

**DEVELOPMENT OF A DROPLET BREAKUP MODEL CONSIDERING
AERODYNAMIC AND DROPLET COLLISION EFFECTS**

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SUMMARY:

A model is currently under development to predict the occurrence and outcome of spray droplet breakup induced by aerodynamic forces and droplet collisions. It is speculated that these phenomena may be significant in determining the droplet size distribution in a spray subjected to acoustic velocity fluctuations. The goal is to integrate this breakup model into a larger spray model in order to examine the effects of combustion instabilities on liquid rocket motor fuel sprays. The model is composed of three fundamental components: a dynamic equation governing the deformation of the droplet, a criterion for breakage based on the amount of deformation energy stored in the droplet and an energy balance based equation to predict the Sauter mean diameter of the fragments resulting from breakup. Comparison with published data for aerodynamic breakup indicates good agreement in terms of predicting the occurrence of breakup. However, the model significantly overpredicts the size of the resulting fragments. This portion of the model is still under development.

TECHNICAL DISCUSSION:

The work to be discussed here is part of an ongoing numerical study of several aspects of the interaction between transverse acoustic fluctuations and atomized liquid sprays. Therefore it is relevant to the study of combustion instabilities in liquid propellant rocket motors since it is known that these instabilities result from a coupling between the combustion and fluid dynamic processes of the motor and the chamber acoustic resonance modes. It has been conjectured that for a spray subjected to acoustic waves, the displacements of the droplets due to the acoustic velocity fluctuations may have a significant impact on the spray pattern and droplet size distribution downstream of the injector.

In a previous study [Wert (1992)], numerical solutions were obtained for a model of a nonevaporating, pressure-atomized spray subjected to a transverse, one-dimensional acoustic field. This model only examined potential droplet agglomeration. Examination of the results showed an increase in mean droplet size downstream of the injector compared to the same spray injected into a quiescent medium. An issue not addressed in this earlier work, however, is that of possible drop breakup downstream of the near-injector primary atomization zone. Just as acoustic velocity fluctuations were shown to enhance droplet coalescence, therefore increasing droplet size, so too may these fluctuations lead to enhanced droplet fragmentation.

Downstream drop breakup, or secondary atomization, can occur through two processes, both of which

are of potential importance for acoustically perturbed sprays:

1. Aerodynamic breakup where the relative velocity between the drop and the continuous phase is sufficient to fragment the drop.
2. Collision-induced breakup where the energy of the colliding drops is sufficient to fragment the drops.

To examine the importance of these two fragmentation modes, a breakup model is currently under development. When completed, this submodel will be integrated into the overall spray model. Previous efforts to model droplet breakup have focused on only the aerodynamic breakup mode [O'Rourke and Amsden (1987) and Ibrahim et al. (1990).] However, what is clearly needed is a model able to treat both aerodynamic and collision-induced modes. The remainder of this discussion will describe the droplet breakup model in its current state of development and provide some preliminary comparisons with experimental data.

The droplet breakup phenomenon was approached from the standpoint of energy conservation; thus, the analysis began by integrating the differential mechanical energy conservation equation over the volume of a drop of arbitrary shape. The velocity of a fluid element within the drop was then decomposed into two components: a mean velocity, equal to the velocity of the droplet mass center, and a fluctuating component that is nonzero for a deforming droplet. Substituting this decomposition into the energy equation and subtracting out the terms for the mean droplet energy (much like developing the turbulent kinetic energy equation), yielded an integro-differential equation governing the deformation velocity field of the droplet. This equation contains terms related to the temporal variation of the deformation kinetic energy, the surface tension energy generation rate, the dissipated energy due to viscous effects and an energy source term that must be constituted to account for aerodynamic surface forces and droplet collision.

While the energy equation gives a necessary condition that the deformation velocity components must satisfy in order to satisfy mechanical energy conservation, it is not possible to use this equation to solve for the deformation velocity field within the drop. To do this analytically would require the solution of the Navier-Stokes equations subject to the boundary conditions at the drop surface. Clearly a generalized analytical solution is not possible and a full numerical solution of the flow field within each spray droplet is not practical for implementation into an overall spray model. Thus it was necessary to specify an appropriate deformation velocity field. To do this, the droplet was viewed prior to breakup as deforming in one of two fundamental modes:

1. From a sphere to an oblate spheroid. This approximates the flattening of the droplet experienced initially in the aerodynamic breakup mode [Nigmatulin (1991) and Clift (1978).]
2. From a sphere to a prolate spheroid. When fragmentation occurs after the temporary coalescence of two colliding droplets, the droplet initially deforms into a shape much like a prolate spheroid before further deforming into a dumbbell shape and fragmenting [Ashgriz and Givi (1987) and (1989).]

By including both prolate and oblate deformation modes, the model can account for the initial stages of both aerodynamic and collision-induced breakup effects.

A velocity field was subsequently developed which not only satisfies both of the above mode shapes,

but which satisfies incompressible continuity as well. Substituting this field into the deformation mechanical energy equation yielded a second-order, nonlinear ordinary differential equation. This equation governs the temporal variation of the streamwise axis of the spheroid, $2b$:

$$\frac{\rho_d V_d}{10} \left[2 + \left(\frac{a}{b} \right)^2 \right] \frac{db}{dt} \frac{d^2 b}{dt^2} - \frac{3}{2} \frac{a^2}{b^3} \left(\frac{db}{dt} \right)^3 + 4 \pi \sigma b S \left(\frac{b}{a} \right) \frac{db}{dt} + \frac{5}{2} \mu_d \frac{V_d}{b^2} \left(\frac{db}{dt} \right)^2 = E_i \quad (1)$$

where ρ_d is the drop density, V_d is the drop volume, $2b$ is the streamwise axis length, $2a$ is the cross-stream drop diameter, σ is the surface tension, $S(b/a)$ is a function of spheroid geometry, μ_d is the drop viscosity and E_i is the energy input source term. From left to right, the terms are: the deformation kinetic energy term, the surface tension energy term, the energy dissipation term and the energy input source term.

The development of a deformation velocity field allowed the explicit evaluation of all the terms of the deformation mechanical energy equation except one, the energy input source term, E_i . This term must incorporate both aerodynamic and collision effects. To evaluate the aerodynamic energy source term required knowledge of the pressure distribution on the droplet surface as a function of spheroid shape and relative velocity. In the paper of Masliyah and Epstein (1970), the authors reported numerically-determined surface pressure distributions at $Re = 1$ and $Re = 100$ for spheroids of various major to minor axis ratios. It should be noted that Reynolds numbers of the order of 100 are typical for sprays. Integration of the vector dot product between the surface pressure force and the surface velocity over the drop surface area yielded the aerodynamic energy input rate. At present, this has been done for the oblate data only ($b/a < 1$) as this is of most concern for aerodynamic-induced breakup. For simplicity, the derived points were correlated by the expression

$$\frac{E_{i,aero}}{\pi a^2 \left(\frac{1}{2} \rho_c U^2 \right) \frac{db}{dt}} = - \left[\left(1.037 - 0.388 \left(\frac{b}{a} \right) \right) f_1 + 0.854 f_2 \right] \left(\frac{Re}{6} \right)^{-0.11} \quad (2)$$

where $E_{i,aero}$ is the aerodynamic energy input term, ρ_c is the continuous phase density and U is the relative velocity while f_1 and f_2 are unit step functions such that $f_1=1$ for $b/a > 0.5$ and $f_2=1$ for $b/a < 0.5$. The Reynolds number is based on the cross-stream diameter, $2a$. Equation 2 correlates the data to within 2 % for the points at $Re = 100$. Note the weak Reynolds number dependence. The strongest dependence is on the spheroid geometry manifested through the axis ratio, b/a .

Equation 1 governs only the lowest-order deformation mode of a droplet prior to breakup. The final stages of droplet fragmentation are dominated by the development of higher-order modes (e.g. the dumbbell-shaped breakup of a droplet formed by two colliding droplets.) The reader is referred to Nigmatulin (1991) for a discussion of the various aerodynamic breakup modes. Since analytical treatment of these higher order modes was not desired for the sake of simplicity, the conditions under which a droplet fragments were specified in terms of a critical deformation energy level of the modeled fundamental modes. It is postulated that a single

critical deformation energy level for breakup exists for both collision and aerodynamic-induced breakup.

To estimate this critical energy level, the binary fuel droplet collision data of Ashgriz and Givi (1989) was used. In their work, the authors observed collisions of pairs of fuel droplets having various relative velocities and relative sizes. The critical energy level for breakup was derived by applying an energy balance to the test case in which the droplets just had sufficient relative velocity such that the droplet formed from the coalesced pair fragmented. From this energy balance, it was possible to derive the critical dimensionless energy:

$$\frac{E_{d,crit}}{\sigma D_o^2} = 1.48 \quad (3)$$

Here $E_{d,crit}$ is the critical deformation energy, which comprises the deformed kinetic and surface tension energies. This energy is nondimensionalized by the product of the drop surface tension and the square of the spherical diameter of the fragmenting drop, D_o .

Together, equations 1, 2 and 3 form the basis for predicting whether aerodynamic-induced breakup will occur. As a test, the model predictions were compared with droplet breakup data available in the literature. In the recent work of Hsiang and Faeth (1992), the authors conducted experiments on the properties of drop deformation and secondary breakup for shock wave initiated disturbances. To recreate the shock condition in the model, a step velocity change was specified. Noting that equation 1 is a second-order equation, the two specified initial conditions were that the drop was initially spherical and that it possessed no deformation kinetic energy ($b = 0$ and $db/dt = 0$, respectively.) Equations 1 and 2 were solved numerically using Heun's method. Care was taken to ensure a time step independent solution.

The model was used to determine what step change in velocity was necessary to bring about droplet breakup. This was done for several of the fluids considered by Hsiang and Faeth. Figure 1 shows the critical Weber number, $\rho_c U_o^2 D_o / \sigma$, necessary to bring about breakup of the drop as a function of the Ohnesorge number, $\mu_f / (\rho_o D_o \sigma)^{0.5}$ where U_o is the imposed step velocity change. The Ohnesorge number is a measure of the ratio of liquid viscous forces to surface tension forces. The points are the predictions of the model while the solid line is from the data presented by Hsiang and Faeth (1992), which includes data from past studies. For We above the line, the droplet is predicted to fragment; however, for We below the line, the drop merely undergoes deformation and oscillation. The model reasonably predicts the variation in the critical Weber

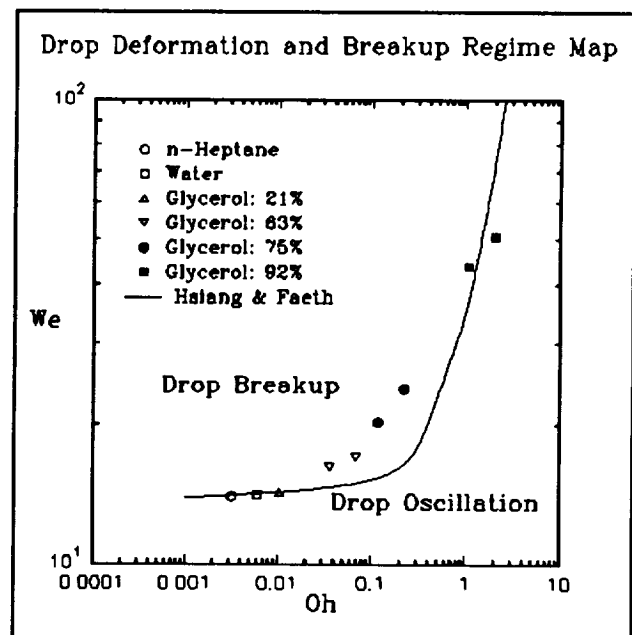


Figure 1. Deformation and breakup regime map.

number with increasing drop viscosity effects. The worst agreement is around $Oh = 0.2$, where the model predicts a critical We that is about 40 % high. It should be noted, however, that for sprays $Oh \leq 0.01$ is expected. For this range the agreement between the model and experimental data is excellent. Since the critical breakup energy was derived from considerations of drop collision data, its success in predicting aerodynamic breakup lends support to the hypothesis that, at least for small effects of viscosity, the critical breakup energy applies equally well to both collision and aerodynamic-induced fragmentation.

Having found the model able to adequately predict the occurrence of aerodynamic breakup, it was necessary to prescribe a method for predicting the outcome of breakup. For this, the simple energy balance method recommended by O'Rourke and Amsden (1987) and Ibrahim et al. (1990) was used. In this method, the deformation energy of the droplet (both kinetic and surface tension energy) is equated to the surface energy of a monodisperse group of spherical droplets. Thus the deformation energy is converted into surface energy of the fragments. Performing this energy balance allows the prediction of the size of the fragments, which is taken to be the Sauter mean diameter, SMD, of the fragments.

The results of using this method are shown in figure 2. The points are the model predictions, the solid line is the best-fit line provided by Hsiang and Faeth (1992) and the dashed lines represent the spread in their data. Examining figure 2 it is seen that the model predicts the trend of the data quite well, but significantly overpredicts the size of the SMD resulting from breakup. This was not unexpected. Recall that the oblate spheroid deformation model treats only the initial stages of

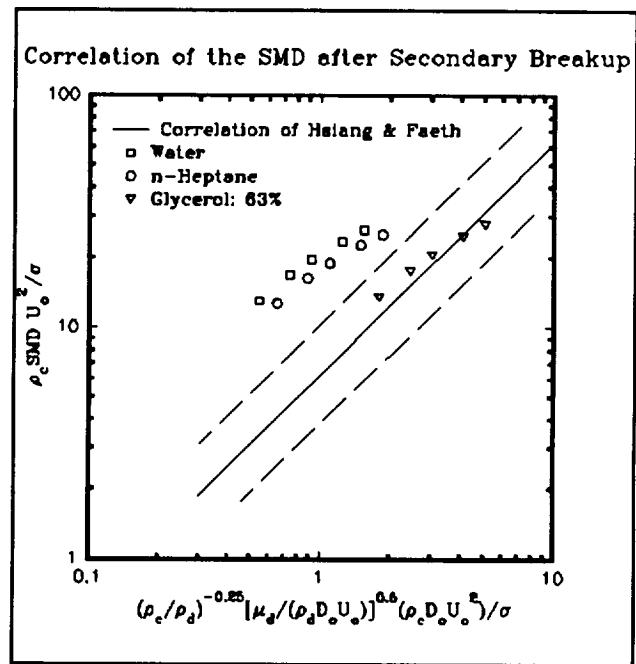


Figure 2. Correlation of the SMD after breakup.

droplet deformation. The higher-order deformation modes that ultimately lead to breakup are neglected in favor of the critical energy criterion of equation 3. Thus the model neglects the energy that enters the droplet through the aerodynamic forces acting on the higher-order deformation modes. It is believed that the neglect of this energy, which would be available to generate additional droplet surface area thus producing smaller fragments, is the source of the overprediction of the SMD. An attempt to account for the energy that enters the droplet as a result of these higher-order modes is under development.

Work that remains to be done on the model includes the derivation of E_i for droplet collision, further comparison of model predictions with available experimental data and integration of the breakup model into the larger spray acoustics model.

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