STRUCTURE AND DYNAMICS OF PREMIXED FLAMES IN MICROGRAVITY

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Introduction

In this report we describe the research performed at the Naval Research Laboratory in support of the NASA Microgravity Science and Applications Program over the past three years with emphasis on the work performed since February 1992, the beginning of the current project. The focus of our research has been on investigating fundamental combustion questions concerning the propagation and extinction of gas-phase flames in microgravity and earth-gravity environments. Our approach to resolving these fundamental questions has been to use detailed time-dependent, multidimensional numerical models to perform carefully designed computational experiments. The basic questions we have addressed, a general description of the numerical approach, and a summary of the results are described in this report. More detailed discussions are available in the papers published which are referenced herein.

A systematic study which isolates the various processes that could lead to flame instabilities and extinction is needed to gain a better understanding of flammability limits and flame dynamics in microgravity. Numerical simulations, in which the various physical and chemical processes can be independently controlled, can significantly advance our understanding of flame instabilities and flammability limits on earth and in a microgravity environment. In the past three years, we have addressed a number of basic issues aimed at resolving some of the important aspects of flame structure and propagation. Some of the issues we have addressed using our numerical simulations are: the effects of heat losses and buoyancy forces on the structure and stability of flames(both burner-stabilized and flames in tubes), the existence of flammability limits in the absence of external losses or buoyancy forces in the system, and the extinguishment process at the downward-propagation limit.

Computational Tools

Two computational models developed at NRL, FLIC2D and FLAME1D, have been used in the work reported here. Both the numerical models are time-dependent and solve the multispecies coupled partial differential reactive-flow equations. These models include a detailed chemical kinetics mechanism coupled to algorithms for convection, thermal conduction, viscosity, molecular diffusion, thermal diffusion, and external forces. The external force, gravity, can be in any direction relative to flame propagation and can have a range of values. Energy sources and sinks may also be prescribed as a function of time. All of the chemical and physical processes are solved sequentially and then coupled asymptotically by timestep splitting [1].

FLIC2D, a two-dimensional model, has been used extensively to study cellular flames [2,3], the effects of gravity and heat losses on the structure and dynamics of lean hydrogen-air flames [4-8]. FLAME1D has been applied to various studies of flame phenomena including calculations of burning velocities, minimum ignition energies and quenching distances, effects of curvature and dilution, and flammability limits [9-11]. This one-dimensional model is generally used to test new sub-models such as for radiation and chemistry before implementing them in the multidimensional model. It is also used to study physical and chemical phenomena in which multidimensional effects are secondary. Space restriction does not allow the elaboration of the models here but details can be found in previous reports [9,12]. These models are also continuously evolving. Some of the recent additions to the models are the inclusion of wall effects and radiation, heat losses to a burner, moving adaptive grids and a parallel implementation of chemistry solver.

Summary of Research

Our recent research can be broadly divided into four categories: (a) dynamics of cellular flames [3], (b) effects of gravity, heat losses and viscosity on flame instabilities and structure[4-6], (c) extinguishment process at the lean-flammability limit[7,8] and (d) instabilities near the rich-flammability limit[13]. Each of these categories are briefly discussed below.

Dynamics of Cellular Flames

Our initial simulations [2] of cellular flames were in qualitative agreement with experimental observations on the stability of flames in lean and rich hydrogen-oxygen-nitrogen mixtures [14] and were also able to identify the thermo-diffusive instability mechanism as the primary mechanism responsible for the formation of cellular flames in hydrogen-oxygen-nitrogen mixtures in most systems. We then used the simulations to investigate the cell-split limit phenomena observed in the NASA drop tower [15] experiments.

We simulated the structure and dynamics of flames in a series of mixtures with 15% or less hydrogen in air. We observed brisk formation of cells and their subsequent splitting in lean mixtures with more than 11% hydrogen. In leaner mixtures with 9.5-11% hydrogen, the formation and splitting of cells is less vigorous. For mixtures with 9% or less hydrogen, a single cell is formed which does not split at all. For these mixtures, even calculations for very long times (0.4 seconds) in larger systems (10.2 cm channel width) did not show any indications of cell-splitting.

Heat losses have been postulated as a mechanism that can cause a cell-split limit. However, the simulations in this study do not include any loss mechanism; yet such a limit is still observed. This suggests that external loss mechanisms are not required and that the cell-split limit is actually an intrinsic feature of the lean hydrogen-air mixture itself. However, the actual mixture at which cell splitting ceases may be affected by losses.

Effects of Gravity, Heat losses and Viscosity on Flame Instabilities and Structure

We have performed a systematic series of investigations to isolate and study the role of gravity, heat losses and viscosity on the structure and stability of flames. In the first series, we isolated the effects of gravity by comparing upward- and downward-propagating flames to zero-gravity flames in idealized two-dimensional systems in which the effects of viscosity and heat losses to the wall can be ignored [4,5].

These simulations showed that the effects of gravity become more important as the lean flammability limit is approached. In mixtures with 12% or more of hydrogen in air, gravity plays only a secondary role, with the stability and structure of the flame controlled primarily by the thermo-diffusive instability mechanism. However, in leaner hydrogen-air mixtures gravity becomes more important. Upward-propagating flames are highly curved and evolve into a bubble rising upwards in the tube. Downward-propagating flames are flat or even oscillate between structures with concave and convex curvatures. The zero-gravity flame shows only cellular structures. Cellular structures which are present in zero gravity can be suppressed by the effect of buoyancy for mixtures leaner than 11% hydrogen. These observations have been compared to theoretical and experimental observations [4] and have been explained on the basis of an interaction between the processes leading to buoyancy-induced Rayleigh-Taylor instability and the thermo-diffusive instability. These results also indicate that the instability mechanisms can interact in a quite complex manner, and even though one mechanism can mask the other, in certain regimes, both can be equally important.

In many practical applications as well as in the determination of flammability limits, flames are confined. Heat and radical losses will occur to the confining walls and the flow will also have to come to rest at the surface of the walls. Our simulations indicate that viscous effects play only a secondary role when the walls are assumed to be isothermal. However, heat losses to the walls play a dominant role resulting in the formation of additional cellular structures near but slightly displaced from the walls.

We also investigated how gravity modifies the structure and dynamics of flames in an isothermal, two-dimensional channel [6]. Heat losses are found to significantly modify upward- and downward-propagating flames. In the upward-propagating case, instead of a single bubble rising in the tube, a two-fingered flame is observed. This flame has some features similar to experimentally observed flames in lean hydrogen-air mixtures. The downward-propagating flame is also quite different when the effect of heat losses are considered. In this case, a flame is "visible" only in the central portion of the channel(see figure). Again, this flame is qualitatively similar to some near-limit flames in experiments. Therefore, we decided to do further simulations including the effects of heat losses to isothermal walls to gain some insight into the dynamical behavior observed experimentally in flames near extinguishment.

Extinguishment Process at the Lean-Flammability Limit

The experimentally observed flammability limit is between 9 and 10% for downward flame propagation in lean Hydrogen-air mixtures. Therefore further simulations including the effect of wall heat losses were carried out for flames in 10%, 9.75%, 9.5% and 9% hydrogen-air mixtures. The computational results show that a downward propagating flame in an isothermal channel has a flammability limit of around 9.75%. The details of the extinguishment process in this mixture has been analysed and found to be in excellent agreement with experimental observations.

In experiments, the flame is first observed to halt its downward propagation and then actually move back up into the burnt products[16]. From the simulations we can understand the reason for this observed behavior. The simulations indicate that the flame is quenched at the walls and tongues of colder gases, comprised mainly of burnt products flow down the sides. At the same time, there is an upward motion of the gases at the center of the channel, causing the flame to rise up into the burnt products. Further simulations also indicate that the dilution of the unburnt mixture with the products of combustion is an essential step in the extinguishment

Our earlier simulations have shown that a flame can propagate downward in a 9% mixture in a channel with adiabatic walls and cellular flames occur in this mixture in a zero-gravity environment. These observations taken in conjunction with our current simulations indicate that both heat losses and gravity are simultaneously required to cause the observed limit. A general conclusion from this work is that detailed numerical simulations that include wall heat losses can adequately simulate the dynamics of the extinguishment process in downward-propagating flames [8]. At the upward-propagation limit, the flames are highly three-dimensional and therefore must await the development of a three-dimensional model for a complete description.

Instabilities Near the Rich-Flammability Limit

A fundamental question that has not yet been fully resolved is the existence of an intrinsic flammability limit in a zero-gravity environment. In the absence of buoyancy forces, there are many competing factors such as preferential diffusion, flame chemistry, conductive and radiative heat losses, the aerodynamics of burnt gases, and flame stretch that can cause or modify flammability limits. Numerical simulations provide an ideal way to systematically isolate and evaluate the role of various factors.

We have conducted a systematic study of flames in rich hydrogen-air mixtures[13]. Because these flames are nearly one-dimensional, we conducted these investigations with the FLAME1D code. The numerical simulations indicate that a steady burning velocity is not obtained for very rich hydrogen-air mixtures. As the amount of hydrogen is increased, at first a damped oscillation is observed in the flame and burning velocities, and then with further increase in the amount of hydrogen, an undamped oscillation with a complex set of frequencies is observed. Simulations with a simplified one-step irreversible chemical reaction do not show these oscillations, suggesting that chemical kinetics plays a strong role in inducing these oscillations. Further analysis shows that the oscillations are due to a competition for H atoms between chain branching and chain-terminating reactions. However, the limiting mixture predicted by these simulations is beyond the experimentally observed limit. These differences may be because of the neglect of phenomena such as stretch and radiative heat losses.

Simulations of spherically expanding flames suggest that stretch effects (due to curvature) will cause the oscillations to occur in less rich mixtures than that observed for planar flames. Further calculations including multidimensional effects and radiative and conductive heat losses are needed to quantitatively determine the flammability limits in zero-gravity as well as to more fully understand the significance of the instability induced by chemical kinetics.

Work in Progress

The calculations discussed above have lead to a better understanding of the structure and propagation of flames. We now understand the reasons for some of the observed differences in the structure of upward and downward propagating flames. We also have a detailed description of the extinguishment process in downward-propagating flames and rich hydrogen-air flames. However, these simulations have also brought up a number of unresolved issues which need to be examined. Four major issues which need to be addressed are: (1) What is the role of radiation in near-limit flame phenomena, especially for hydrocarbon flames ? (2) Will the extinguishment process and the relative importance of various instability mechanisms be the same for hydrocarbon flames as for hydrogen flames ? (3) Are burner-stabilized flames significantly different from freely propagating flames ? and (4) How does three-dimensionality modify the observations from the two-dimensional simulations ?

These are the issues that we are currently focussing on in our research efforts. We have implemented a sub-model that accounts for radiation from water in our one-dimensional flame code. Simulations using this model indicate that for the wide range of hydrogen-air mixtures (from lean to rich), radiative loss plays only a minor role in modifying the flame properties. A sub-model to account for radiation losses from CO_2 is being developed for inclusion in our studies of hydrocarbon flames.

Detailed reaction mechanisms are available for some hydrocarbons but the cost of including such mechanisms in time-dependent, multidimensional simulations is very high. The solution of the chemical rate equations would take a significant portion of the computer time because of the large number of species and the large number of rate equations involved in a mechanism consisting of hundreds of elementary reactions. The major advances being made in parallel computing will probably be the crucial factor enabling us to simulate the hydrocarbon flames to the same level of detail as we do with the hydrogen flames. Currently, we are working on a parallel-processing approach for doing our multidimensional flame simulations. Meanwhile, continuing efforts are also being made to reduce the cost of doing detailed multidimensional simulations.

One approach to reducing the cost of multidimensional flame simulations is to use a greatly simplified reaction mechanism. However, some important phenomena may be missed by using a overly simplified mechanism. An intermediate approach is to use a skeletal mechanism [17, 18] which retains many characteristics of the detailed reaction mechanism. Results from using such a skeletal mechanism can then be compared to those using the more reduced reaction mechanisms to evaluate their validity and performance. With this approach in view, we are implementing and testing the skeletal mechanism for methane in FLAME1D. After this, we plan to incorporate the hydrocarbon chemistry along with the radiation model in FLIC2D and use it to simulate the structure and dynamics of multidimensional flames in hydrocarbons.

Currently, we have also begun to simulate burner-stabilised flames in order to address the effects of the burner on the structure and stabiity of cellular flames. Preliminary results indicate that the tendency to cellular structure can be significantly affected by the presence of the burner. A freely-propagating flame exhibiting vigorous cell-splitting can be stabilised at an inflow velocity lower than the normal burning velocity to suppress the formation of cells. Factors such as the details of the boundary-conditions imposed at the burner and the inflow velocity appear to play a significant role on the observed flame dynamics.

Many other interesting flame phenomena observed in microgravity are fully three-dimensional. The development of simplified but validated radiation and chemistry models along with advances in parallel computing of reacting flows are required to simulate the detailed dynamics of such flames.

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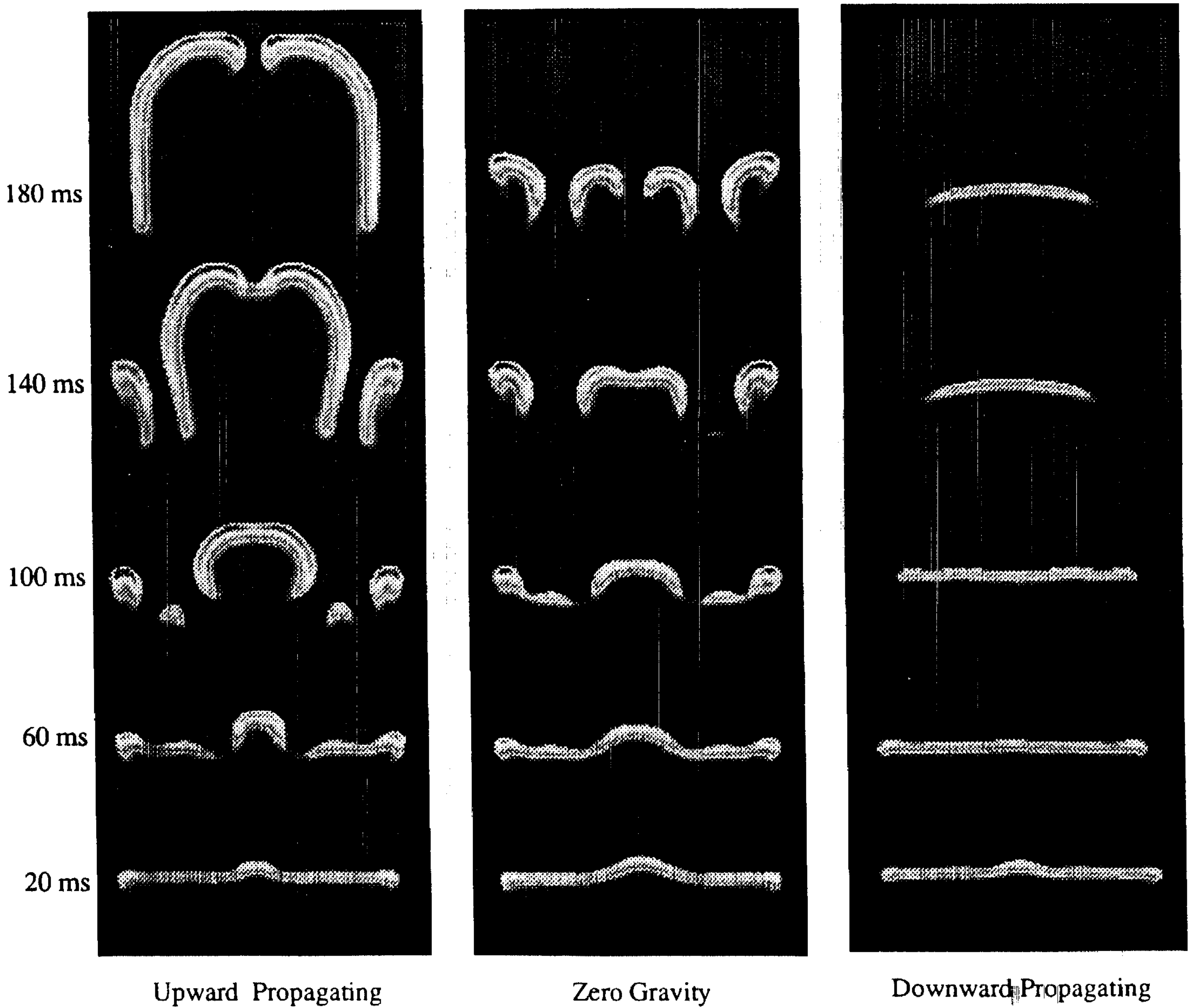

Comparison of OH concentration in upward-, zero-gravity and downward- propagating flames with heat loss to walls.

See Color Plate D-3