Combustion of Moving Droplets and of Droplets Suspended within a Convective Environment: Transient Numerical Results

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Numerical Model

The problem considered is that of a single-component liquid fuel (n-heptane) droplet undergoing evaporation and combustion in a hot, convective, low pressure, zero-gravity environment of infinite expanse. For a moving droplet, the relative velocity (U_{∞}) between the droplet and freestream is subject to change due to the influence of the drag force on the droplet. For a suspended droplet, the relative velocity is kept constant.

The governing equations for the gas-phase and the liquid-phase consist of the unsteady, axisymmetric equations of mass, momentum, species (gas-phase only) and energy conservation. Interfacial conservation equations are employed to couple the two phases. Variable properties are used in the gas- and liquid-phase. Multicomponent diffusion in the gas-phase is accounted for by solving the Stefan-Maxwell equations for the species diffusion velocities. A one-step overall reaction is used to model the combustion [1].

The governing equations are discretized using the finite volume and SIMPLEC methods. A colocated grid is adopted. Hyperbolic tangent stretching functions are used to concentrate grid points near the fore and aft lines of symmetry and at the droplet surface in both the gas- and liquid-phase. The discretization equations are solved using the ADI method with the TDMA used on each line of the two alternating directions. Iterations are performed within each time-step until convergence is achieved. The grid spacing, size of the computational domain and time-step were tested to ensure that all solutions are independent of these parameters. A detailed discussion of the numerical model is given in [2,3].

Results and Discussion

The numerical model was used to investigate the combustion of a n-heptane droplet with an initial diameter (d_0) of 500 μm . Two cases were studied: a) a moving droplet, and b) a suspended droplet within a convective environment. The results presented here are for an ambient temperature (T_{∞}) of 1000 K, an ambient pressure (P_{∞}) of 1 *atm*, an initial droplet temperature (T_0) of 297 K and initial Reynolds numbers (Re_0) of 8, 10 and 50.

Table 1 compares the lifetimes of both moving and suspended n-heptane droplets for the Reynolds numbers considered. The table contains interesting results that need to be explained. For example, the lifetime of a moving droplet with $Re_0 = 50$ is longer than the lifetimes of moving droplets with initial Reynolds numbers of 8 and 10. Furthermore, for the same initial Reynolds number, the suspended droplet burns out faster than its moving droplet counterpart in two cases ($Re_0 = 8, 50$), while for $Re_0 = 10$, the result is opposite. In the remainder of this section, the results presented in Table 1 will be discussed in more detail.

Figure 1 shows the time history of the dimensionless droplet diameter squared $(d/d_0)^2$, Reynolds number, Damköhler number and evaporation constant (*K*) for a suspended and a moving droplet with $Re_0 = 8$. The suspended and moving droplet developed envelope flames at approximately the same time (t = 30 ms). Considering the droplet lifetimes (231 and 240 ms), this happened at a very early stage. Once the envelope flame formed, it remained for both droplets until the end of their lifetimes. Thus during most of the droplet lifetime, both the suspended and the moving droplet experience the same flame configuration. This implies that the two droplets will exhibit similar burning behavior and thus similar lifetimes. Figure 1(a) shows that to be true. The droplets in both cases have very similar diameter squared time histories.

	$Re_0 = 8$	Suspended	$t_d = 231 \ ms$
$P_{\infty} = 1 atm$		Moving	$t_d = 240 \ ms$
$T_{\infty}=1000\ K$	$Re_0 = 10$	Suspended	$t_d = 335 \ ms$
$T_0 = 297 K$		Moving	$t_d = 243 \ ms$
$d_0 = 0.5 mm$	$Re_0 = 50$	Suspended	$t_d = 250 \ ms$
		Moving	$t_d = 316 \ ms$

Table 1: n-heptane droplet lifetimes for suspended and moving droplets.

Figure 1(b) shows the time history of the instantaneous Reynolds number (*Re*) for both cases. Both Reynolds numbers decrease monotonically with time however, they decrease at different rates. The Reynolds number is defined as $Re = d(t)U_{\infty}(t)/v_{\infty}$, where d(t) and $U_{\infty}(t)$ are the instantaneous droplet diameter and freestream velocity. The freestream velocity remains constant for the suspended droplet. As a result, the Reynolds number changes only with the droplet diameter. However, for the moving droplet, the droplet diameter decreases, and the droplet velocity decreases due to drag. Thus the Reynolds number for the moving droplet decreases faster than that for the suspended droplet.

The higher Reynolds number associated with the suspended droplet implies a stronger convection. This results in a higher evaporation constant for the suspended droplet than for the moving droplet as shown in Figure 1(d). At the beginning of the droplet lifetime, the evaporation constants for the two cases are very close and both increase rapidly due to the high temperature environment. A difference between the evaporation constants appears at about one tenth of the lifetime due to the difference in the convective strength for the two cases. At the relatively low initial Reynolds number of 8, the difference in the evaporation constants between the suspended droplet and the moving droplet remains small during the entire droplet lifetime. As a result, the droplet lifetimes for the two cases are very close.

Figure 1(c) compares the instantaneous Damköhler numbers for the two cases. Here, Damköhler number is defined as:

$$Da = \frac{R(t)}{U_{\infty}(t)} A \rho_{\infty}^{a+b-1} W_{f}^{1-a} \left(\frac{1}{W_{o}}\right)^{b} \exp\left(-\frac{E_{a}}{R_{u}T_{\infty}}\right)$$

where W_o and W_f are molecular weights for the fuel and oxygen, and a, b, A, and E_a are constants. The Damköhler number is proportional to the ratio of droplet diameter to instantaneous freestream velocity. This ratio is the characteristic convective time-scale. Thus, Da is proportional to $d(t)/U_{\infty}(t) = t_{conv}$. Figure 1(c) shows that the Damköhler number for the suspended droplet decreases with time, while for the moving droplet case it increases slowly with time. The former result is expected since for the suspended case, U_{∞} is constant while the droplet diameter decreases. This results in a monotonic decrease in Da. For the moving droplet case, both d(t) and $U_{\infty}(t)$ decrease. The resulting trend in Damköhler number is not obvious. For $Re_0 = 8$, it seems that the droplet velocity decreases slightly faster than the droplet diameter.

For $Re_0 = 50$, both droplets ignite in the wake areas far downstream. After ignition, for the

moving droplet case, the flame moves toward the droplet slowly, and finally forms an envelope flame (at approximately t = 270 ms) near the end of its lifetime. For the suspended droplet, no envelope flame is developed throughout its lifetime, and the wake flame remains at approximately the same location for most of the droplet's lifetime. At t = 237 ms the wake flame trailing the suspended droplet extinguishes. Thus, a pure evaporation process dominates in both cases. In the absence of envelope flames, the difference in Reynolds number histories between the two cases (*Re* is smaller for the moving droplet due to its deceleration) is the only cause for their different lifetimes shown in Table 1.

The combustion behavior for the two cases at $Re_0 = 10$ is quite different from the cases discussed above. Although the Reynolds number for the suspended droplet is again higher than that for the moving droplet throughout the droplet lifetime, the lifetime of the suspended droplet is approximately 40% longer than that of the moving droplet. The big difference in droplet lifetimes, is caused by the difference in flame configurations. The moving droplet develops an envelope flame at an early stage (t = 40 ms) of its lifetime. In contrast, the suspended droplet exhibits a transition flame (the flame partially surrounds the droplet) during most of the droplet lifetime. As a result, the front of the droplet is exposed to the ambient temperature, leading to a longer lifetime for the suspended droplet.

The results presented above for the three different Reynolds numbers seem to suggest that a moving droplet tends to develop an envelope flame at some stage during its lifetime, whereas a suspended droplet develops an envelope flame only at low initial Reynolds numbers. The flame configurations present in a burning droplet are a function not only of the Reynolds number, but of the Damköhler number as well.

For all three initial Reynolds numbers, the Damköhler number for suspended droplets always decreases with time, while Da for moving droplets always increases with time. The Reynolds number decreases with time for both moving and suspended droplets. Figure 2 shows the quasi-steady solutions for flame configurations as a function of Da and Re for a n-heptane droplet with a diameter of 500 μm . The quasi-steady solutions were obtained using a previously developed code [3] that was modified to include the current multicomponent diffusion formulation and kinetics parameters. The x's correspond to the quasi-steady solutions and the dash-dot lines on the figure indicate the predicted boundaries between the different flame configurations. Note that these flame configuration boundaries are for a fixed diameter as compared to the decreasing diameter present in the unsteady problem. Since both Da and Re scale with diameter, we would expect the flame configuration boundaries to move down and to the left on the figure for decreasing diameter.

Figure 2 also shows the actual paths of the moving (indicated with 'M') and suspended (indicated with 'S') droplets in the Da - Re plane. When $Re_0 = 8$, an envelope flame forms for both the moving and suspended droplet very early in the droplet lifetime. For $Re_0 = 10$, both droplets ignite to form a transition flame near the start of the droplet lifetime. The decrease in the droplet diameter coincides with the aforementioned shift (to the left and down) in the configuration boundary between an envelope and a transition flame. The increasing Damköhler number present for the moving droplet case causes a rapid change from a transition to an envelope flame while the decreasing Damköhler number for the suspended droplet results in a transition flame configuration throughout the droplet lifetime. One can also see from the figure that in the $Re_0 = 50$ the moving droplet may eventually form an envelope flame whereas the suspended droplet may not form an envelope flame.



Figure 1: Comparison between moving droplet and suspended droplet combustion for $Re_0 = 8$ ($d_0 = 500 \ \mu m$ and $T_{\infty} = 1000 \ K$).



Figure 2: Flame configurations in the Damköhler vs. Reynolds number plane: $d = 500 \, \mu m$.

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