

The Effects of Detailed Chemistry and Transport on Microgravity Droplet Combustion

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Abstract - A brief overview of recent advances in the theoretical study of microgravity droplet combustion is presented. Much of this work has centered on the development and utilization of spherically-symmetric transient numerical models which consider detailed gas phase chemistry and transport as well as energy and/or species transport within a regressing condensed phase. Numerical results for microgravity combustion and vaporization of methanol, methanol/water, heptane, and heptane/hexadecane droplets are summarized along with refinements in chemical kinetics and the development of a new two-dimensional axi-symmetric model.

1. INTRODUCTION

In recent years, a joint program with F. A. Williams at the University of California San Diego has been in progress to study microgravity droplet combustion. This program includes microgravity droplet experiments and theoretical studies using asymptotic and numerical methods. At UCSD asymptotic methods have been used to investigate the flame structure and extinction of n-heptane [1,2] and methanol droplets [3]. Meanwhile, theoretical efforts in this laboratory have centered on the development of transient numerical models. These models consider detailed gas phase chemistry and transport, condensed phase transport, condensed phase surface regression, and, where applicable, condensed phase surface chemistry. Much of the work has utilized a transient, spherically symmetric, moving finite element approach originally developed by Cho, *et al.* [4,5]. This modeling approach has been used to successfully simulate the microgravity combustion and/or vaporization of methanol droplets [6], methanol/water droplets [7,8], n-heptane droplets [9], n-heptane/n-hexadecane droplets [10], and carbon particles [11,12]. These studies have led to new and exciting discoveries in fields which are generally considered mature.

The results which will be briefly summarized in this paper repeatedly underscore the effects of detailed coupling between gas phase chemistry, gas phase transport, liquid phase transport, and phase equilibrium. For instance, the methanol and methanol/water results show that the droplet extinction diameter depends not only on the gas phase chemical and transport rates but on the rate of liquid mass transport as well. Moreover, even during "quasi-steady" combustion when the observed burning rate is essentially constant, a closer examination of the gas phase chemical heat release reveals a continuously varying flame structure. This result suggests a shift in the gas phase kinetic routes as the diffusional residence time decreases with decreasing droplet diameter. Finally, new regimes of droplet combustion and carbon particle oxidation have been predicted wherein traditional quasi-steady assumptions are no longer valid.

These discoveries have prompted continued numerical and experimental research efforts. A spectral element approach is being utilized to develop a 2-D axi-symmetric model which will be initially applied to the study of microgravity droplet combustion in the presence of forced convection [13]. Also, a new n-alkane reaction mechanism has been developed which contains significantly more detail than the semi-empirical mechanisms used in the n-alkane studies mentioned above [14]. Finally, continued ground-based 2.2 second drop tower and 5 second Zero Gravity Facility experiments are being conducted in conjunction with the numerical modeling described in this paper [15]. Ultimately, this research effort is focused on development and analysis of the space-based DCE and FSDC experiments which are scheduled to fly aboard upcoming shuttle flights. The DCE and FSDC will be used to study the microgravity combustion of isolated, pure n-heptane droplets and fiber supported, bi-component droplets of several fuels including methanol/water and heptane/hexadecane.

2. THE EFFECT OF TRANSIENT VAPORIZATION ON THE IGNITION OF DROPLETS

In order to minimize the disturbance by an ignition source on a droplet deployed in microgravity, a substantial effort has been made in the past to understand the interactions between the ignition source (a spark, for instance) and the droplet [16]. However, little was understood about the instantaneous evolution of the gas phase surrounding a droplet after deployment into the microgravity environment. Accordingly, in 1993 a numerical study was performed by Marchese and Dryer [17] to determine whether it was possible to achieve pure gas phase ignition in the region surrounding a droplet, or if it was always necessary to supply additional energy to the droplet surface to raise the droplet surface temperature thereby increasing the mass fraction of fuel in the gas phase.

The fact that methanol and n-heptane have flash temperatures of 11.5 °C and -4 °C respectively would suggest the possibility of achieving pure gas phase igni-

tion in the region surrounding such droplets deployed in air at 25 °C. However, experiments have shown that, under the same experimental conditions, methanol droplets are much more difficult to ignite than n-heptane droplets [15]. The modeling results have indicated that, although, methanol has a flash temperature of 11.5 °C, it would be extremely difficult to achieve pure gas phase ignition of a methanol droplet in the 1 mm size range deployed in air. As the definition of the flash temperature would suggest, initially a 25 °C droplet is surrounded by a thin layer of fuel/air mixture which is within the flammability limits of methanol/air. The modeling results show that for short time periods after deployment the mere divergence of the flow field results in a finite gas phase location wherein the gas mixture falls below its lean flammability limit. Due to the stoichiometry of the methanol/air system, this location is at most one radius from the droplet surface. Moreover, as the droplet vaporizes, the high latent heat of vaporization of methanol causes the surface temperature to rapidly drop. The gas phase location of the lean flammability limit thus moves closer to the droplet surface. After only several seconds, the droplet surface temperature falls below the flash temperature at which time the entire gas phase surrounding the droplet is outside the lean flammability limit.

Figure 1 shows the gas phase location of the lean flammability limit for 25 °C droplets of methanol and n-heptane instantaneously immersed in atmospheric pressure air at 25 °C. These results suggest that only a precisely timed and located ignition source would be able to achieve pure gas phase ignition for the methanol/air system. An ignition source located outside the locus of flammable mixture would require an ignition energy much greater than the minimum gas phase ignition energy as additional energy would have to be supplied to raise the droplet surface temperature.

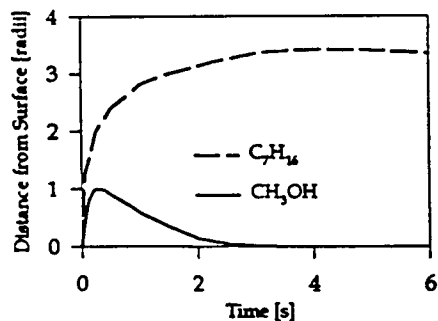


Figure 1. Gas phase location of lean flammability limit in radii from the droplet surface for 1 mm droplets dispersed in air.

The results for n-heptane show precisely why it is less difficult to ignite n-heptane droplets than methanol droplets. Firstly, the stoichiometry of the n-heptane/air system results in a lean limit locus which is much farther from the droplet surface than the methanol/air system. Furthermore, while the vaporization of an n-heptane droplet does cause its surface temperature to drop, it

does so to a much lower extent since the latent heat of vaporization of n-heptane is roughly 1/4 that of methanol. These results suggest that, since the gas phase surrounding an n-heptane droplet remains flammable at distances of 3 radii from the droplet surface, pure gas phase ignition should exist for the n-heptane/air system. Thus, the overall energy necessary to ignite an n-heptane droplet should be close to the minimum gas phase ignition energy of n-heptane.

3. COMBUSTION OF METHANOL AND METHANOL/WATER DROPLETS

The time-dependent, spherically symmetric combustion of bi-component liquid droplets of methanol and water has been simulated by Marchese and Dryer [7,8] using the finite element chemically reacting flow model mentioned above. The computations utilize the detailed multi-component molecular transport approach of Coffee and Hiernel [18] and the comprehensive methanol oxidation mechanism of Held, *et al.* [19] (89 forward chemical reactions and 21 species) to solve the gas phase energy and species equations. In addition, a semi-empirically-formulated binary vapor-liquid equilibrium relation is used to describe the phase change at the droplet surface. The conservation equations of energy and species are also solved within the droplet interior.

The numerical results for initially pure methanol droplets reproduce experimental observations wherein flame-generated water dissolves into the droplet during combustion. The results indicate that the extent of water absorption and its effect on both the quasi-steady burning rate and flame extinction phenomena are strongly dependent on the liquid mass Peclet number (defined as the ratio of the regression rate of the droplet surface to the effective mass transport rate of water within the liquid droplet).

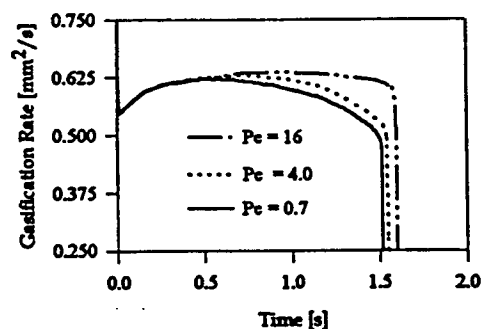


Figure 2. Instantaneous burning rate for 1000 micron initial diameter pure methanol droplets in air at 1 atm.

Figure 2 shows the instantaneous burning rate obtained from calculations in which the effective liquid phase mass diffusivity is parametrically varied resulting in various average liquid mass Peclet numbers. This figure shows that increased liquid mass transport results in increased deviation from d^2 -law behavior (i.e. gasification rate is not constant). Furthermore, as shown in

Fig. 3, increased mass transport promotes droplet extinction.

Fig. 3 suggests two extinction diameter limits. For $Pe_{l,m} \gg 1$, the extinction diameter approaches that value which would be observed if water were insoluble in methanol. For $Pe_{l,m} \ll 1$, the extinction diameter approaches that value which would be observed if the mass transport rate of water into the droplet were infinitely fast with respect to the surface regression rate.

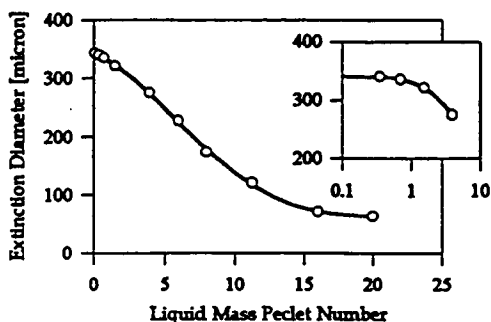


Figure 3. Variation in extinction diameter with liquid mass Peclet number for 1000 micron methanol droplets in 1 atm air.

From experimentally measured and correlated transport data the average liquid mass Peclet number for the combustion of methanol/water mixtures in air can be shown to be > 20 . Therefore, Fig. 3 suggests that if the interior of the liquid droplet were truly spherically symmetric and circulation-free, the effect of water dissolution on quasi-steady combustion and flame extinction would be minimal. However, considerable water uptake during methanol droplet combustion has been measured independently by Choi, *et al.* [20], and Lee, *et al.* [21]. Numerical modeling which simulates the conditions of the above experiments suggest that the liquid mass Peclet number present in these experiments was approximately 10. This decreased Peclet number suggests the presence of circulation within the liquid droplet which may be attributed to several sources, including the deployment technique and/or thermocapillary effects. Indeed, in a similar experimental configuration, Winter, *et al.*, [22] detected the presence of internal droplet circulation using laser induced fluorescence.

Methanol/water mixtures of 0-50% initial water content have also been modeled. These results show that for low liquid mass Peclet number, the water content at extinction is insensitive to the initial water content. Conversely, for high liquid mass Peclet number, the water content at extinction varied directly with the initial water content. Consequently, the extinction diameter is a weaker function of initial water content in the former situation than in the latter.

The low Peclet number results agree with suspended droplet results of Choi [23] which showed that a final water content of 80-85% was relatively insensitive to the initial water content. This result is not surprising since natural convection present in these experiments would not only have resulted in substantial internal droplet

circulation, but may also have increased the rate at which flame-generated water arrived at the droplet surface.

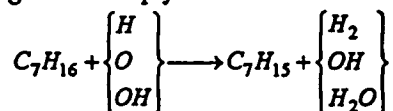
The numerical results suggest a series of drop tower droplet combustion experiments using methanol/water mixtures. The outcome of these experiments, which are presently underway [15], will indicate the magnitude of the liquid mass transport rate present in these and the future DCE space-experiments which will utilize similar deployment techniques.

4. COMBUSTION OF HEPTANE AND HEPTANE/HEXADECANE DROPLETS

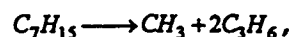
The results of the previous section provide valuable insight into much of the phenomena governing multi-component liquid droplet combustion although only one of the liquid components is a fuel. Moreover, the results suggest that, while the liquid phase effects of diffusional resistance and volatility differential might be studied analytically with infinitely fast, or simplified gas phase chemistry, a full understanding of ignition, quasi-steady burning, and extinction requires accurate gas phase chemical kinetics.

In a subsequent study by Marchese and Dryer [10], binary mixtures of *n*-heptane (C_7H_{16}) and *n*-hexadecane ($C_{16}H_{34}$) have been modeled to extend the previous numerical results to systems in which both liquid components are fuels. These fuels were chosen due to the existence of experimental data [24,25], an available semi-empirical chemical kinetic mechanism for *n*-heptane [26], and the substantial volatility differential between the two components.

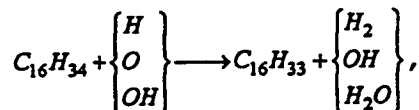
The gas phase chemical kinetics are modeled using the semi-empirical approach of Warnatz [26]. This approach had been utilized to generate a 32-species, 96-step *n*-heptane mechanism which accurately predicted laminar pre-mixed flame propagation. More recently, this mechanism has formed the basis for numerical studies on steady counter flow diffusion flames [27] and steady spherically symmetric diffusion flames [28]. The Warnatz model for *n*-heptane oxidation assumes that the predominant route of *n*-heptane consumption is abstraction of a hydrogen atom by O, OH, and H, thereby forming a generic *n*-heptyl radical:



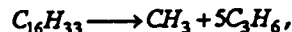
The principal empiricism in the Warnatz model is the description of the *n*-heptyl radical decomposition into the unlikely products of methyl radicals and propene in fixed ratio,



rather than the expected mixture of β -scission products, C_2H_4 , C_2H_5 , C_3H_6 , C_4H_8 , CH_3 , and C_5H_{10} . A similar approach is also applied to model the gas phase *n*-hexadecane chemistry. Hydrogen abstraction from *n*-hexadecane,



followed by the decomposition of n-hexadecyl into fixed proportions of methyl radicals and propene,



have been added to the original 96-step mechanism.

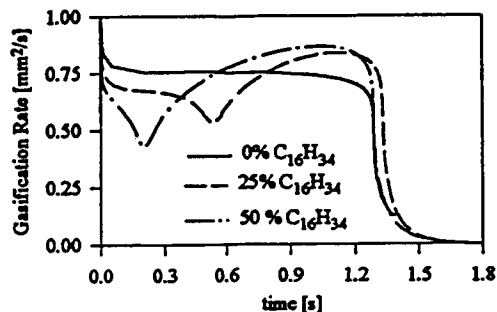


Figure 4. Instantaneous gasification rate, for 1000 micron initial diameter heptane/hexadecane droplets in 23% $O_2/77\% N_2$ at 0.164 atm ($Pe=10$).

Figure 4 is a plot of the instantaneous gasification rate for 1 mm heptane/hexadecane droplets in an oxidizing environment of 23% $O_2/77\% N_2$ at 0.164 atm. As Fig. 4 suggests, the pure n-heptane droplet closely exhibits its classical d^2 -law droplet combustion behavior as the gasification rate is constant over the majority of the droplet lifetime. For mixtures of n-heptane/n-hexadecane, the gasification rate varies continuously during the droplet lifetime. The gasification rates of the 25% and 50% hexadecane droplets reflect three distinct periods of quasi-steady combustion. The first period constitutes the preferential gasification of heptane, which is the more volatile component. The second period begins when the heptane is depleted from the droplet surface. Once this occurs, the droplet heats up toward the boiling point of hexadecane resulting in a decrease in gasification rate. During the final period, the gasification rate increases as the liquid phase species gasify at fixed ratio due to the high liquid mass Peclet number.

As in the methanol/water studies, the results are found to vary depending on the value of the liquid mass Peclet number. Figure 5 shows results of computations performed to determine the effect of increased liquid mass transport. In these computations an effective liquid mass diffusivity is parametrically varied over an order of magnitude such that the average liquid mass Peclet number varied from 1 to 10. This figure suggests that the net observable effect of increased liquid mass transport is to delay the onset of the secondary droplet heating period. Once again, these results suggest that isolated droplet experiments using these fuels might be utilized to determine the effective Peclet number present in the experiments. Finally, the numerical model predicts droplet extinction diameters of 187, 225, and 312 microns for average liquid mass Peclet numbers of 10, 5, and 1, re-

spectively. This effect underscores the intimate coupling between the liquid and gas phase processes.

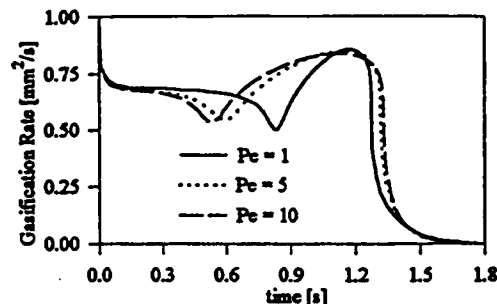


Figure 5. Instantaneous gasification rate, for 1000 micron initial diameter 25% hexadecane droplets in 23% $O_2/77\% N_2$ at 0.164 atm ($1 \leq Pe \leq 10$).

5. A NEW REACTION MECHANISM FOR N-ALKANE DROPLET COMBUSTION MODELING

In the studies summarized in Section 3, the gas-phase chemistry is modeled using the comprehensive (89 step, 21 species) gas-phase chemical kinetic mechanism of Held and Dryer [19]. The results show the effects of complex chemistry which would not have been observed if the gas phase were modeled using single-step activation energy asymptotics. For instance, the results suggest that, rather than merely increasing leakage through a thin reaction zone, the reduction in diffusional residence time with droplet diameter results in a gas-phase flame structure that continuously evolved throughout the droplet lifetime. Figure 6 shows the local gas-phase chemical energy release surrounding a 1500-micron droplet deployed in a microgravity environment of 50% $He/50\% O_2$, at 0.5 atmospheres at three times during the droplet lifetime. The continuous variation in flame structure, as indicated by the changing energy release pattern, suggests a shift in the gas phase kinetic routes with diffusional residence time. This result is consistent with recent microgravity n-heptane droplet studies of Jackson

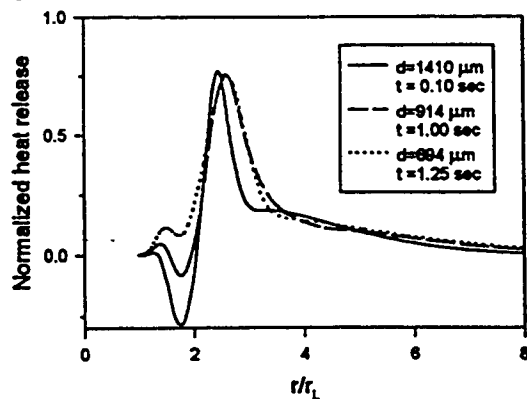
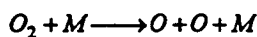


Figure 6. Gas-phase heat release profile surrounding a 1500 micron methanol droplet at 0.25, 0.50, and 1.00 seconds after ignition. (50% $O_2/50\% He$, $P=0.50$ atm)

and Avedesian [29] which showed that sooting propensity decreased significantly with droplet size. It was sug-

gested that the decreasing diffusional residence time with decreasing initial droplet diameter results in less time for production of soot precursors on the fuel side of the diffusion flame. Such arguments are complicated, however, by an additional time scale associated with thermophoretic soot collection.

The n-heptane oxidation mechanism of Warnatz which has been used in the studies presented above in Section 4 lacks sufficient detail to capture some of the interesting transient phenomena observed in the methanol/water studies. In addition to possible flame structure variations, the model is not well-equipped to handle droplet ignition. As mentioned previously, the Warnatz mechanism postulates only one consumption route for the fuel—abstraction by H, O or OH, followed by thermal decomposition of the resulting heptyl radical (C_7H_{15}) to propene and the methyl radical (CH_3). Since, initially, only fuel, oxygen, and inert exist in the gas phase, the only initial source of radicals in this mechanism is via oxygen dissociation. Indeed, droplet ignition is not obtained for any initial conditions when the reaction:



is suppressed.

Four difficulties are perceived with regard to the use of the Warnatz mechanism in diffusion-flame modeling in general, and specifically in time-dependent droplet calculations. First, as mentioned above, the absence of a thermal decomposition route for the n-heptane presents difficulties in the study of ignition phenomena. Second, the treatment of the n-heptyl radical as a single species, rather than a mixture of isomers, results in a non-realistic distribution of olefinic intermediate species. The mechanism overemphasizes the importance of propene reactions, rather than those of the expected mixture of Beta-scission products which are, in fact, observed in n-heptane/air diffusion flame structures [30] and flow reactors [31]. Third, the C_1 - C_3 submechanism is in need of updating with current reaction paths and rate constants. The propene submechanism, in particular, lacks any abstraction routes, which are likely to be an important reaction path under combustion conditions. Finally, the kinetics are insufficient for eventual grafting of additional reactions to describe sooting effects.

A recent experimental and modeling effort by Held, *et al.* [14] has been directed toward providing a more detailed treatment of the decomposition of both the parent fuel, n-heptane, and the four isomeric heptyl radicals, while still retaining a relatively simplified view of the overall kinetics. Because each species added to a mechanism adds another differential equation to be solved in the kinetic system, while a new reaction only adds another term to an existing equation, a model may be extended by additional reactions without significant computational penalty. A major goal of the model development is the increase in site-specific detail, while maintaining a relatively small number of species. Also, the C_1 - C_3 mechanism has been updated to a detailed kinetic mechanism developed in previous and ongoing work [19,32]. The final reaction mechanism consists of 241 re-

actions among 37 species, an increase of 145 reactions, but only 5 species.

To support the development of this mechanism, a series of n-heptane oxidation and pyrolysis experiments have been performed using a variable pressure flow reactor. The calculated and measured species profiles for a rich oxidation case shown in Fig. 7. The agreement is excellent, both in terms of overall reaction rate and intermediate distribution. Similar calculations using the full Warnatz mechanism yield characteristic reaction times on the order of 300 sec, compared to the 0.5 second time scale of the experiments.

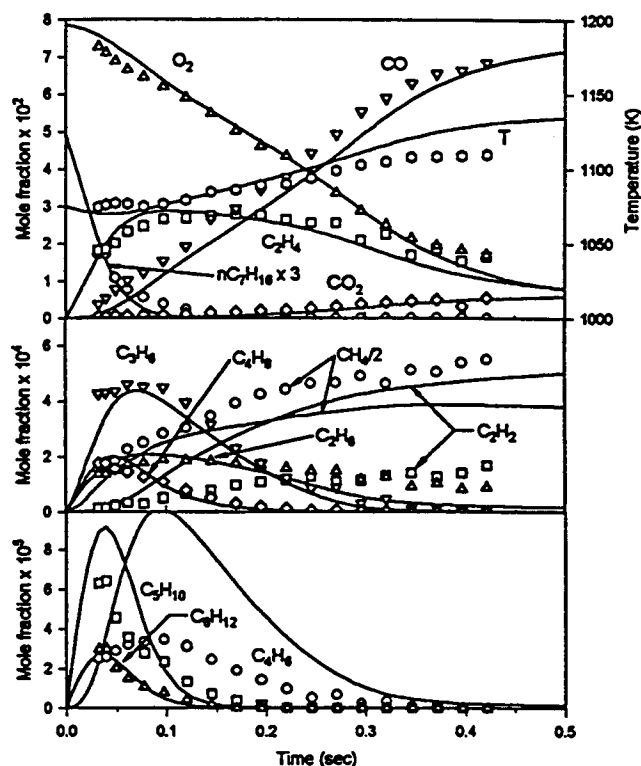


Figure 7. Measured (symbols) and calculated (lines) species and temperature profiles for n-heptane oxidation.

6. TWO-DIMENSIONAL MODEL DEVELOPMENT

The success of the spherically symmetric modeling has prompted the development of a transient, axis-symmetric, 2-D droplet combustion model [13]. The model has been developed mathematically by applying an asymptotic expansion on the square of the mach number, thereby suppressing all acoustic waves. In this formulation, the thermochemical system (species and energy equations) and hydrodynamic system (momentum and mass conservation equations) are decoupled in time. The governing equations are spatially discretized using the spectral element method. Time integration is performed using a fifth-order, fully implicit backward difference method with a general, sparse Jacobian algorithm. To date, the diffusion problem has been tested using a dif-

fusion operator based on the mixture fraction formulation of Kee, *et al.* [33]. The thermochemistry solver is currently being coupled with the momentum solver to analyze the 2-D, axi-symmetric convection situation.

7. CONCLUSIONS

Recent studies using sophisticated transient numerical models which consider detailed chemistry and transport have led to new and exciting discoveries in the field of droplet combustion. Refinement of chemical kinetic, equilibrium, and transport sub-models continues along with the development of a new 2-D axi-symmetric droplet combustion model.

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