STRUCTURE AND DYNAMICS OF DIFFUSION FLAMES IN MICROGRAVITY

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Introduction

The objectives of this project are to gain insight into diffusion flames by modeling various configurations related to ongoing experimental investigations in the microgravity combustion science program. The emphasis of the work is to understand the structure and dynamics of diffusion flames. Improving our fundamental understanding of diffusion flames is most relevant to issues related to fire safety and fire prevention because most fires consist of diffusion flames.

Work on this project started in May 1994.

Near-limit Oscillations

From recent experiments of candle flames conducted in a reduced gravity environment [1], [2], the following observations were made:

- the flame shape is nearly a hemisphere as opposed to the elongated tear drop shape observed under normal gravity conditions
- the flame standoff distance is quite large; at the base of the flame that distance is about 5mm compared to 1mm in normal gravity conditions
- the flame is steady during most of the process, however, as the oxygen in the chamber is consumed, spontaneous oscillations develop prior to extinction
- the burning rate and the flame temperature are considerably reduced when compared with their values in normal gravity.

The goal of our current efforts is to shed light on these observations and in particular on the oscillations that occur during the last stages of the burning.

In microgravity the candle flame bears some similarity to the diffusion flame that surrounds a burning liquid droplet. Both have a spherical shape and both depend on the heat conducted back to the condensed phase. Hence their structure and dynamical properties are likely to be similar. In our first attempt to model the above observations we have therefore analyzed the droplet problem. To simulate the experimental conditions we consider the burning to occur in a reduced oxidant environment, i.e. the ambient mass fraction of the oxidant, X_{∞} , is assumed small. Under these conditions the flame standoff distance is relatively large and the burning rate is reduced. The combustion field is now divided into a near-field, where fuel vapor in the absence of oxidant is transported outward by convection and diffusion, and a broad chemically reactive far-field where convection is effectively negligible. For steady burning the mass burning rate \dot{m} is expressed in the form

$$\dot{m} = \frac{4\pi a\lambda}{c_p} \left\{ \ln\left(1+B\right) + \frac{1}{L} \left(\frac{QX_{\infty}}{\nu_X W_X}\right) \frac{\mu}{1+B} \right\}$$
(1)

where a is the droplet radius, λ and c_p are the thermal conductivity and specific heat (at constant pressure) of the mixture, $B = c_p (T_{\infty} - T_s)/L$ is the transfer number for pure vaporization with T_s, T_∞ the surface and ambient temperatures respectively, L is the latent heat of vaporization and $Q/\nu_X W_X$ is the heat of reaction per unit mass of oxidant consumed (the subscript X identifies the oxidant). The parameter μ , obtained by numerically solving the reactive-diffusive far-field equations, depends on the physico-chemical parameters and in particular on the Damköhler number δ representing the ratio of diffusion time to chemical reaction time. We note that in the absence of heat loss $\mu \to 1$ as $\delta \to \infty$; eq. (1) then reduces to the classical expression for the burning rate (e.g. [3]) when expanded for small X_{∞} . The dependence of the mass burning rate μ on the Damköhler number δ is shown in Fig. 1. The response curve exhibits different characteristics depending on the ambient oxidant concentration X_∞ and on the heat loss parameter h. For moderate values of X_∞ the familiar S-shaped response curve is obtained. However, by reducing the oxidant concentration the response curve becomes monotonic connecting the weakly burning state where $\mu \sim \delta^{1/2}$ (for small δ), to the equilibrium limit where μ tends to a constant ≤ 1 as $\delta \to \infty$. The asymptotic value reached for large δ depends of course on the heat loss parameter h. The steady problem in the absence of heat loss and with a unity Lewis number has been previously discussed in [4], as part of a complete discussion of a droplet combustion analysis.

The change in shape of the response curve has significant implications regarding the dynamics of the flame. For example, the concept of abrupt extinction is associated with the S-shaped response curve. If the Damköhler number δ is slowly decreased, say in an experiment, the upper branch corresponding to an intense burning is followed down to the turning point δ_E where the response jumps to the lower branch corresponding to a weak burning or an extinguished state. The point $\delta = \delta_E$ (which, in general, does not have to be the turning point) is associated with extinction. In contrast, a monotonic response curve indicates that the transition from an intense to a weak burning takes place in a gradual way. Behind this description is the assumption that the middle branch of the S-curve is unstable and therefore cannot be realized in practice. The monotonic curve on the other hand is often assumed to be stable for all δ . This hypothesis appears to be true when there is no heat loss.

In the presence of heat loss, however, it is found that part of the monotonic curve may become unstable (see Fig. 2). When perturbations proportional to $\exp(i\omega t)$ are sought, one finds that growing modes are possible for δ below some critical number. Furthermore, at the onset of instability $\mathcal{R}e(\omega) \neq 0$ implying that a growing oscillatory mode develops. The frequency of oscillations is given by

$$\mathcal{R}e(\omega) = lpha rac{\lambda eta^{-2}}{
ho_{\infty} c_p a^2}$$

where $\beta = E/RT_{\infty}$ is the activation energy parameter, assumed large, and α is an O(1) number. By slowly decreasing δ below its critical value, only a small change in the frequency (i.e. in α) is detected but the amplitude grows continuously. It is therefore anticipated that as the amplitude becomes sufficiently large the flame extinguishes. Hence near limit oscillations, similar to the one observed in the microgravity candle flame experiment [2], may result in the presence of heat loss.

Future plans include examining other source of perturbations which may also yield flame

oscillations. For example, near-limit oscillations have been observed in candle flames under normal gravity conditions at relatively low pressures [5]. It has been suggested that the presence of convective flows may be responsible for these oscillations. Although this does not appear to be the mechanism responsible for the oscillations in the microgravity experiments [2], it would be of interest to incorporate weak buoyant flows as a source of perturbations in the analysis in order to better understand the difference between these two environments. Attempt will also be made to model the candle flame itself, which more closely resembles a spherical cap rather than a complete sphere.

Flame Front Instabilities

Studies of intrinsic instabilities in flames have been predominantly concerned with premixed systems. A manifestation of an intrinsic instability is the spontaneous development of cellular structures, which is commonly observed in premixed flames. The competing effects of thermal and mass diffusivities play a central role in the development of cellular flames. One might therefore expect that they play a similar role in diffusion flames as well. However, very little has been done on the subject. The lack of experimental work in this area may be attributed to the fact that it is difficult to generate in the laboratory a one-dimensional diffusion flame free of the stabilizing influence of stretch. The most comprehensive experimental study [6] has been carried out only recently using a slot-jet flame. Using a spherical burner in microgravity a one dimensional spherical flame of sufficiently large size can be produced. This configuration may well be suited for studying the development of flame front instabilities in diffusion flames, both theoretically and experimentally. The goal of our current efforts is to pursue a theoretical study of thermal-diffusive instabilities in diffusion flames.

An important parameter in this study is the Damköhler number δ . In the limit $\delta \to \infty$, known as the Burke Schumann limit, the chemical reaction is concentrated in a thin sheet separating a region where there is fuel but no oxidant from a region where there is oxidant but no fuel. The requirement that fuel and oxidant do not co-exist and the requirement that fuel and oxidant must flow into the flame sheet from opposite sides in stochiometric proportions, are sufficient conditions for complete determination of the combustion field including the instantaneous shape and location of the flame sheet. Stability analyses of simple flame configurations show that under such conditions the flame sheet is absolutely stable.

The situation is different when there is a leakage of fuel and/or oxidant. The mathematical formulation in this case is based on the assumption that δ is large but such that $\hat{\delta} = \delta \beta^{-3} \exp(-\beta/T_f)$, where $\beta \gg 1$ is the activation energy parameter and T_f is the flame temperature for complete combustion, is O(1). The reduced Damköhler number $\hat{\delta}$ plays an important role in this description. The inner structure for a steady one-dimensional flame has been discussed by Linan [7]; it depends on two parameters $\hat{\delta}$ and γ . (Of practical interest is $|\gamma| < 1$; depending on its sign γ stands for the fractional excess of heat that is conducted to the fuel or oxidant side of the reaction zone). Numerical integration of the structure equation reveals the dependence of the combustion field on these parameters. The Burke Shumann limit is recovered when $\hat{\delta} \to \infty$. By reducing $\hat{\delta}$ a small leakage of fuel and/or oxidant develops and the flame temperature decreases. This behavior persists with the reactants leakage and the flame temperature reduction increasing continuously, until extinction occurs at $\hat{\delta} = \hat{\delta}_{ex}$.

For a steady one-dimensional flame the parameter $\hat{\delta}$ is a constant determined by the underlying flow field. For example, in a counterflow $\hat{\delta}$ is proportional to the imposed strain

rate. For a general three-dimensional corrugated flame $\hat{\delta}$ is only determined locally, for example in terms of the local orientation of the reaction sheet and the local fuel and oxidant concentrations, or in terms of the local gradients of the mixture fraction [3]. We have thus extended Linan's analysis to allow for temporal and spatial variations. To complete the mathematical formulation expressions for the reactant leakages and their dependence on $\hat{\delta}$ must be identified. Fig. 3 shows the results of the numerical integration of the structure equation for $\gamma > 0$. For $\gamma < 0$ the role of the fuel and oxidant are interchanged. Expressions for the leakages that best interpolate the numerical data of Fig. 3 take the form

$$Y_* \sim (\beta \hat{\delta})^{-1} \exp\left[-C_F (\hat{\delta} - \hat{\delta}_{ex})^a\right]$$
(2)

$$X_* \sim \beta^{-1} \exp\left[-C_X (\hat{\delta} - \hat{\delta}_{ex})^b\right]$$
(3)

where C_F, C_X, a, b depend only on γ . Clearly Y_* and X_* vanish as $\hat{\delta} \to \infty$. When $\gamma = 0$, equal amounts of fuel and oxidant leak through the reaction zone. As $\gamma \to 1$, however, the fuel leakage at extinction becomes excessively large, i.e. $Y_* = O(1)$, and the oxidant leakage becomes negligibly small, i.e. $X_* = 0$. The reverse is true when $\gamma \to -1$. This general formulation is suitable for investigating the stability of simple flame configurations. Preliminary results indicate that depending on the fuel and oxidant Lewis numbers instabilities leading to cellular structures may arise. This appears to be consistent with the experimental results of [6]. A systematic study is being carried out to identify the stability boundaries in terms of the relevant parameters.

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Fig.1 - The dependence of burning rate on the Damkohler number for selected values of $\gamma \sim X_{\infty}$; calculated for h = 0.



Fig.2 - Response curves for selected values of $\gamma \sim X_{\infty}$ with h = 1. The dark segments correspond to the unstable states where the oscillations occur.



Fig.3 - Fuel and oxidant leakages through the reaction zone for selected values of γ . For $\gamma < 1$ the role of fuel and oxidant are interchanged.