Prepared By: Hayley H. Shen, Ph.D.
Academic Rank: Associate Professor
Institution: Clarkson University
Department of Civil and Environmental Engineering

NASA/MSFC:
Office: Propulsion Laboratory
Division: Propulsion Systems
Branch: Performance Analysis

MSFC Colleague: Charles F. Schafer, Ph.D.

Contract No: NGT-01-008-021
The University of Alabama
Liquid fuel combustion process is greatly affected by the rate of droplet evaporation. The heat and mass exchanges between gas and liquid couple the dynamics of both phases in all aspects: mass, momentum, and energy. Correct prediction of the evaporation rate is therefore a key issue in engineering design of liquid combustion devices. Current analytical tools for characterizing the behavior of these devices are based on results from a single isolated droplet. Numerous experimental studies have challenged the applicability of these results in a dense spray.

To account for the droplets' interaction in a dense spray, a number of theories have been developed in the past decade. These theories were reviewed last summer by the author under the summer faculty fellowship program. Predictions from these theories show significant deviation of the evaporation rate from the single droplet result. Although the applicability of these theoretical results awaits experimental verification, their implementation into CFD codes can already be carried out to assess the magnitude of their effect.

This summer's study was concentrated on two tasks. One was to investigate how to implement the existing theoretical results, the other one was to explore the possibility of experimental verifications.

The current theoretical results of group evaporation are given for a mono-dispersed cluster subject to adiabatic conditions. The time evolution of the fluid mechanic and thermodynamic behavior in this cluster is derived. An example is given in the following figure (Bellan and Cuffel 1983, Fig.5).

\[
V_{Fg}^0 \quad T_g^0 \quad T_d^0 \quad R/R_0
\]

where \(V_{Fg}^0\) is the initial mass fraction of fuel in the gas phase, \(T_{g0}\) and \(T_{d0}\) are the initial droplet and gas temperatures respectively, and \(R/R_0\) is the ratio of current to initial droplet radius, \(\phi = \text{air-fuel mass ratio/stoichiometric air-fuel mass ratio.}\)

The above results are not in the form of a subscale model for CFD codes. In CFD codes, the concept requires that in each time step, the evaporation in each computational cell is
determined by the conditions in the cell. However, the conditions in each cell are solved from conservation laws that include the transport of properties among neighboring cells. Therefore, results from the adiabatic conditions in the current theories must be modified to obtain the necessary subscale model. Moreover, the given theoretical results have been obtained from numerical integrations which covered only a small range of parameters as shown in the previous figure. A much broader range of parameters must be derived for application.

Extension of the current theories to cover a wide range of parameters and deriving a subscale model for CFD codes require a longer period of study than a ten-week's work. An approximate solution has thus been derived and utilized in one of the CFD codes. This approach is discussed below.

In the derivation, the superposition principle is utilized. At first, a single droplet evaporation is modeled by setting the boundary conditions at the droplet surface and at the average midpoint between two droplets. The boundary conditions at the droplet surface are from the usual mass and energy balance law, together with the Clausius-Clapeyron relation. The boundary condition at the midpoint is approximated as the superposition of the condition at that location from two non-interacting droplets. This is illustrated in the following figure.

The result of this approximate solution yields \( \frac{m}{m_0} = 1 - Y_{\text{ambient}} \frac{R}{a} \), where \( m \) and \( m_0 \) are the evaporation rates for a droplet in a cluster and for a single isolated droplet respectively. This result is a first order approximation in terms of \( Y_{\text{ambient}} \) and \( R/a \).

Since the above formula only depends on the current local information, it can be used as a subscale model to test the effect of group evaporation. However, the average distance \( a \) between neighboring droplets is not available from current experimental data. Therefore, this formula cannot be utilized at the moment. An estimated distance between droplets is obtained by spreading all droplets equally in the computational cell. Using the mass flow rate and drop size distribution from a pressure-atomized spray, reported by Drallmeier and Peters (1991), the estimated distance between droplets yields \( Y_{\text{ambient}} \frac{R}{a} = 0.1\% \). Which is too low to produce any effect. This shows that it is very important to obtain the correct constitution of the clusters to evaluate the group evaporation effect.
In order to demonstrate the potential significance of the group effect in spray calculations, a parametric study was carried out utilizing the MAST code, developed by C.P. Chen at UAH. Three different evaporation rates have been used. The spray data given in Drallmeier and Peters (1991) is simulated. The total mass flux downstream from the injector is plotted in the following figure. The evaporation rate utilized to calculated the three curves are assumed to be constant fractions of the evaporation rate for a single isolated droplet. Three different fractions: 1, 0.8, and 0.5 are used.

In reality, the farther from the injector, the smaller the drop size, and the smaller the value $R/a$, while the value $Y_{ambient}$ increases. These characteristics result from the evaporation process. Therefore, the modification of the evaporation rate should not be constant as assumed above. The curves however are valuable for assessing the potential effect of group evaporation. As shown in the above figure, from no group effect to 50% of group effect, the mass flux can deviate by about 30%. Therefore correct account for evaporation in a cluster is important for liquid fuel engine designs. Further analytical work must be initiated to investigate this important mechanism.

Many theoreticians have strongly suggested the need for experimental work to verify their results. However, true spray evaporation is a very difficult phenomenon for accurate measurements. The idealized conditions used in theories, such as uniform, spherical droplets homogeneously distributed in space, are impossible to realize in the laboratory. Thus, even if measurements can be accurately made, the data may be ambiguous for verifying theories.
An alternative technique is proposed. Large crystal growth is a diffusion controlled process, similar to droplet evaporation. The mathematical structure of the two processes are identical in the growth/decay for the case of a single isolated particle. The $D^2 \cdot t$ law (D is the particle diameter and t is time), for the rate of growth/decay, has been verified in numerous experimental works for both phenomena. The observation and measurement of crystal growth is comparably much easier than droplet evaporation. Idealized conditions such as uniform, spherical, and homogeneously distributed particles are possible to create for crystal growth. A setup utilizing salt, distilled water, and ice as a temperature controlling material for boundary condition, with a nucleation controlled ice growth in a distilled water bath, is a candidate for such experiment. Comparison of growth rates between a single ice particle and a lattice of ice particles can be used to verify the theoretical prediction of the group evaporation effect.

One difficulty in the proposed experiment is the natural convection effect associated with temperature variation in the material. Such effect is not included in the idealized theoretical model and must be eliminated. From the product $\text{GrPr}^2$ (Gr is the Grashof number and Pr is the Prandtl number), which represents the time scale for diffusion vs that of natural convection, it is estimated that the natural convection can be neglected for small temperature gradients and small ice particles. For instance, a temperature difference of 0.01°C between the distilled water bath and the boundary, and an ice particle growing in the size range of 1mm, yield $\text{GrPr}^2<1$. Such condition is barely achievable in the laboratory. However, if successful, the potential of such experiment for verifying the convective group evaporation is great. Since in forced convection, the natural convection effect becomes negligible, the above limitation can be relaxed considerably. In spray combustion, forced convection is probably much more dominant. Experimental work in such case is therefore of more practical value.

In conclusion, more analytical work is required to extend the current group evaporation theories for a subscale model to be used in CFD codes. In view of the difficulty in idealized evaporation experiments, large crystal growth is a promising alternative for experimentally studying the group effect. Due to the similarity between droplet evaporation and large crystal growth, results from the group crystal growth may be usable for verifying the theories in group evaporation.

REFERENCES