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The collision behavior of droplets of low surface tension fuels simulating near-critical droplet collision in high-pressure engines, and of droplets of dissimilar fluids simulating the atomization of unlike reactants, were experimentally studied. Results showed that the low-surface tension fuels do not readily disintegrate, while the dissimilar fuel droplets can actually merge. These collision dynamics were also computationally simulated using the techniques of front tracking and molecular dynamics. The computer algorithms developed for droplet collision were also extended to simulate the dynamics of wrinkled flames in complex flows, including flame-vortex interaction and the development of the Landau-Darrieus cells.

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DROPLET COLLISION IN LIQUID PROPELLANT COMBUSTION

(Grant No.: F49620-97-1-0205)

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Narrative

For the subject grant, experimental and computational research were conducted on the dynamics of droplet collision and flamefront motion. Accomplishments of these two projects are separately discussed in the following.

Droplet Collision Dynamics

The collisional behavior of droplets of low surface tension fuels simulating near-critical droplet collision in high-pressure engines were experimentally studied by adding detergent in conventional liquid fuels. Results show that, contrary to expectation, the colliding droplets spread out but do not readily disintegrate. Coalescence, however, was relatively difficult. Further experiments are being conducted to define the transition to splashing collision.

Collision of non-similar fluids was also experimentally investigated in order to understand the efficiency of impinging atomization of two jets of unlike reactants such as fuel and oxidizer. An unexpected result was observed in that when the two fluids are rheologically immiscible, they actually merged and form a single droplet upon collision at moderate Weber numbers. While it is not clear if mixing at the molecular level occurred, they were certainly mixed at the macroscopic level of the droplet. It is expected that the ability to mix two nominally immiscible fluids could have significant technological implication. Discussion has been initiated with material scientists to identify possible applications.

Droplet collision was simulated using two computational approaches, namely front tracking and molecular dynamics. By using the front tracking technique, the collision sequence in different collision regimes was simulated, the history of pressure and viscous dissipation within the droplet was spatially resolved, and the energy partition among the various modes was identified. By using molecular dynamics, bouncing and coalescence were successfully simulated for the first time

without the artificial manipulation of the inter-droplet gaseous film. Furthermore, splashing collision was also observed.

Flame Dynamics

Considerable efforts were expanded in the development of computational algorithms for the simulation of flame surfaces. The specific emphasis here is the recognition that much of previous efforts in flame simulation did not account for thermal expansion in crossing the flame front. Since heat release across the flame is significant, leading to substantial disparities in the gas density, assumptions of constant density flames are quantitatively inadequate in describing flame dynamics. Furthermore, since density jump across and interface also induces the Landau-Darrieus instability, neglecting thermal expansion also physically falsifies the phenomena of interest.

Two front-tracking algorithms were developed. The first adopts the multi-fluid approach used for the droplet collision simulation. Specifically, in droplet collision there is a great density disparity between the gas and the liquid, which are separated by a sharp deformable interface. This is similar to the situation of a wrinkled flame sheet separating the high-density unburnt gas from the low-density burnt gas. The second algorithm emphasizes the need for a sharp interface, recognizing that the interfaces in existing algorithms actually consist of several numerical grids and hence are not true discontinuities. The algorithm developed is believed to be the most accurate in the simulation of sharp interfaces.

By using these two algorithms, several flame dynamics problems were simulated, including flame-vortex interaction and flamefront instability in large-scale flows. In particular, it was found that wrinkling of a flame surface in the presence of a vortex is very much influenced by the Landau-Darrieus instability instead of the motion of the vortex itself, and that the wrinkling due to large-scale flows can suppress the formation of small-scale instabilities.

Publications

1. "A Front Tracking Method for the Motion of Premixed Flames," by J. Qian, G. Tryggvason, and C. K. Law, *Journal of Computational Physics*, Vol. 144, pp. 52-69 (1998).

2. "A Numerical Method for Solving Incompressible Flow Problems with a Surface of Discontinuity," by B.T. Helenbrook, L. Martinelli, and C.K. Law, *Journal of Computational Physics*, Vol. 148, pp. 366-396 (1999).

3. "The Role of Landau-Darrieus Instability in Large Scale Flows," by B.T. Helenbrook and C.K. Law, *Combustion and Flame*, Vol. 117, pp. 155-169 (1999).

4. "Molecular Simulation of Droplet Collision in the Presence of Ambient Gas," by S. Murad and C. K. Law, *Molecular Physics*, Vol. 96, pp. 81-85 (1999).