UNSTEADY NUMERICAL SIMULATIONS OF THE STABILITY AND DYNAMICS OF FLAMES

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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 (from Feb. 1992) with emphasis on the work performed since the last microgravity combustion workshop. The primary objective of our research is to develop an understanding of the differences in the structure, stability, dynamics and extinction of flames in earth gravity and in microgravity environments. Numerical simulations, in which the various physical and chemical processes can be independently controlled, can significantly advance our understanding of these differences. Therefore, our approach is to use detailed time-dependent, multi-dimensional, multispecies numerical models to perform carefully designed computational experiments. The basic issues 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.

Some of the basic issues we have addressed recently are 1) the relative importance of wall losses and gravity on the extinguishment of downward-propagating flames, 2) the role of hydrodynamic instabilities in the formation of cellular flames, 3) effects of gravity on burner-stabilized flames, and 4) effects of radiative losses and chemical-kinetics on flames near flammability limits. We have also expanded our efforts to include hydrocarbon flames in addition to hydrogen flames and to perform simulations in support of other on-going efforts in the microgravity combustion sciences program. Modeling hydrocarbon flames typically involves a larger number of species and a much larger number of reactions when compared to hydrogen. In addition, more complex radiation models may also be needed. In order to efficiently compute such complex flames recent developments in parallel computing have been utilized to develop a state-of-the-art parallel flame code. This is discussed below in some detail after a brief discussion of the numerical models.

Numerical Models

Most of the computations discussed in this report have been performed using the two-dimensional time accurate flame code, FLIC2D [1]. Some issues that do not require a multidimensional solution are addressed using FLAME1D [2] . Both of these codes developed at NRL solve the multispecies coupled partial differential reactive-flow equations. These models include a detailed chemical kinetics mechanism coupled to algorithms for convection, thermal conduction, radiation, viscosity, molecular diffusion, thermal diffusion, and external forces. The

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external force, gravity, can be in any direction relative to flame propagation and can have a range of values. All of the chemical and physical processes are solved sequentially and then coupled asymptotically by time step splitting [3]. Space restriction does not allow the elaboration of the models here but details can be found in previous reports [1,2].

Summary of Research

Our recent research can be broadly divided into the following topics: (a) the extinguishment of downward-propagating flames [4], (b) role of hydrodynamic instabilities [5], (c) burner-stabilized flames [6,7], (d) effects of radiative losses of flames near flammability limits, (e) development of a parallel flame code [8], and (f) cellular structure of methane flames [9]. Each of these topics is discussed briefly below.

The Extinguishment of Downward-Propagating Flames

In the continuation of our research on the similarities and differences between zero-gravity and earth gravity flames, we have studied the detailed dynamics and mechanism of extinguishment of downward-propagating flames in two-dimensional channels [4]. The details of the extinguishment process in this mixture has been analyzed 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[10]. 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. This sets up a recirculatory flow which causes an upward motion of the gases at the center of the channel, causing the flame to rise up into the burnt products. Further analysis of the simulations also indicate that the dilution of the unburnt mixture with the products of combustion is an essential step in the extinguishment process. This mechanism may explain the extinguishment of flames in other fuel-air mixtures also (during downward propagation). Currently, this is being tested for flames in lean methane-air mixtures.

The actual limit obtained from the computations for a downward propagating flame in an isothermal channel is around 9.75% and is in good agreement with experimental observations. Our earlier simulations have shown that a flame can propagate downward even in a 9% mixture in a channel with adiabatic walls indicating that heat losses to the walls are essential to the observed limit. Cellular flames are also observed to occur in this mixture, both in simulations and experiments, 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.

Role of Hydrodynamic Instabilities

Recently, we have been able to clarify the relative role of hydrodynamic and thermo-diffusive effects for hydrogen flames[5]. In earlier simulations, rich hydrogen-oxygen-nitrogen (3:1:16) flames were flat in 2 cm and 5.1 cm wide systems even in zero-gravity, while theory would predict them to be non-planar due to the hydrodynamic instability. Recently, when the system size was increased to 9 cm, the flame indeed developed a curved structure due to hydrodynamic effects. These results imply that except for very large systems (system size/flame thickness greater than about 20), the diffusive transport effects dominate the hydrodynamic effects in hydrogen systems. Whether this is true for hydrocarbon systems is a matter that needs to be investigated.

Furthermore, even this flame curvature due to the hydrodynamic instability is suppressed if gravity effects (downward) are turned on, indicating that the hydrodynamic instability is indeed a weak effect. The structure of these flames are also quite different from the classical cellular flame structure.

Burner-Stabilized Flames

We have systematically explored the effects of different burner boundary conditions (Hirschfelder, isothermal, etc.) on the structure and dynamics of both one- and two-dimensional flames stabilized on burners. The different boundary conditions are different ways of characterizing the heat losses to the burner. In addition to reproducing well known features of burner-stabilized flames, these simulations have been used to isolate the role of heat losses, gravity and burner boundary conditions.

Our one-dimensional simulations [6] have shown that, for high inlet velocities, the structure of burner-stabilized flames is similar to that of unconstrained flames. However, for low inlet velocities, the inflection point is absent in the temperature profiles. The characteristic "C-shaped" curve, suggesting two flame temperatures for each flame stand-off distance, is observed as predicted by theory. However, this does not mean that there are two solutions, as suggested by some investigators. An unique solution is seen if the stand-off distance is plotted as a function of the inlet velocity. We conclude that the inlet velocity should be considered as the independent variable, rather than the stand-off distance, as is sometimes done in theoretical analyses. For a Hirschfelder burner, blow-off occurs at a much lower velocity than for the isothermal burner cases studied. In all cases, the blow-off velocity is higher than the burning velocity of an unconstrained flame at the room/coolant temperature. In general, the blow-off velocity corresponds to the burning velocity of an unburnt mixture initially at the burner temperature.

Our two-dimensional flame simulations show that a flame can be stabilized at inlet velocities much higher than the 1-D blow-off velocities because of the curvature of the flame. Cell formation occurs for high inlet velocities but new cells are not formed by cell splitting, as observed in the unconstrained case. At low inlet velocities, cellular structure is suppressed due to increased heat losses and a flat flame is established on the burner. Similar behavior is observed for the isothermal and Hirschfelder burners but at different inlet velocities. The observed differences with the two different burner boundary conditions imply that a characterization of the burner used in experiments is required to make meaningful comparisons with experiments.

The suppression of cellular structures for low inlet velocities occurs in both zero-gravity and downward-propagation burner-stabilized flames. This, in conjunction with our earlier observations on unconstrained flames in these mixtures in zero-gravity indicates that heat losses to the burner are more dominant than gravity in determining the structure and dynamics of these flames [7]. This observation is also in agreement with the conclusions of Dunsky and Fernandez-Pello [11].

Flammability Limits

As discussed earlier, we have a detailed description of the behavior of flames at the downward-propagation limit and both conductive heat losses and gravity are found to be required simultaneously to explain the observations. Similar studies of zero-gravity and upward-propagating flames must await the development of a three-dimensional flame model. Meanwhile, we have also been studying the issue of fundamental flammability limits in a zero-gravity environment using one-dimensional simulations of flames in mixtures that are not expected to show multidimensional structures.

Results from the numerical simulations indicate that a steady burning velocity is not obtained for very rich hydrogen-air mixtures [12]. 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. 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. We speculated earlier that these differences may be because of the neglect of phenomena such as stretch and radiative heat losses.

Simulations of spherically expanding flames indicate 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 radiative heat losses indicate that radiation can indeed shift the apparent flammability limit to less rich mixtures. However, the oscillations observed in the burning velocities are still present even when the effects of radiative heat losses are included. Uncertainty in the chemical-kinetic parameters and multidimensional effects may also play a role in the absolute value of the limiting mixture. Further calculations are currently being carried out to more fully understand the effects of these parameters on the rich flammability limit.

Calculations of flames in lean methane-air mixtures using the one-dimensional flame code show that with radiative losses, a zero-gravity flammability limit of about 5.15% is obtained which is in agreement with experimental data from drop-tower tests. Without radiative losses, flame propagation can be observed in much leaner mixtures.

Development of a Parallel Flame Code

Detailed three-dimensional flame simulations, or even two-dimensional simulations of complex hydrocarbon flames, need a tremendous amount of computer resources. It appears that more cost-effective and efficient computations can be carried out taking advantage of the developments in parallel computing. Therefore, a major research effort was undertaken in the past year to develop and test a parallel version of the multidimensional flame code. The parallel version includes the same physics and employs the same numerical methods used in the vectorized code described above.

The parallel version of the flame code has now been implemented on the Intel Paragon and the IBM SP2 computers. A good test of the parallelism is the scaling of the computation time with the number of processors. Figure 1 shows the timings of the important processes for the computation of a downward-propagating methane-air flame. For this methane computation on a 256 X 256 grid, it requires 50 nodes of the Intel Paragon to equal one CRAY C-90 processor. All processes except the fluid convection scale well. The fluid convection does not scale due to the large amount of communication and scalar code required by the multigrid solution procedure. The chemistry takes 60 - 70% of the total time; thus it is very important that a good load balance is achieved. As shown in the figure, the chemistry module scales extremely well with the number of processors. If a large number of processors are utilized, these computers have the capability to solve a two-dimensional problem with detailed chemistry or even three-dimensional problems with some simplifications.

Cellular Structure of Methane Flames

Cellular structures in methane flames have been studied using a moderately detailed reaction mechanism, popularly called the "skeletal mechanism" involving 16 species and 35 reactions. This mechanism has been used as the starting point for deriving systematically reduced mechanisms. It is unlikely that the reduced mechanisms will provide satisfactory results if the skeletal mechanism itself is unsatisfactory. Simulations of flames in lean methane-air mixtures using this mechanism did not show prominent cellular structures as observed in lean hydrogen-air mixtures. The cellular structures may not have been prominent because the Lewis number of the mixture, though less than one is close to unity (0.9). Theoretical analysis [13] indicates that the deviation from unity is an important parameter determining the cellular structure of flames. The Lewis number can be decreased by adding carbon dioxide as a diluent. Therefore, further simulations were carried out with carbon dioxide dilution.

A 56.5% carbon dioxide diluted methane mixture with an equivalence ratio of 0.5 is particularly interesting since it has a burning velocity of about 7.5 cm/s which is close to the burning velocity of near-limit CO2 diluted mixtures studied experimentally. Figure 2 shows the time evolution of the OH mole fraction at 15 ms intervals. The vertical scale in this figure has been expanded two times for clarity. The variations in the OH concentration along the flame are not as large as in hydrogen-air flames making the cellular structures appear more like ripples on the flame. Though the Lewis number of this mixture is small (0.7), it is still large than those of lean hydrogen-air flames (~0.3) and probably accounts for the differences in the flame structure. The cellular structures are however much more prominent than in lean methane-air flames indicating that the deviation of the Lewis number from unity is important in determining the size and strength of the cellular structures, in accordance with the theory [13].

The size of the cells observed in the simulations, 5 cells in a 5.1 cm channel, is in good agreement with experimental observations (elsewhere in this volume) of Ronney, 10-11 cells in a 10 cm diameter tube. However, the limiting mixture though having a comparable burning velocity to those in experiments, is quantitatively different. The dilution limit observed in the computations is about 56.5% CO_2 while the experimental limit is between 57.4-58.3% dilution. While there are details in the configuration used in the experiments and simulations, the uncertainties in the chemical parameters could also account for such differences. Further studies with the one-dimensional flame code indicates small changes in the third-body efficiencies used in the chemical reaction scheme could significantly alter the limit mixtures and burning velocities. The skeletal mechanism used may also be inadequate for mixtures diluted with large amounts of CO2. Further studies with more comprehensive reaction mechanisms will be useful to resolve this issue.

Work in Progress and Future Plans

Currently, the detailed mechanism of the extinguishment of downward-propagating methane-air flames is being studied using the newly developed parallel version of the flame code. This study will help confirm if the mechanisms observed earlier in the extinguishment of lean hydrogen-air flames is also true for methane. A similar study for a higher hydrocarbon such as propane may also be needed to generalize the observation.

The studies of flames with CO_2 dilution suggest that some simulations with more detailed methane mechanisms is needed before moving on to more reduced reaction mechanisms. Even with the development of the parallel version of the flame code, simplified mechanisms will be needed to simulate transient three-dimensional phenomena such as the breakdown of flame strings to flame balls. Three-dimensional simulations are also needed to predict extinguishment of upward-propagating and zero-gravity flames. So a major effort in the next year will be to develop and test a three-dimensional version of the flame code.

Recently, collaborations have also been established with the group at the University of Michigan to perform simulations that are complementary to the experiments being planned such as the interaction between a vortex and a flame in a premixed gas in a tube. The collaboration has already produced some interesting results on unsteady diffusion flames that can be found elsewhere in this volume.

Acknowledgments

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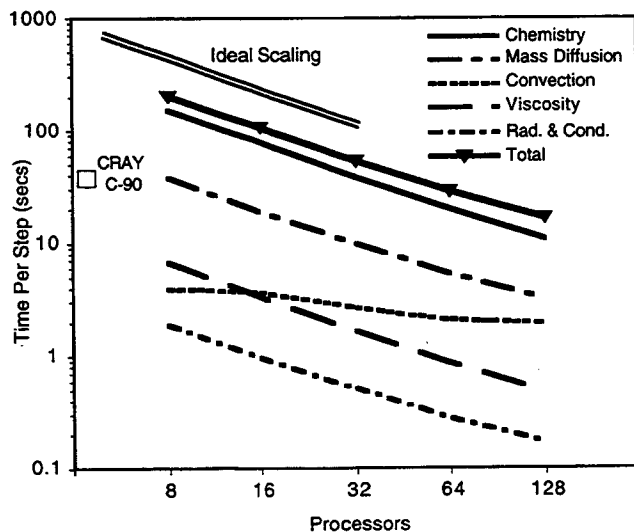13. Pelce,P. and Clavin, P., J. Fluid Mech., 124:219-237, 1982.
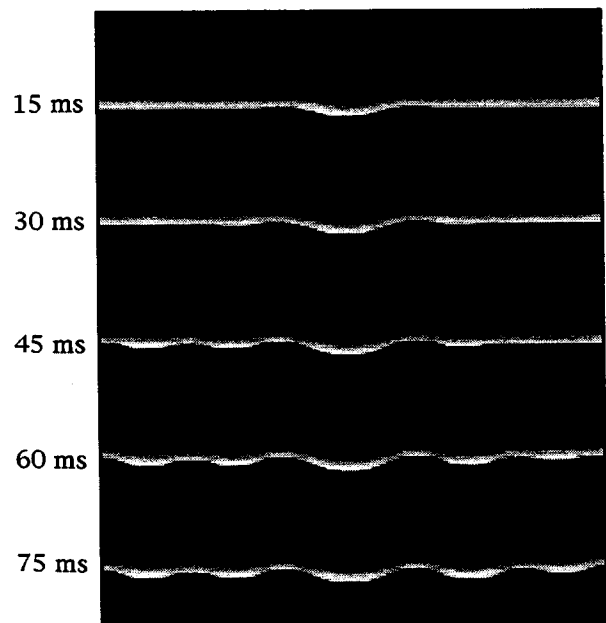

Fig. 1. Computation times on Intel Paragon.

Fig. 2. Cellular structures in a 56.5% Methane - CO2 Flame