998) and Senecal *et al.* (1998) have applied the sheet breakup model to both inwardly—and outwardly—opening pressure-swirl fuel injectors. The overall, qualitative agreement between the predictions and the measured spray are shown in Figure 10, which presents the calculated spray droplet distributions and photographs of Parrish (1997) for three times after the start of injection. It is evident that the numerical results capture the exterior vortex ring that entrains droplets upward and away from the main spray.

Figure 11 presents the measured and computed spray penetration for both the main spray and the pre-spray (see Fig. 10) as functions of time. In addition, the measured and computed local SMD in a plane 39 mm downstream of the injector and perpendicular to the spray axis is shown in Figure 12.

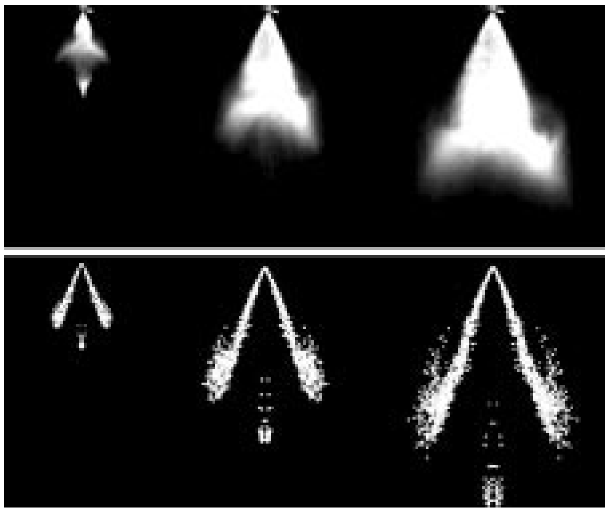

Figure 10

Comparisons of photographs (top) and computer model predictions (bottom) for 0.7, 1.7 and 2.7 ms after the start of injection (from left to right). The numerical results present a two-dimensional slice through the spray to show the spray structure.

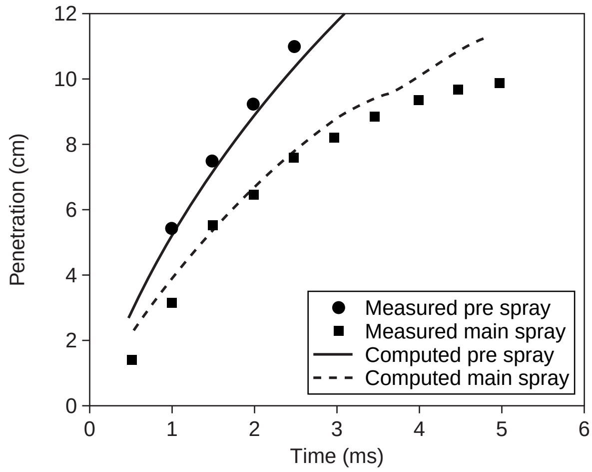

Figure 11

Measured and predicted spray penetration for the main spray and pre-spray as functions of time.

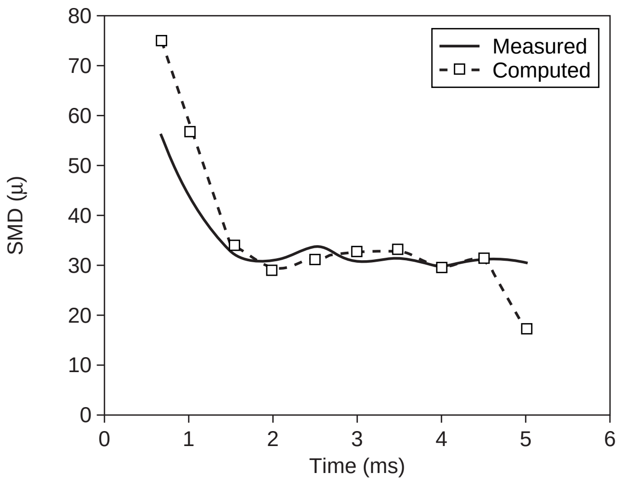

Figure 12

Measured and predicted Sauter mean diameter. Drop sizes are averaged over a plane 39 mm downstream of the injector.

Figure 13

GDI engine concept with pressure-swirl injector.

It is seen that the model gives excellent predictions of penetration and drop size.

Sheet spray breakup models have been applied to model stratified charge GDI engines by Li *et al.* (1999). Spray is targeted onto a shaped piston to direct the charge toward the sparkplug, as indicated in Figure 13. The ignition, flame kernel growth and combustion details are found to depend strongly on the injector spray orientation and on the injection timing.

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REFERENCES

Amsden, A.A., O'Rourke, P.J. and Butler, T.D. (1989) Kiva-II: A Computer Program for Chemically Reactive Flows with Sprays. *Los Alamos Report* LA-11560-MS.

Arcoumanis, C., Gavaises, M., and French, B. (1997) Effect of Fuel Injection Processes on the Structure of Diesel Sprays. *SAE Paper* No. 970799.

Bai, C., and Gosman, A.D. (1995) Development and Methodology for Spray Impingement Simulation. *SAE Paper* No. 950248.

Benedict, R.P. (1980) *Fundamentals of Pipe Flow, Wiley, New York.*

Dan, T., Takagishi, S., Senda, J. and Fujimoto, H. (1997) Organized Structure and Motion in Diesel Spray. *SAE Paper* No. 970641.

Dec, J.E. (1997) A Conceptual Model of DI Diesel Combustion Based on Laser-Sheet Imaging. *SAE Paper* No. 970873.

Dombrowski, N. and Johns, W.R. (1963) The Aerodynamic Instability and Disintegration of Viscous Liquid Sheets. *Chem. Eng. Sci*. **18**, 203.

Georjon, T.L., and Reitz, R.D. (1998) A Drop Shattering Collision Model for Multi-Dimensional Spray Computations. Accepted for publication, *Atomization and Sprays*.

Habchi, C. and Baritaud, T. (1997) Modeling Atomization and Breakup in High Pressure Diesel Sprays. *SAE Paper* No. 970881.

Hagerty, W.W. and Shea, J.F. (1955) A Study of the Stability of Plane Fluid Sheets. *J. Appl. Mech*., **22**, 509.

Han, Z., Parrish, S., Farrell, P.V. and Reitz, R.D. (1997) Modeling Atomization Processes of Pressure-Swirl Hollow-Cone Fuel Sprays. *Atom. Sprays*, **7**, 663.

Hountalas, D.T. and Kouremenos, A.D. (1998) Development of a Fast and Simple Simulation Model for the Fuel Injection System of Diesel Engines. *Advances in Engineering Software*, **29**, 13-28.

Huh, K.Y. and Gosman, A.D. (1991) A Phenomenological Model of Diesel Spray Atomization. *Proceedings of International Conference on Multiphase Flows*, Sept. 24-27, Tsukuba, Japan.

Kong, S.C., Han, Z.W. and Reitz, R.D. (1995) The Development and Application of a Diesel Ignition and Combustion Model for Multidimensional Engine Simulations. *SAE Paper* No. 950278.

Li, G., Fan, L., Han, Z. and Reitz, R.D. (1999) Modeling Fuel Preparation and Stratified Combustion in a Gasoline Direct Injection Engine. To appear *SAE Congress*.

Li, X. and Tankin, R.S. (1991) On the Temporal Instability of a Two-Dimensional Viscous Liquid Sheet. *J. Fluid Mech*. **226**, 425.

Liu, A.B. and Reitz, R.D. (1993) Mechanism of Air-Assisted Liquid Atomization. *Atomization and Sprays*, **3**, 1, 55-75.

Naber, J. and Reitz, R.D. (1988) Modeling Engine Spray Wall Impingement. *SAE Paper* No. 880107.

Nurick, W.H. (1976) Orifice Cavitation and Its Effects on Spray Mixing. *J. Fluids Eng*., **98**, 681-687.

Ohrn, T.R., Senser, D.W. and Lefebvre, A.H. (1991) *Atomization and Sprays*, **1**, 2, 137-153.

O'Rourke, P.J. and Amsden, A.A. (1987) The TAB Method for Numerical Calculation of Spray Droplet Breakup. *SAE Paper* No. 872089.

Parrish, S.E. (1997) Spray Characterization in a Motored Direct-Injection Spark-Ignited Engine. *Ph.D. Thesis*, University of Wisconsin, Madison.

Patterson, M.A. and Reitz, R.D. (1998) Modeling the Effects of Fuel Spray Characteristics on Diesel Engine Combustion and Emissions. *SAE Paper* No. 980131.

Pelloni, P. and Bianchi, G.M. (1999) Modeling the Diesel Fuel Spray Breakup by Using a Hybrid Model. Submitted *SAE Congress*.

Pilch, M. and Erdman, C.A. (1987) Use of Breakup Time Data and Velocity History Data to Predict the Maximum Size of Stable Fragments from Acceleration-induced Breakup of a Liquid Drop. *Int. J. Multiphase Flow*, **13**, 741-757.

Reitz, R.D. (1987) Modeling Atomization Processes in High-Pressure Vaporizing Sprays. *Atomization and Spray Technology*, **3**, 309-337.

Sarre, C.K., Kong, S.C. and Reitz, R.D. (1999) Modeling the Effects of Injector Nozzle Geometry on Diesel Sprays. To appear *SAE Congress*.

Schmidt, D.P., Nouar, I., Senecal, P.K., Hoffman, J., Rutland, C.J., Martin, J. and Reitz, R.D. (1999) Pressure-Swirl Atomization in the Near Field. To appear *SAE Congress*.

Senecal, P.K., Schmidt, D.P., Nouar, I., Rutland, C.J. and Reitz, R.D. (1998) *Modeling High Speed Viscous Liquid Sheet Atomization*, in preparation.

Squire, H.B. (1953) Investigation of the Instability of a Moving Liquid Film. *Brit. J. Appl. Phys.*, **4**, 167.

Su, T.F., Farrell, P.V. and Nagarajan, R.T. (1995) Nozzle Effect on High Pressure Diesel Injection. *SAE Paper* No. 950083.

Tanner, F.X. (1997) Liquid Jet Atomization and Droplet Breakup Modeling of Non-Evaporating Diesel Fuel Sprays. *SAE Paper* No. 970050.

Tennison, P.J., Georjon, T.L., Farrell, P.V. and Reitz, R.D. (1998) An Experimental and Numerical Study of Sprays from a Common Rail Injection System for Use in an HS-DI Diesel Engine. *SAE Paper* No. 980810.

Weber, C. (1931) On the Breakdown of a Fluid Jet. *ZAMP*, **11**, 136.

Final manuscript received in March 1999