Numerical Analysis of Unsteady Droplet Gasification Mechanism in Hot Environment

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Abstract

Canonical fluid dynamic analysis is applied to account for the contributing physical mechanisms and the order of magnitude of the transient moving droplet gasification rate based on energy and species conservation equation as eigenvalues in the general aerothermochemical environment. The results show women, with sufficient analytical self-organized thermo-fluid-chemical mechanisms of dynamic evolution, sequenced by preheating of exterior gaseous mixture and interior liquid, gasification, ignition, combustion, and stages of transient developments of flame structure. Physical mechanisms and exterior interior binding reveal that there are gasification contribution partition changes caused by the convective and conductive transport processes, thermal accumulation and time-dependent variation of Spalding-Godsave (S-G) potential accompanied by the dynamic evolution. We found that both the exterior/interior convection and transient heating in the early phase play key roles in preheating period. This is followed by the gaseous phase ignition, exothermic chemical reaction and transient flame configuration, which control the gasification rate. In the full transient period, the external flow field’s contribution starts at approximately 86\% of the intrinsic gasification contribution to 100\%, whereas the interior flow commences with -10\% of intrinsic field gasification rate, but vanishes to nearly zero, respectively, when the quasi-steady state is reached.

1 Introduction

The interfacial exchanges of mass, energy and momentum between a liquid fuel droplet and its gaseous environment are the fundamental processes of profound importance in the vaporization and combustion of fuel sprays and multi-phase fluid flow involving phase change. Celebrated isolated droplet gasification law, pioneered by Spalding (1955), successfully predicts the burning rate of a spherical diffusion flame stabilized in a uniform oxidizing atmosphere of a stationary droplet. Success of the Spalding’s law, of an isolated, stationary droplet gasification law, has served as the foundation of modern droplet theory but more importantly it has inspired the new research directive toward the understanding of droplet behaviors under general thermofluidchemical mechanisms of dynamic evolution, manifested by the interfacial exchange between the exterior and interior flow fields of a regressing droplet in the critical stage of the commencement of droplet combustion.

Of particular importance is the transient phenomena of preheating, ignition, flame developments of a droplet, which is suddenly exposed to a hot stream. The critical issues of interest, here, are the knowledge on the nature and impacts of the exchange mechanisms and their intercoupling on the dynamic and combustion evolution, manifested by the interfacial exchange between the exterior and interior flow fields of a regressing droplet in the critical stage of the commencement of droplet combustion.

The objectives of this paper are to examine the details of the evolutionary developments, identification of major mechanisms of exchange processes, which are prompted by fluid processes that occur in the exterior and interior flows, and their percentile contributions on the global rate processes and exchange processes throughout the injection to the state of quasi-steady state combustion. We adopt the canonical theory of fluid dynamics, which was devised by Chiu [1] for the axiomatic presentations of the structures and interface exchange rates of the flow fields in terms of eigenvalues and eigenfunctions of the Dirichlet's problems governed by the systems of non-linear partial differential equations. The theory serves to the identification of all the exchange mechanisms, binding mechanisms, together with the percentile contribution of each mechanism on the construction of the flow field and the rate processes, thereby yielding information on the specific importance of each contributing mechanism on the flow structure and rate processes during the transient process. Canonical theory yields startling universal and simple analytical framework with mathematical exactness and elegant structural construction which capture the roles played by full non-linear mechanisms in the coupled systems of Navier-Stokes equation. The method has been successfully applied in various problem areas including droplet combustion, and boundary layer flow [1-4].

2 Canonical formulation

The detailed account of the canonical formulation is reported, elsewhere see for example Chiu [4], and thus will not be reproduced here, however the canonical law of exchange for the single droplet gasification rate in general fluid environment (GFE) is presented below.

Briefly, the equations governing the flow of a reacting gas over an isolated, gasifying droplet depicted in Figure 1, are given by the conservation laws expressed in Shvab Zeldovich formalism. The law of gasification of an isolated droplet moving in GFE is expressed in terms of the eigenfunctions of the conservation equations of $J_{\alpha\ell}$ or those of $J_{\alpha i}$ as follows:
The transient analysis of hot air flow over an n-octane \((\text{C}_8\text{H}_{18})\) droplet is performed by applying the canonical fluid dynamic theory to interpret the physical sub-mechanics which drives the interfacial heat and mass exchanges. The grid systems for the exterior flow and interior flow are 75x41 and 25x41 respectively. The droplet surface temperature is initially 300K and the hot environment is at 1000K. The droplet with radius 100µm is exposed in the hot environment at Reynolds number 68. The transient droplet combustion simulation is conducted with the convective time step approximately at 2.5x10^{-6} sec.

### 3.1 Law of drag force modulation

Upon releasing the droplet in the hot flow stream, the drag force reduces the droplet relative velocity \([5]\). Hence, the latter velocity has been updated in each time step by the drag modulation. The total drag consists of pressure drag, friction drag and thrust drag, refer to \([5]\).

The decrease in the relative velocity \(\Delta u_{re}\) is calculated from the deceleration rate \(du_{re}/dt\) as following:

\[
\frac{du_{re}}{dt} = \frac{3}{8} \frac{\rho}{\rho_0} \frac{U^2}{C_D} \frac{S_{dr}}{D_{dr}} \frac{\Delta u_{re}}{dt}
\]

Thus, the next time far field velocity \(u(x,r,t+\Delta t)\) is obtained by the following equation,

\[
u(x,r,t+\Delta t) = u(x,r,t) + \Delta u_{re}
\]

### 3.2 Canonical theory analysis

In order to understand the time historical development of the transient droplet gasification, the calculations of the canonical physical submechanisms \(m\) are performed to investigate the order of magnitude of each contribution and the interpretations are described in the following paragraphs.

When the 100 µm droplet with Reynolds number 67.86 is exposed in the hot convective environment, it starts to be heated up and vaporize by a preheated air. In Figure 2, the interior temperature contour plot indicates that the heat transfer from the gas phase prompts the internal thermal circulation, induced by Hill’s vortex motion inside the droplet. The fuel vapor is carried behind the droplet and mixes with the oxidizer.
to form the combustible mixture, then ignition occurs initially located at tenfold radius with the wake flame configuration. As time evolves, the chemical reaction enhances and total drag force modulates the relative velocity between the gas and liquid phase, thus the initial wake flame moves toward the droplet. At characteristic time 3000, the transition flame is formed around the droplet ambience as shown in Figure 3 and the flame begins to envelope the whole droplet surface. At t=3000, the envelope flame is observed which indicates the combustion type transits from the premixed combustion to the diffusion combustion type.

In the transient analysis of droplet combustion, the interior heat-up period and total drag modulation dominate the initial transient period of droplet lifetime. By inspecting Figure 2, at t=150, the interior heat conduction is dominated by the diffusion effect inside the droplet. After internal circulation flow is formed, due to the relative velocity between two phases, the convection effect takes over the interior heat transfer, but when the velocity difference becomes smaller, after t=300. The diffusion effect becomes a dominant factor.

By performing the canonical droplet calculations, the physical sub-mechanisms contributing to droplet gasification are identified and shown in Figures 4 and 5. Details of the canonical analysis follows: Firstly, we investigate the accumulation of S-G potential, m9 which yields the negative contribution and tends to reduce the gasification rate. The reason is that the heat from the exterior flow provides for droplet heat up to raise the surface temperature to the boiling temperature. When the latter state is reached, at approximately, t=3000 the m10 has no contribution.

The convective transport and dissipation of S-G potential, m0 increases the degree of mixing and heat transfer inside the droplet, thus this value has positive contribution to the gasification rate as shown in Figure 4. The m0 competes against the m10 value along the time, and both become no net contribution after the boiling temperature is reached. It appears that m0 and m10 form a micro-equilibrium configuration at each stage.

After the peak value of m0 and m10, the interior flow becomes more stable and ignition occurs behind the droplet as described above. Thus, chemical reaction term, m6 will dominate the overall aerothermal behaviors. At the beginning, the conductive transport of S-G potential, m1 only accounts for major percentile contribution, but after commencement of combustion, the m1 value remains at a constant value, but smaller in percentile contribution compared to others sub-mechanisms. The reason for the nearly constant m1 value of this contribution is that the Spalding gasification is uniquely determined by the states of the gaseous environment and the droplet surface.

The m1 value indicates that the variable property induces the residual transport of S-G gasification potential. After onset of ignition, the m1 value decreases gradually. As flame type becomes transition flame, the m3 value becomes negative contributing to the droplet gasification rate.

Referring to the formula of convective transport of S-G potential, $-m_{3} = \phi^\Psi_{\alpha T} V\ln(1+\gamma)$, it has the positive contribution when the velocity is in the direction opposite to that of the temperature gradient. Before onset of ignition, there exists positive contribution to the gasification rate due that the directions of hot air velocity and temperature gradient are in the opposite direction. But after ignition, the hot flow velocity is in general in the same direction as the local temperature gradients, thus the m3 contribution becomes negative. Physically speaking, the Stefan flow forms around the droplet surface and blocks the convective heat transfer to the droplet surface.

After ignition, the chemical reaction contribution, m6 becomes dominant compared to other submechanisms. And during transition flame period, there is a sharp increase and reaches the peak at formation of envelope flame. Furthermore, according to the evolutional figure of accumulation and time dependent variation of S-G potential, m8 and time variation of pressure, m2, both values have negative contributions to the droplet gasification, but each of them is small compared to the reference gasification rate against time.

The values of $\Psi_{\alpha T}$ and $\Psi_{\alpha T}^{*}$ reflects the extent of the contribution of intrinsic contribution by the exterior and interior flow processes. It is observed that when the droplet temperature increases during preheating, $\Psi_{\alpha T}$ decreases, hence each interior contribution decreases and ultimately vanishes when the gradient and the temporal change of the flow variables vanish. It indicates that the gasification is fully contributed by the exterior field. Further, the exterior factor $\Psi_{\alpha T}$ increases towards unity as the droplet temperature approaches the boiling temperature. The evolutional figure of two factors is shown in Figure 6. The interior factor becomes zero as the interior thermal equilibrium is attained. At the beginning, the value of exterior factor is 0.86 due that the temperature difference between two phases remains. As the interior equilibrium reaches, the theoretical value of exterior factor should be unity. But at t=2100, the exterior factor equals to 0.96. The small difference compared to the theoretical value is caused by the intrinsic temperature difference although the envelope flame surrounds the droplet and interior thermal equilibrium is attained.

4 Conclusions

From the canonical theory analysis, we conclude that droplet preheating by the preheated air convection toward droplet, interior-exterior thermal binding, and micro-thermal equilibration in droplet interior, are the principal mechanisms of gasification in the preheating period, which occupies approximately one-third of time required to reach quasi-steady state droplet gasification. Following preheating period, the exterior heat conductive transfer in polar angular direction and weak exothermic reaction enhance gasification whereas the exterior convection tends to reduce gasification rate. Ignition occurs shortly after the micro-equilibrium is established within the droplet interior. After ignition, the droplet interior temperature reaches to nearly the boiling temperature and effects of internal circulation diminish. In the evolution stage, the interior flow makes negative contribution to gasification which diminishes from approximately −10 %, at the beginning of the total gasification, to nearly 0 % within the characteristic time of 2100. The effect of convective transport in the external flow appear to have slightly larger negative contribution than that of conductive transfer, whereas the exothermic reaction and Spalding rate become the positive contributing factors beyond t = 5700. The change in flame configuration also plays critical role in transient droplet combustion rate and structure.

5 Acknowledgements

The author will acknowledge the financial support from National Science Council under the contract No. NSC93-2212-E-006-005 and NSC96-2623-7-244-002-D.

References

Figure 1. Schematic of elemental volume over which canonical analysis of single droplet gasification is applied.

Figure 2. Temperature contour plot of interior liquid phase at characteristic time from 50 to 300, (a)-(f).

Figure 3. Time histories of normalized droplet gasification against the characteristic time with major scenario contour plot.

Figure 4. Time series scenarios of the droplet interior gasification sub-mechanisms along characteristic time.

Figure 5. Time series scenarios of the droplet exterior gasification sub-mechanisms along characteristic time.

Figure 6. Time histories of the exterior (a) and interior (b) surface modulation factors.