NUMERICAL INVESTIGATION OF DROPLET HEATING, VAPORIZATION, AND IGNITION OF METHANOL AND LOX DROPLETS IN A CONVECTIVE FLOW FIELD

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Abstract

A two-dimensional computer code for the simulation of heating, vaporization, ignition, and subsequent combustion of cold droplets injected in a hot uniform gas flow is developed. The numerical simulation of the processes is performed in an axisymmetric configuration for spherical droplets with boundary fitted grid point systems. Detailed models for the relevant processes are employed; in particular, detailed chemical reaction systems are used. Both methanol droplets in hot air as well as liquid oxygen droplets in gaseous hydrogen are studied. The first chemical system is relevant in diesel engine combustion, and typical conditions at 30 bar are investigated. The liquid oxygen/hydrogen system is studied at 10 bar, and the inlet liquid oxygen (LOX) droplet temperature is cryogenic (85 K) – this condition is found in liquid rocket propulsion. The computer code accounts for physical properties in this temperature range through addition of a data base for LOX/hydrogen to the commonly used NASA polynomials in the temperature range between 300 and 5000 K. For the LOX droplets in gaseous hydrogen, also two neighboring droplets are considered, and the influence of droplet spacing on ignition is investigated.

Introduction

A detailed knowledge of the processes associated with droplet vaporization, ignition, and combustion is a prerequisite for the understanding of spray combustion in, e.g., oil burners, diesel engines, or in liquid rocket propulsion. Some studies of the fundamental physical-chemical mechanisms associated with droplet vaporization and combustion can be found in the literature [1, 2, 3, 4]. The fluid-dynamical processes are reasonably well known [2, 3, 4] whereas the ignition and combustion of single and multiple droplets in convective flow fields are not well understood.

Stapf *et al.* [5] apply a two stage model for the group ignition and combustion of heptane in air at high pressure (50 bar). The overall droplet group ignition model that comprises up to 10 droplets employs a one-step chemical reaction scheme and the detailed processes around a single droplet are described with a detailed chemical reaction scheme. This model gives a good overall structure of the processes, but it neglects the effects of both multispecies transport and chemical reactions on neighboring droplets since the one-step reaction scheme typically presumes a Lewis number of unity.

The scope of the present paper is the investigation of one and two droplet ignition using detailed models for both multispecies transport and detailed chemical reactions. Since these gas phase processes are the major focus of interest, rather simple models are used to describe the fluid dynamics and transport of droplets. Here the droplets are assumed to be and remain fixed throughout the processes involved, and the present study focuses on two droplets of equal initial size.

The present study concerns the heating, vaporization, and ignition of single methanol droplets in a convective air stream at 30 bar. This pressure level is typical for the self-ignition in diesel engines. Moreover, the same processes are investigated for a liquid oxygen (LOX) droplet in gaseous hydrogen at 10 bar. This condition prevails in liquid rocket propulsion [6, 7]. The injection temperature of the liquid in such system is cryogenic, and the physical properties in this temperature and pressure regime are included. Both the heating, vaporization, and ignition of a single droplet and two droplets in a tandem are studied. Parametric dependencies of ignition time with initial droplet size, gas injection velocity, and gas temperature are presented for the single LOX droplet. Moreover, the influence of a neighboring droplet on ignition time is investigated. The information obtained by the detailed

models employed in the study may be used for the development of sub-models for spray combustion in complex combustion systems.

Model

The computer code developed for the present study is an axisymmetric, twodimensional, time-dependent code which allows the study of heating, vaporization, and combustion of droplets injected in preheated flows. In order to improve the numerical efficiency, boundary fitted grid point systems are used.

Major features of the model are detailed chemical reactions in the gas phase for both methanol/air and hydrogen/oxygen and detailed transport in the gas phase. The physical properties in the gas phase are evaluated from NASA thermochemical tables which are extended by JSME tables for the low temperature and high pressure conditions for the LOX [8, 9]. The liquid phase equations comprise droplet heating and vaporization where the diffusion–limit model has been employed which requires numerical resolution of the droplet interior.

The numerical solution procedure as well as detailed formulations of the governing equations and boundary conditions are given in Ref. [8].

Single Droplets

A methanol droplet at 300 K is placed in a uniform gas stream at 1500 K. The pressure is 30 bar which is typical for self-ignition in a diesel engine. The initial droplet diameter is 50 μ m and the initial gas velocity equals 25 m/s. After 11.56 µs ignition (evaluated from the profile of the gas temperature) occurs, and the left part of Fig. 1 shows the gas temperature at this time. Ignition occurs in the wake of the droplet as is anticipated from the gas phase composition. Ignition occurs at locations where the reactants are mixed and the gas temperature is high enough for self-ignition to occur. The last condition is fulfilled everywhere around the droplet at some distance from its surface whereas the first one determines the ignition location in the present situation. It is observed that ignition does not occur on the axis of symmetry but at some distance in radial direction. This behavior is explained looking at a zoom of the gas phase velocity field shown on the RHS in Fig. 1. The figure reveals a recirculation zone in the wake region of the droplet that establishes shortly before ignition occurs. This means that air from the downstream region is carried into this area which again causes the gas phase composition to be leaner on the axis in the wake region compared to the regime at somewhat higher radial distances. The phenomenon of flow separation in the wake region of a droplet has been discussed by Sirignano [2], and here its influence on the ignition location becomes obvious. Thus, the gas phase velocity field has a strong impact on the ignition location in this configuration. A study to further investigate this phenomenon is carried out where the initial gas velocity is reduced to 10 m/s. This situation is shown in the left part of Fig. 2. Here, no recirculation occurs and ignition is located on the axis of symmetry. The remainder of the paper concerns the heating, vaporization, and ignition of liquid oxygen (LOX) droplets in a convective hydrogen flow.

First, a single liquid oxygen droplet with an initial diameter of 25 μ m and an initial temperature of 85 K is placed in a laminar uniform flow of hot hydrogen at 1500 K and 10 bar. The initial velocity of the gaseous hydrogen is 20 m/s. These conditions are relevant to liquid rocket propulsion [6, 7].



Figure 1: Methanol droplet: Contour plot of the gas temperature (left) and the gas streamlines (right) at ignition.



Figure 2: Left: Methanol droplet: Zoom of the gas phase temperature at ignition for an initial gas velocity of 10 m/s. Right: LOX droplet: Parametric dependence of ignition time versus initial droplet diameter for an initial gas temperature of 1500 K; initial gas velocity 25 m/s (filled circles), 70 m/s (open circles).



Figure 3: LOX droplet: Left: Oxygen profile prior to ignition (t = 2.1 μ s); Center: Temperature profile during ignition (t = 2.8 μ s); Right: OH profile after ignition (t = 3.2 μ s).

Figure 3 shows the heating, vaporization and ignition characteristics prior to ignition (left), during ignition (center) and after ignition (right). Prior to ignition, the oxygen profile reveals the diffusion of molecular oxygen into the gas phase. In contrast to the corresponding process for methanol droplets, the vaporized oxygen is found almost circular around the droplet in this situation. There are some major differences between the systems that are observed. First, the pressure of the methanol droplet vaporization is 30 bar whereas the pressure in the LOX droplet case is 10 bar. A reduced pressure goes along with lower density and a higher molecular diffusion velocity in the gas phase. Moreover, the Lewis number of gaseous hydrogen is considerably lower than unity, and therefore the vaporized oxygen has a higher freedom of diffusion compared to the methanol vapor under the conditions investigated in the first part of the paper. At the same time, the chemical time scales of the hydrogen/oxygen system are small compared to the methanol/air system and ignition occurs at 2.8 μ s for the LOX droplet in hydrogen. There is no recirculation zone, and ignition occurs in the wake region of the droplet on the axis of symmetry as shown in Fig. 1. The flame quickly propagates to build an envelope flame as can be seen from the profile of the OH mass fraction displayed on the RHS of Fig. 3 at 3.2 μ s. The flame is not circular around the droplet due to convection in the gas phase.

For the LOX droplet in gaseous hydrogen, a parameter study has been performed where the ignition time versus intial droplet size, inlet gas velocity, and initial gas temperature has been investigated. The RHS of Fig. 2 shows the ignition time for two inlet gas velocities of 25 and 70 m/s, respectively. The higher initial gas velocity causes a quicker transport of vaporized liquid into the wake region of the droplets, and an ignitable mixture establishes faster. This leads to shorter ignition times for all initial droplet diameters as long as there is no recirculation zone in the wake region of the droplet. Moreover, Fig. 2 shows that there is a minimum ignition time for a droplet diameter of somewhat smaller than 50 μ m. This effect is well known from studies of both single droplet and spray ignition [10, 11]. In the case of small droplets it takes more time for an ignitable mixture to build up whereas for large droplets, the droplet heating process consumes a considerable amount of time.

A reduction of the gas temperature from 1500 K to 1400 K prolongs ignition. For both initial gas velocities, the values of ignition time for an initial droplet diameter of 25 and 50 μ m is somewhat more than a factor of three higher compared to the values shown on the RHS in Fig. 2.

Two Droplets

The computational domain as well as the numerical grid for the two-droplet situation is given in Fig. 4. The droplets are assumed to remain fixed in space throughout the compution which is reasonable in the present low Reynolds number situation of the gas phase.

Figure 5 shows a contour plot of the gas temperature for the situation of a droplet distance of five droplet diameters. The downstream droplet causes a small recirculation zone in the wake region of the leading droplet (not shown). This is mainly due to the presence of the downstream droplet. It affects both the gas phase velocity profile as well as the vaporizing oxygen: The existence of the downstream droplet reduces the downstream convection of the leading droplet, and the ignition location is somewhat away from the axis of symmetry which is typical for situations where recirculation in the wake region occurs, c.f. Fig. 1. The downstream droplet ignites on its upstream side where the ignition location also is shiftet somewhat away from the axis of symmetry. The gas velocity field has established after about 0.42 μ s, and ignition occurs at 1 μ s.



Figure 4: Computational domain and curvilinear mesh used in the simulations for two droplets, here with the initial distance of 150 μ m.



Figure 5: Temperature profile for a droplet distance of 250 μ m during ignition (t = 1.0 μ s).



Figure 6: Temperature profile for a droplet distance of 150 μ m during ignition (t = 1.3 μ s).



Figure 7: HO₂ profile for a droplet distance of 150 μ m during ignition (t = 1.3 μ s).

Figure 6 shows the gas phase temperature for a two-droplet situation with a distance of 150 μ m which equals three times the initial droplet diameter. Here ignition also occurs in the wake region of the leading droplet, and the second droplet ignites on its upstream side. The droplets are considerably closer together, and the vaporization of the downstream droplet leads to a cooling down of the gas phase that affects ignition time of the leading droplet: The ignition time in this situation is 1.3 μ s which is longer than in the two-droplet case with a larger distance. Here the effect of droplet interaction obviously is stronger: Not only the gas phase velocity profile but also the gas phase temperature is affected by the presence of the second droplet. A comparison with the single droplet vaporization of LOX in hydrogen discussed in Figs. 2–3 reveals that the ignition of the single droplet wake region is not prevented by the presence of another droplet which leads to a longer time for an ignitable gas phase mixture to build. After ignition, the flame propagates in the two-droplet situation of Fig. 6 and there is no separate flame associated with each droplet, but rather, a merged, single connected flame surface forms after 2.2 μ s (not shown). Thus, the combustion mode has changed from single to a group combustion of the two droplets.

The ignition and combustion model employed in the present study also is suitable to predict other species profiles during vaporization, ignition, and combustion since a detailed chemical reaction mechanism is employed. The H_2O , OH, O, and H profiles more or less follow the profile of the gas temperature, and they are not displayed here. However, it is interesting to look at the profile of HO_2 during ignition. Figure 7 shows a contour plot of the mass fraction of HO_2 during ignition, and a somewhat complex situation is found. The HO_2 presists in regions that are hot but not too hot due to the stability of the molecule, c.f. Fig. 6. The maxima of the mass fraction of HO_2 are to be found right between the two droplets as well as at some distance away from the droplets in the radial direction.

These are the areas where combustion occurs and radicals are build leading to the production of HO_2 in regions where the gas temperature is not too high for that species to exist. A similar picture is obtained for the H_2O_2 profile (not shown). The figure demonstrates the complex processes and interaction of the gas velocity field, the vaporization, droplet heating, and combustion.

Conclusions

A detailed numerical study of single droplet heating, vaporization, and ignition of methanol and LOX droplets in a convective air and hydrogen gas stream, respectively, has been performed. Parametric dependencies of ignition time versus initial droplet size have been obtained for different initial gas velocities and gas temperatures. Also, the combustion mode of two interacting LOX droplets have been studied, and the transition from two individual droplet combustion mode to group combustion mode has been successfully simulated.

It is evident that in dense sprays where the droplets are rather close, the interaction of the droplets plays an important role for the overall combustion process. Thus, further parametric studies with respect to the droplet separation distance can be a tool to improve models for the ignition and combustion of dense sprays.

Acknowledgements

The authors thank Dr. D. Preclik from ASTRIUM for discussions concerning the physical properties' data base for cryogenic inlet temperatures of the H_2/O_2 system. The work was supported in part by the DARA GmbH.

References

- [1] Faeth, G. M., Proc. Comb. Inst. 26:1593-1612 (1996).
- [2] Sirignano, W. A., Fluid Dynamics and Transport of Doplets and Sprays. Cambridge University Press (1999).
- [3] Bellan, J., Prog. Energy Combust. Sci. 26, 381-416 (2000).
- [4] Chiu, H. H., Prog. Energy Combust. Sci. 26: 329-366 (2000).
- [5] Stapf, P., Dwyer, H. A., Maly, R. R., Proc. Combust. Inst. 27:1857-1864 (1998).
- [6] Sender, J., Lecourt, R., Oschwald, M., Haidn, O. J., Proc. ILASS-Europe'97, Florence, Italy, 145-154 (1997).
- [7] Gicquel, P., Vingert, L., Proc. ILASS-Europe'99, Toulouse, July 5-7 (1999).
- [8] Aouina, Y., Gutheil, E., Maas, U., Riedel, U., Warnatz, J., Combust. Sci. and Tech., 173:1-29 (2001).
- [9] Schlotz, D., Gutheil, E., Combust. Sci. and Tech., 158:195-210 (2000).
- [10] Gutheil, E., Combust. Flame, 93:239-254 (1993).
- [11] Aggarwal, S. K., Prog. Energy Combust. Sci., 24, 565-600 (1998).