Numerical Investigation of Droplet Vaporization and Combustion Models Spray Combustion

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INTRODUCTION In spray-combustion numerical computation, the droplet vaporization model is usually assumed by simple empirical or analytical formula based on the studies of quasi-steady single-droplet vaporization and combustion in a stagnant or convective flow. By employing this formula in spray-combustion computation, the droplet vaporization rate in which the historical states of the droplet was neglected is presumed to obtain unique values. For instance, the correction formula for droplet vaporization in a convective flow was proposed by Faeth and Lazar [1]. Recent studies of Chen [2] and Jiang et al. [3,4], however, indicate that multiple solutions of flame configurations and vaporization rates exist under certain flow conditions for a fuel droplet vaporizing in purely oxidizing or reactive flows. The flame configuration and the associated vaporization rate depend upon the initially assumed state around the droplet and the process it experiences. This result clearly suggests that an appropriate evaluation for the droplet vaporization rate involves not only the instantaneous ambient conditions around the droplet, but also the historical processes the droplet undergoes. It is thus apparent that the existing popularly-adopted droplet vaporization models, such as that proposed by Faeth and Lazar [1], fail to account for such important multiple flame-configuration effects.

In practical spray-combustion processes, spray droplets are generally generated from a relatively cool region near the fuel nozzle, and the droplet temperature is initially lower than its wet-bulb point before entering the hot combustion zone. The droplet is inevitable to experience the heat-up process during its early stage of lifetime. With a quasi-steady assumption, the transient effects of the droplet heat-up process on vaporization rates was not taken into account. These effects can be so significant as shown later by the present study that they should not be ignored. Furthermore, the quasi-steady analyses can not account for the transient variation in the vaporization rate as the droplet's ambient conditions change rapidly. The objective of the present study is thus to demonstrate where and how the existing droplet vaporization models fail in estimating the droplet vaporization rate in spray-combustion computations and then to make suggestions for modifying the models.

FORMULATIONS The physical problem is described to represent a convective air-flow over a vaporizing spherically-shaped droplet. Axisymmetric gas- and liquid-phase flows are numerically simulated by solving the time-dependent Navier-Stokes equations. The fuel droplet is assumed to vaporize in an environment without gravity. The ambient pressure is assumed to be well below the critical value of the fuel droplet. Effects of thermal radiation and droplet deformation are also neglected, since at low pressures those are of secondary importance. Furthermore, since the Weber number for a typical case in the present study is approximately 1.0 (<<20), a nearly spherical droplet can be assumed [5]. Fick's law is assumed in the species diffusion velocity. Variations in specific heat, viscosity, diffusion coefficient, and thermal conductivity over temperature have been taken into account through the appropriate kinetic-theory models or correlations from Reid et al. [6]. The specific heat of the gas mixture is evaluated from the ideal gas mixing rule. The governing equations of the gas-phase include continuity equation, momentum equation, energy equation, species conservation equation and equation of state. The liquid-phase consists of the same governing equations of the gas-phase but it excludes the species conversation equation and equation of state. The general form of governing equations for both phases are given below

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial}{\partial x}(\rho u\phi-\Gamma_\phi\frac{\partial\phi}{\partial x})+\frac{1}{r}\frac{\partial}{\partial r}(r\rho v\phi-r\Gamma_\phi\frac{\partial\phi}{\partial r})=S_\phi \tag{1}$$

The initial conditions corresponding to the sudden injection of a cold droplet into a uniform flow are:
(i) gas phase:

$$u = u_\infty,\ v = 0,\ p = p_\infty,\ T = T_\infty,\ \rho = \rho_\infty,\ Y_f = 0,\ Y_o = Y_{o,\infty}$$

(ii) liquid phase:

$$u = v = 0,\ T=T_0, Y_f=1,\ Y_o=0,\ p = p_\infty,\ \rho =\rho_0$$

The boundary conditions in term of spherical coordinates (r_f,Θ)originating from the fuel-droplet center are given as follows:

(i) upstream inflow($r_f = r_{f,\infty}$, $0 \le \theta \le \pi/2$)

$$u = u_\infty , v = 0, T_g = T_\infty , Y_f = 0, Y_o = Y_{o,\infty}$$

(ii) Downstream outflow($r_f = r_{f,\infty}$, $\pi/2 \le \theta \le \pi$)

u_∞,v, T_g, Y_f and Y_o are extrapolated from the inner region.

(iii) axis of symmetry ($0 \le r_f \le r_{f,\infty}$, $\theta = 0$ or π)

$$v = \frac{\partial T}{\partial r} = \frac{\partial u}{\partial r} = \frac{\partial Y_o}{\partial r} = \frac{\partial Y_f}{\partial r} = 0$$

(iv) droplet surfcae ($r_f = r_s$)

$$\dot{m}'' = \dot{m}'' Y_f - \rho_g D_g \left(\frac{dY_f}{dr}\right)_{s,g} \tag{2}$$

$$\dot{m}'' Y_o = \rho_g D_g \left(\frac{dY_o}{dr}\right)_{s,g} \tag{3}$$

$$\lambda_g \left.\frac{dT}{dr}\right)_{s,g} = \lambda_l \left.\frac{dT}{dr}\right)_{s,l} + \dot{m}'' L \tag{4}$$

$$\mu_g \left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r_s} + \frac{1}{r_s}\frac{\partial v_n}{\partial \theta}\right]_{s,g} = \mu_l \left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r_s} + \frac{1}{r_s}\frac{\partial v_n}{\partial \theta}\right]_{s,l} \tag{5}$$

$$(v_{g,\theta})_s = (v_{l,\theta})_s \tag{6}$$

$$\rho_g (v_{g,n} - v_{s,n}) = \rho_l (v_{l,n} - v_{l,n}) = \dot{m}'' \tag{7}$$

$$\ln\left(\frac{p_{g,s}}{p_{ref}}\right) = \frac{L}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T_{g,s}}\right) \tag{8}$$

Eq.(2) to Eq.(7) are obtained from the species, energy, shear stress and mass-flux conservation at the interface. Since phase equilibrium is assumed at the droplet surface, the Clausius-Clapeyron relation, Eq. (8), is employed to relate the vapor pressure to the temperature of the vaporizing droplet. The temperature along the droplet surface thus is not uniform.

NUMERICAL METHODS The governing equations of the gas and liquid phases are discretized into their algebraic counterparts based on the finite-volume method, and the SIMPLER algorithm [7] is applied to solve the gas and liquid flow fields. The line-by-line TriDiagonal-Matrix Algorithm, featuring a back-and-forth sweep that alternates direction, is used as the equation solver, and incorporates the block correction procedure [8] for increasing the computational efficiency. The power-law scheme is used for the convective and diffusive flux over the control volume surface. In order to reduce the truncation errors due to the non-uniform grids, the grid mesh of physical domain is obtained by the hyperbolic tangent distribution method [9]. The grid system consists of 51×41 grids for the gas-phase flow, and 25×41 grids for the liquid-phase flow. Since the governing equations are not only highly nonlinear, but also coupled, the solution is obtained by underrelaxing each variable and using an iterative procedure. Both phase solutions are iterated until the interface conditions are satisfied. The solution for the interface variables is solved by employing an efficient Newton-Raphson scheme. Finally, the relative velocity between the gas-phase flow and the droplet gradually decreases with time due to the drag.

RESULTS AND DISCUSSIONS An n-ocatane (C_8H_8) fuel droplet in an air convective flow serves as the basis for the present study. The ambient gas pressure is 1 atm and the initial ambient temperature is 1000 K. The initial relative velocity between the droplet and the free stream is selected to be 40 m/sec. The initial droplet temperature and droplet radius are 300 K and 100μm, respectively. In the early stage, since most of the heat transferred between the two-phase is used to heat up the droplet, only a small fraction of the heat vaporizes the fuel droplet. This results in the reactivity and temperature around the droplet being low. As time elapses, more fuel vapor is emitted and reacts with the hot air in the downstream region of the droplet, leading to the ignition of a trailing wake flame therein. As the relative velocity between the droplet and the ambient air decreases with time due to the drag, the leading zone of the wake flame moves forward against the flow. The flame thus evolves from a wake-one, to a side-one, and then to an envelope-one. The temporal evolution of the flame configuration and the associated droplet vaporization flux are presented in Fig.1. It is interesting to note that the vaporization flux exhibits a marked increase when the flame evolves from a transition-type to an envelope-type. This result clearly implies that the vaporization rate is deeply related to the flame configuration.

The results predicted by two selected quasi-steady models are compared with those of the present study in Fig. 2, to demonstrate the limitation of quasi-steady models for the analysis of a transient droplet burning in spray combustion. The first selected quasi-steady model was proposed by Faeth and Lazar [1] which has been described previously. This model can be applied to both vaporization and combustion cases. However, an

ignition criterion has to be employed to determine the droplet burning status before the vaporization or combustion model is chosen. The second quasi-steady model was proposed by Chen [2] and Jiang et al. [3]. This model includes the lower- and upper-branch solutions corresponding to an initially non-burning and burning droplet, respectively. In the early stage of the droplet lifetime, all the quasi-steady models fail in the prediction of the droplet vaporization flux. This result is not surprising since the quasi-steady models do not take account of the droplet heating and tend to overestimate the vaporization flux. Among the quasi-steady models, the vaporization model of Faeth and Lazar [1] substantially underestimates the droplet vaporization flux when an envelope flame occurs. The lower-branch solution of Chen [2] and Jiang et al. [3] offers the best match in trend with the present transient solution. However, without considering the droplet heat-up process, the lower-branch solution tends to release more fuel vapor initially and to ignite the droplet at an earlier instant. As a result, the envelope flame appears earlier and the vaporization flux is over-predicted. The predictions by the upper-branch solution of Chen [2] and Jiang et al. [3] and the combustion model of Faeth and Lazar [1] are even worse, since both solutions' presumption of an initially burning droplet is far apart from the initial droplet status. It is interesting to note that despite of their poor agreement with the present transient solution during the early stage of the droplet lifetime, the predictions by all the quasi-steady models except the vaporization model of Faeth and Lazar [1] are in good agreement with the present transient solution during the final stage of the droplet lifetime when an envelope flame encloses the fuel droplet and the heat for droplet heating is minimal.

The transient effects are also important when the droplet experiences a sudden change in its ambient conditions. This is illustrated in Figs. 3, where the vaporization flux predicted by the quasi-steady models are compared with the transient solution for an assumed situation in which the temperature of the approaching flow changes suddenly from 1000 K to a lower value of 600 K at a non-dimensional time of 4000 when an envelope flame has been established enclosing the droplet. As the flow temperature changes, the predicted vaporization flux decreases immediately for all solutions. An examination of the predicted flame configuration of the transient solution reveals that as the flow temperature reduces to 600 K at the non-dimensional time of 4000, the envelope flame can still be sustained around the droplet. It is also true for the upper-branch solution. Therefore, the predictions by the upper-branch solution and the combustion model are in agreement with those of the transient solution. The envelope flame, however, cannot be sustained in the lower-branch solution for such low flow temperature, resulting in a lower prediction in the vaporization flux. The same story is also found in the prediction by the vaporization model of Faeth and Lazar [1].

CONCLUSIONS The transient burning process of a convective droplet in air was predicted, using detailed numerical simulations for both gas- and droplet-phase flows. The flame configuration of a droplet suddenly placed in a hot air starts with pure vaporization, and progresses through a wake flame, a transition flame, and then an envelope flame. The Reynolds number decreases as the droplet burning proceeds because of vanishing droplet-size and slip-velocity. The droplet vaporization flux increases with time through the whole droplet lifetime. The quasi-steady models were found to be inadequate in the initial droplet heat-up period when the heat transfer from the ambient is mainly contributed to heating other than vaporization. As an envelope flame is exhibited around the droplet in the final stage of the droplet lifetime, the predictions by the quasi-steady models except the vaporization model of Faeth and Lazar [1] are in good agreement with the transient solution. The quasi-steady models, except the upper-branch solution, fail in predicting the flame configuration as the ambient temperature drops suddenly.

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FIGURES:

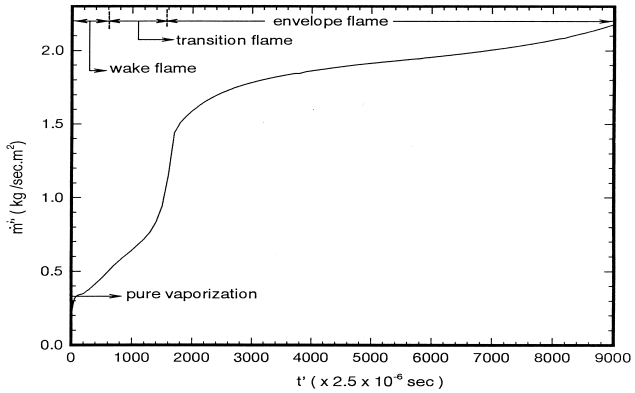

Fig. 1 The vaporization flux verse time predicted at the droplet radius 100μm.

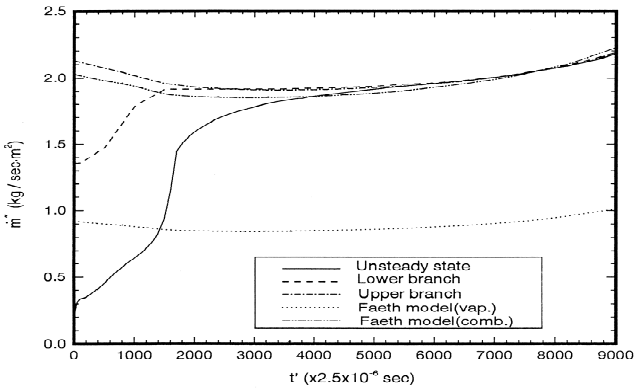

Fig.2 Comparison of the droplet vaporization flux at the droplet radius 100μm verse time predicted between present transient analysis and quasi-steady analysis.

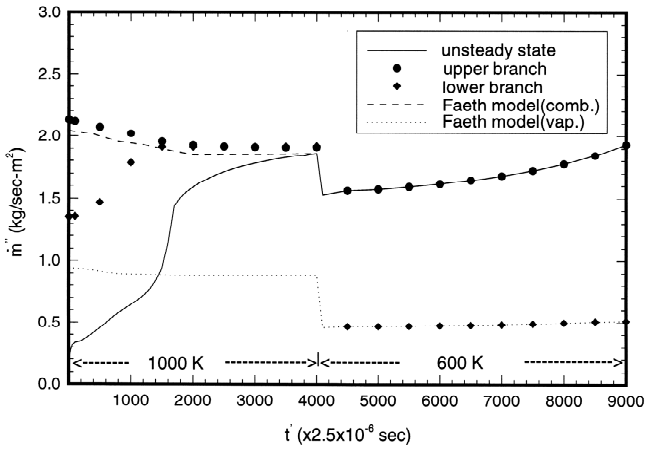

Fig. 3 Comparison of the droplet vaporization flux at the droplet radius 100μm from flow temperature 100 K to 600 K verse time predicted between present transient analysis and quasi-steady analysis.