PROJECT SUMMARY

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One of the major problems in turbulent combustion is to predict the turbulent burning velocity, which can be increased by the turbulence compared to the laminar burning velocity. This requires the solution to a reacting flow problem, where the turbulence is coupled to the chemical reaction. The difficulties lie in the fact that many disparate spatial and temporal scales are present in the convection-reaction-diffusion system. The investigator studies several simplified flame/flow interactions, where fluid flows have separate large and small scales. The particular aspects considered are the diminished enhancement of turbulent burning velocity when the turbulence intensity is increased above a certain value (the bending phenomenon), and the onset of flame quenching when the turbulence is too strong. The focus is on the often ignored interaction between small scale fluid flow and chemical reaction. The approach is to solve the system in two stages: (1) a small scale problem is solved with full interaction between chemistry and fluid flow to generate the local burning velocity, which can be quite different from the laminar burning velocity; (2) at the large scale level, this local burning velocity is used, together with the large scale fluid velocity, to move the flame front, where it is treated as an interface. The turbulent burning velocity is then estimated and the bending phenomenon is analyzed. The investigator uses the projection method for viscous fluid and implicit second-order upwind finite difference methods for the chemical reaction or the front evolution respectively, at two different scale levels. The objective is to assess the effects of small scale fluid flows on the turbulent burning velocity when the turbulent intensity is large. In another project, the investigator develops a free boundary formulation to model an experiment for chemical fronts propagating in a Hele-Shaw cell, under buoyancy effects. In this model, a mechanism that produces fingers that are different from those in the classic viscous fingering phenomenon is identified. The objective is to obtain the wavelength criterion for the fingers which is distinctive in the experiment. The investigator uses a potential theory formulation to solve a simplified model and the level set (G-equation) formulation to solve a more complete model. A method for the evolving temperature that captures its correct jumps across the front is developed. The wavelength of the fingers are important for understanding flame instability caused by buoyancy effects.

Computational Studies of Flame-Flow Interactions

Jingyi Zhu

Introduction

Turbulent combustion is probably the most important area in combustion science, yet to this day no comprehensive theory has been developed. The reasons for this include the extremely complicated fluid and chemical reaction systems and the lack of a theoretical understanding of the turbulence phenomenon itself. However, the advent of fast computers and state-of-the-art numerical methodologies developed in the last several decades offer new hope that breakthroughs on these problems will be made in the near future.

Here, we focus on the problem of flame-flow interaction for some idealized systems and propose to work on two important aspects of this problem: predicting the turbulent burning velocity in premixed flames, and buoyancy effects in front propagation. There is a long history of investigation of these issues from both theoretical and experimental approaches, obviously due to their practical importance. Now, numerical simulations are playing more and more important roles and continue to make great progress in understanding these interactions.

In premixed flames, the turbulent burning velocity S_T, which is defined as the mass consumption rate per unit cross-section area divided by the reactant fluid density, is found to increase as the turbulent flow intensity u' increases [70]. However, increasing u' beyond certain level increases S_T very little and may lead to complete quenching of the flame [1]. This is the so-call "bending" phenomenon [7, 56]. Various attempts had been made in the past to study the effect of u' on S_T [16, 32, 3, 4, 73, 66, 12], mostly with the assumption that the combustion happens in the flamelet regime, where the laminar flame structure is preserved for the local wrinkled flame in turbulence. Under this assumption, several factors have been identified and studied: such as the effect of thermal expansion [3, 21]; the effect of flame stretch [52, 59]; and the effect of the kinetic energy spectrum of the flow field [32, 73, 65, 31]. The results show that they are responsible for the bending phenomenon. However, none of the above factors is seen to lead to the quenching phenomenon under the flamelet assumption [56]. To find the mechanism that will eventually lead to flame quenching, we propose to study the effects of combustion in a different mode: the distributed combustion mode [42], in which the flame structure is substantially changed by the small scale fluid flow, and how it affects the turbulent burning velocity. The rationale is that even if a typical turbulent combustion operates mostly in the flamelet mode, still, there may be a portion of the flame where there is a transition to distributed combustion, which would contribute to the bending phenomenon and eventually could cause certain portions of the flame to quench. This effect has been discussed by Ronney and Yakhot [55] in an analysis of the flame broadening effects with certain turbulence models. Substantial Direct Numerical Simulations have been performed on flame flow interactions [33, 9, 59, 53]. However, a detailed numerical study of the complete reaction-diffusion-convection system in distributed combustion regime has not been reported in the literature. We propose here to proceed in two stages to study the flame-flow interactions at both the small scale and large scale levels, by using the latest numerical methodologies and taking advantage of the huge advance in computational speed on available computers.

From a numerical point of view, the main difficulty in turbulent combustion is the many disparate spatial and temporal scales present in the system. To solve the complete fluid and chemical reaction system satisfactorily is still impossible on existing computers. With a turbulent flow field, even adaptive grid methods do not seem to help much since turbulent flames appear almost everywhere in the region. Our approach is to borrow some ideas from large eddy simulation (LES) where only the large scale parts are resolved in calculations and the small scale effects are taken care of through modeling. In the first stage we will choose some simplified models at a small scale, identify the mechanisms that are common to more complicated systems, and try to understand them as fully as possible. At this level there is a full interaction between the fluid flow and the chemical reaction in that the flame structure is dominated by the small scale flow. We will develop reliable numerical algorithms to obtain important information that will be useful at larger scales. We propose several efficient implicit methods to deal with the small scale interactions between the fluid and the chemistry, which can have different nonlinearities. Particular attention will be paid to the validity of Huygens principle, which is widely used in flamelet approximations.

In the second stage, the information obtained from such small scale models will then be integrated into the large scale problem in a G-equation [47, 71, 36, 50] setting, but with a variable local burning velocity that is valid when the flame thickness changes substantially due to the local flow. The turbulent burning velocity will then be estimated at this level and compared to similar results from the flamelet model. We will be looking in particular for the bending phenomenon in our results. The first stage can be viewed as generating corrections to account for the small scale effects that have been ignored in the flamelet formulation. Our approach has the advantage that both regimes are covered and the switch is done automatically.

The above two stages constitute the first two parts of the proposal. The third part is an independent problem which deals with buoyancy effects in premixed flame propagation. It is a model for a particular experiment [58] associated with buoyancy effects in chemical front propagation in a Hele-Shaw flow. The purpose of this study is to understand the role buoyancy plays in flame instability, which is a very important issue in practical concerns such as accidental fire. The interesting point of this problem is that it is one of very few combustion problems where a fairly complete mathematical model can be obtained which is feasible to solve numerically. Some work for a simplified model is already done and the results are very encouraging. The approaches for the complete model are proposed here.

1 Premixed Flame Propagation in Distributed Combustion

1.1 Physical Problem

Premixed combustion can be divided into different regimes according to the relationships between the various spatial and temporal scales. There are three important time scales in turbulent premixed combustion processes: (1) the large-eddy turnover time scale (t_i) that is determined from the integral length scale of the turbulence (L_I) and the turbulence intensity u'; (2) the small-eddy cutoff time scale t_k (the Kolmogorov time scale in inertial-range turbulence), its ratio to t_i is proportional to the turbulent Reynolds number Re_L; and (3) the chemical time scale t_c, which is proportional to D/S_L^2, where D is a characteristic molecular diffusivity and S_L is the laminar burning velocity. The regimes can be identified using the ratios of these three time scales. They can be obtained from the turbulent Reynolds number $Re_L \approx (t_i/t_k)^2$ and the Karlovitz number $Ka \approx t_c/t_k$. The turbulent Reynolds number is always considered large in turbulent combustion and that leaves the Karlovitz number to determine the regime. The flamelet regime [51] (the "thin" flame model) is obtained by assuming $Ka << 1$ which gives $t_c << t_k << t_i$. In this case both fluid flow time scales are much larger than the chemical time scale, so the flow field is not expected to change the basic structure of the reaction layer. The significance of this is that the laminar flame theory can be modified and applied to the fluid-flame interaction. In this regime, flame propagation is described by a convection and a self-propagation with a local burning velocity S_L, modified only by the flame stretch [71], which comes from the curvature and fluid velocity strain rates at the front.

Important though this flamelet regime is, it does not provide a natural mechanism for the flame structure to be altered to lead to flame quenching. On the other hand, in the regime where $Ka >> 1$ ($t_k << t_c$), the distributed combustion regime, the local flow strain rate is sufficient to extinguish the flame front [70]. When a flame is quenched by a turbulent flow, it is very likely that first there is a transition from flamelet to distributed combustion. The transition is not sharp [56], therefore it is useful to consider the intermediate regime where t_c is comparable to t_k. This can be characterized as a chemical reaction that is fast with respect to the integral scale flow, but slow or comparable with respect to the small scale fluid flow. Here, the complication is that we can no longer assume the laminar flame structure for the reaction layer. The flow-flame interaction becomes important even at the reaction layer level. As a consequence, the reaction rate will be modified locally depending on the small-scale flow. If we still treat the layer as a propagating front, the local burning velocity will be quite different from that of the laminar burning velocity. Damköhler proposed that the mean chemical reaction rate might be the same as in the laminar flame, therefore the change in the burning velocity compared with that of the laminar flame is controlled only by the change in the molecular diffusivity due to the turbulence. If we denote the modified burning velocity and the effective diffusivity by S_L^* and D^* respectively, we have

$$\frac{S_L^*}{S_L} = \sqrt{\frac{D^*}{D}}. \tag{1}$$

With this assumption, the change in the burning velocity can be obtained by calculating the effective turbulent diffusivity. In the passive turbulent diffusion case, certain results for the effective diffusivity are available [48, 29, 44]. However, the Damköhler hypothesis has not been verified and in certain cases it is highly questionable. Our purpose here is to numerically study several simplified one-step chemistry systems described below that are coupled to the fluid equations, and obtain estimates for the modified S_L^* for several different chemical reactions.

The one-step chemical reaction system we propose to study that governs a homogeneous premixed combustible mixture is

$$\rho(Y_t + \mathbf{u} \cdot \nabla Y) = \frac{\epsilon}{Le}\nabla^2 Y - \frac{1}{\epsilon} f(Y,T) \tag{2}$$

$$\rho(T_t + \mathbf{u} \cdot \nabla T) = \epsilon \nabla^2 T + \frac{q}{\epsilon} f(Y,T) - CT^4 \tag{3}$$

This system is in an appropriate nondimensional form. Here Y is the concentration of the reactant species, T between 0 and 1 is the normalized temperature (with respect to the burned and unburned temperatures), ϵ is the ratio of the thermal thickness to the turbulent integral length scale L_I with which all the lengths have been nondimensionalized; q is the heat release; the Lewis number Le is the ratio of the thermal diffusivity to the mass diffusivity. We have also included a heat loss term CT^4 that is due to radiation, where the constant C depends on the Stefan-Boltzmann constant and the Planck-mean absorption length [70]. The radiant heat loss is thought to be important in distributed combustion, which can be a major factor in causing flame quenching [56]. In the constant density model where the flow is decoupled, a normalized $\rho = 1$ and a given incompressible velocity field $\mathbf{u}$ are given *a priori*. In the coupled system, we choose to use a low Mach number model for closed vessels where the leading order pressure, the thermal dynamic pressure P, is assumed to be a function of time only. The fluid system can be written as [43]

$$\rho T = P(t) \tag{4}$$

$$\rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \epsilon Pr \nabla^2 \mathbf{u} \tag{5}$$

$$\nabla \cdot \mathbf{u} = \frac{1}{\gamma P} \left[-\frac{dP}{dt} + \frac{\gamma q}{\epsilon Vol(\Omega)} f(Y,T) \right] \tag{6}$$

$$\frac{dP}{dt} = \frac{\gamma q}{\epsilon Vol(\Omega)} \int_\Omega f(Y,T) d\mathbf{x}, \tag{7}$$

with appropriate boundary conditions and initial conditions. Here Pr is the Prandtl number and γ is the specific heat ratio. The temperature T and species Y are coupled to Eqs. (2- 3).

Three different chemical reaction forms will be considered and compared:

- **Arrhenius reaction**

$$f(Y,T) = A\rho Y \exp(-\beta(1-T)) \tag{8}$$

  where the parameter A is the reaction prefactor, β is the reduced activation energy, or the Zeldovich number. This form approximates a one-step exothermic chemical reaction quite well.

The following two cases will be considered for the case where $Le = 1$ and the radiant heat loss is ignored, where one of the normalized unknowns can be eliminated. In this case, we only have to consider the temperature equation.

- **KPP reaction**

$$f(T) = AT(1-T) \tag{9}$$

  for some positive constant A. This is the simplest form that gives the required two states.

- **Piecewise linear form (Clavin and Liñan [17]**)

$$f(T) = \begin{cases} AY, & 0 \le T \le T_*, \\ B(1-T), & T_* \le T \le 1, \end{cases} \tag{10}$$

  where the parameters A and B are the reaction rates in the unburned and burnt states, respectively with the parameter ranges $-\infty < A < \infty$ and $B > 0$. This form allows for three distinct regimes of behavior that can be analyzed [17, 27].

The fluid velocity $\mathbf{u}$ is from a fluid system which we assume may or may not be coupled to the chemical system. We propose to proceed in three steps: (1) prescribe a known incompressible flow field, such as shear and vortex flows; (2) assume the flow satisfies the nonreactive incompressible Navier-Stokes equations; and (3) allow a full interactive system such as the low-Mach number system Eq. (4-7), instead of the fully compressible system.

In the distributed combustion regime, all scales of turbulence are expected to lie inside the flame. In our proposed study, we want to study the intermediate regime that lies between this regime and the flamelet regime with some vortex dominated flows (no attempt is made at this stage to simulate real turbulent flows). Thus the flow scales will run from those smaller than the flame thickness to those comparable to the flame thickness. With our computing capacity, the scale range could be rather limited. An efficient way to introduce flow scales into calculations is to start with a collection of vortices with a range of core sizes. The range of flow scales can therefore be controlled in the calculation.

1.2 Our Previous Work

We have worked on several problems of this type, at a small fluid scale level, in order to obtain understanding of the local flame-flow interaction. Flame quenching by a small oscillatory flow was observed in our previous work with Xin [72], where a bistable nonlinearity and a given incompressible flow were used. It was found that nonuniform media and the mean zero flow can effectively block the chemical wave when the strength of these disturbances is strong enough. In another joint work with McLaughlin [49], we investigated the effects of finite layer thickness on the effective burning velocity, as opposed to the thin flame model described by Huygens principle. In this work, KPP nonlinearity is used and a shear flow with length scale comparable to the flame thickness is combined with a constant mean flow. It is found that the enhanced burning velocity is sensitive to the alignment of the large scale mean flow with respect to the front orientation. Linear and quadratic dependence on the small scale flow intensity u' are observed for different alignments. We also observed that the finite thickness effect results in a smaller burning velocity than that of the thin flame fronts. These observations should be quite useful in the construction of accurate Large Eddy Simulations and demonstrate that the scheme coefficients should be chosen with care.

1.3 Numerical Tools

The basic components in the our numerical solutions are (1) a fluid solver based on the second-order projection method; and (2) an implicit nonlinear solver for the convection-reaction-diffusion system. In the case where the flow field is prescribed *a priori*, the fluid solver is decoupled from the nonlinear solver. The basic structure of the algorithm will extend our work in [72, 49, 78]. The new challenge is to be able to deal with those different nonlinearities that are not covered in our previous works, particularly in the piece-wise linear type where the Newton's method is expected to fail. Here we summarize the essential components involved in our current codes and propose approaches to deal with the new situations.

The fluid solver is an extension of a well-established second-order projection method developed by Bell, Collela and Glaz [10] which is an upgrade of the original projection method developed by Chorin [15]. The extension to the low-Mach number with chemical reaction was carried out by Lai, Bell and Collela [38]. Over the years, we have develop several codes that incorporate this methodology for different applications, involving different geometry and boundary conditions. Our previous applications involve a non-reactive fluid calculation for viscous flows in a channel with a backward-facing step [76], a low-Mach number system with infinitely thin flame front, and a weakly compressible system for enhanced thermal diffusion. The main features of the method are (1) a fractional step approach where a projection step is taken to make a correction so the incompressibility constraint is satisfied; (2) a second-order Gudonov upwind procedure used to treat all the convection terms, including those in the fluid equation and the two reaction-diffusion equations. An improved version, the approximate projection method, was introduced by Almgren, Bell and Szymczak [2], and it has also been implemented in our codes.

The nonlinear solver is based on a Newton's method and we plan to use a well-proven package NKSOL in this project. The package solves a system of nonlinear algebraic equations. In our applications, we discretize the convection-reaction-diffusion systems with second-order truncation errors in both space and time. Both the diffusion and the reaction terms are approximated by the averages of the values of the current step and the next step, leading to a Crank-Nicolson implicit algorithm. The main difficulty is the stiffness of the system when the activation energy is large (the reaction is concentrated along a thin region). Our implicit methods should work well given the resolution required. The piecewise linear case is introduced here in the hope that the resulting nonlinear system is less expensive to solve compared to the exponential form. However, in this case the Newton's method approach will not work since the nonlinearity is not smooth. In [27], a fixed point iteration approach is used in a one-space-dimensional problem. We will develop our own iterative method for two-space-dimensional problems. A typical grid size that we want use will be 512×512.

1.4 Computing Effective Properties

The goal is to compute effective properties of the flame when it interacts with a small scale local flow and a large scale mean flow. They include: the effective burning velocity, its dependence on the effective diffusion coefficients resulting from the flows; and the average reaction rate.

1.4.1 Effective Burning Velocity S_L^*

One of the most significant differences between the regime we consider here and the flamelet regime is that T and Y are no longer monotone across the reaction layer. Here we need some effective quantity to estimate how fast the reaction layer moves in the fluid. For two space dimensional problems where the chemical wave propagates from the left end towards the right, and with periodic boundary conditions in the y direction, we propose to use

$$S_L^* = \frac{1}{L_y}\frac{d}{dt}\int_\Omega Y d\mathbf{x}, \tag{11}$$

where Y is the normalized fuel concentration, Ω is the rectangular computational domain, and L_y is the length of the computational box in y direction. The integral can be viewed as the portion of the mixture which has reacted.

1.4.2 Effective Thickness of the Reaction Layer δ^*

The definition of the reaction layer in the distributed combustion regime is complicated because of the lack of the laminar flame structure. Here we use the region where substantial reaction is taking place as the reaction layer,

$$A_{reaction} = \int_\Omega \chi(\mathbf{x}) d\mathbf{x}, \tag{12}$$

where

$$\chi = \begin{cases} 1, & \epsilon_0 \le Y \le 1 - \epsilon_0, \\ 0, & \text{otherwise.} \end{cases} \tag{13}$$

for some small $\epsilon_0 > 0$ which should be chosen in the calculation. The averaged reaction layer thickness is therefore defined by

$$\delta^* = \frac{A_{reaction}}{L_y} \tag{14}$$

1.4.3 Effective Diffusion Coefficients D^*

In the presence of periodic incompressible flows, the effective transport properties for scalars can be estimated by solving several elliptic equations in nondimensional variables [29, 44] for $\chi_i, i = 1, 2$ (for two dimensions):

$$D\nabla^2\chi_i - \mathbf{u}(\mathbf{x}) \cdot \nabla\chi_i = u_i(\mathbf{x}), \tag{15}$$

where D is the molecular heat or mass diffusivity. The enhanced diffusity is then

$$D^*_{i,j} = D\left(\delta_{i,j} + \frac{1}{A_\Omega}\int_\Omega \nabla\chi_i \cdot \nabla\chi_j d\mathbf{x}\right). \tag{16}$$

Numerically, given $\mathbf{u}$, we need to solve several elliptic equations that have first order terms with variable coefficients. We plan to modify our multigrid Poisson solver to include these first order terms. If we assume the small scale flow to be isotropic, we would only need to calculate $D^* = D_{1,1} = D_{2,2}$. For diffusion of passive scalars in stochastic velocity fields with well-defined energy spectrum, we can follow the approaches in [14].

1.4.4 Average Chemical Reaction Rate ω^*

Damköhler's assumption that the mean chemical reaction rate ω^* might be the same as in a laminar flame (ω_L) will be investigated here. We calculate

$$\frac{\omega^*}{\omega_L} = \frac{\int_\Omega f(Y,T)d\mathbf{x}}{L_y \int_0^{x_L} f(Y_0, T_0)dx}, \tag{17}$$

where (Y, T) is a two-dimensional solution to the distributed combustion problem and (Y_0, T_0) is a one-dimensional solution to the laminar flame problem and x_L is the length of the rectangular domain.

1.5 Objective: Functional Relations

Our objective in this project is to produce functional forms, if they exist, relating the modified burning velocity to the effective flame thickness, the average reaction rate, and the effective diffusivity. We start from the analogy with laminar flames, where $S_L \sim \sqrt{D\omega}$, so

$$\frac{S^*_L}{S_L} = \sqrt{\frac{D^*}{D}\frac{\omega^*}{\omega_L}}. \tag{18}$$

We would like to relate this ratio to the ratio of the layer thickness δ^*/δ and the small scale fluid intensity u', which can be defined as the RMS of the flow field. First we will try to find a functional relationship between D^*/D and δ^*/δ, this will give us the dependence of the latter on the local flow structure given by u' and the energy spectrum. Finally we will investigate the dependence of ω^*/ω_L on δ^*/δ.

2 Small Scale Flow Effects on the Premixed Turbulent Flame Velocity

2.1 The Problem and Our Previous Work

This aspect concerns the prediction of the turbulent burning velocity S_T in some chosen flows. Previous asymptotic theories [16, 46] exploit the advantages of the flamelet model, and use the ratio between the flame thickness and the wrinkling wavelength as a small parameter in the analysis. The effect of the fluid flow on the flame is mostly through flame wrinkling and flame stretch, but the basic flame structure is still the same as that of a laminar flame. When the heat release is small enough so the effects of thermal expansions are ignored, the flame can be treated as a propagating front moving with the flow field. The so-called G-equation [47, 71, 50, 36]

$$G_t + \mathbf{u} \cdot \nabla G = S_L |\nabla G| \tag{19}$$

describes the front dynamics very well. Here a flame front is represented by a level surface of G, $\mathbf{u}$ is a prescribed velocity field, and S_L is the laminar burning velocity from the laminar flame theory. This equation implicitly assumes Huygens principle which specifies that the front propagates in its normal direction with a given speed S_L. We have solved this G-equation numerically in previous work [74, 75] and have obtained a $S_T - u'$ relationship for certain mean zero vortex flows (see figure 1). The flame stretch effects are included in our calculations and it is shown that they contribute to the bending phenomenon. The major question is how much we can rely on this Huygens principle, given the flow interaction. This issue has been explored recently by Embid, Majda and Souganidis [27] in a study of a scalar advection-reaction-diffusion equation with a piecewise linear reaction. It is found that Huygens principle can be violated in situations depending on the directions of the front and the velocity strain. A modification to Eq. (19) is possible by incorporating the flame stretch dependence of the laminar burning velocity. The underlying mechanism is that a wrinkled flame is stretched by the local mean curvature and the fluid velocity strain. As a result, the local flame becomes thinner and a thinner reaction layer will result in a smaller burning velocity, according to laminar flame theory. We recognize that it is the uneven flame thickness along the wrinkled flame that causes nonuniform burning velocity. However, this flame stretch dependence of S_L is known through asymptotic theory for weak flame stretch only [13] and the applicability is limited. It focuses on only one mechanism that causes layer structure modification. A more general dependence is therefore highly desirable and we propose to generate it through numerical simulations.

In the regime that we consider here, there is an effective layer where the small scale fluid flow interacts with the chemical reaction. The thickness of this effective layer is quite different from those of the laminar flame and it is expected to alter the local burning velocity more substantially, compared to the modification caused by flame stretch. Ronney and Yakhot [55] considered the effect of flame broadening on the turbulent burning velocity, by using a Kolmogorov turbulence model at the small scale level. The significant finding there is that at very high turbulence intensity u', the small scale acts to cause a decrease in S_T, compared to a thin flame. This suggests that the increased effective thickness of the reaction layer is one important mechanism for the bending phenomenon.

Another indication that the small scale fluid flow is quite important in the prediction of S_T can be seen in a recent paper of Bourlioux, Klein and Moser [11], where they developed a large eddy simulation algorithm for the G-equation and compared the turbulent burning velocity from their calculation to those in a Direct Numerical Simulation [33] and found the difference is quite substantial. One reason cited is the small ratio between the Kolmogorov length scale (the small scale of the fluid flow) and the flame thickness that is present in the DNS calculation.

2.2 Proposed Approaches

Our approach here is to couple the G-equation with an equation for the local thickness of the flame, replacing S_L in Eq. (19) by S_L^*. The broadened flame will determine how the local burning velocity should vary and this information is therefore used in the G-equation. As a consequence, the local burning velocity, as opposed to the laminar burning velocity, can have a large fluctuation, depending on the local flow. The key to this approach is how we build a functional relationship between the local burning velocity S_L^* and the local flow. The information obtained in Part 1 of this proposal will be used here. With regard to Damköhler's hypothesis, we propose a two-step approach to this issue. In the fluid part, we solve for the large scales only, and the interaction between small scale and large scale is ignored at this time. However, this can be extended to a Large Eddy Simulation with appropriate modeling at the small scale level.

2.2.1 Using Damköhler's hypothesis

In Damköhler's hypothesis, the mean chemical reaction rate is the same as in a laminar flame. This hypothesis is probably more likely to be valid in cases where the activation energy is relatively small (indicated by a small Zeldovich number β, which measures the sensitivity of the reaction rate to the temperature). From Eq. (1) the change in burning velocity is caused by a turbulent diffusivity, which is caused by the small scale fluid flow. In [55], a Kolmogorov turbulence model is used to generate a functional relation between D^*/D and the effective reaction layer thickness δ^*:

$$\frac{S_L^*}{S_L} = \sqrt{X^2 - 2X + 2}, \quad X = \left(\frac{\delta^*}{L_k}\right)^{2/3} \tag{20}$$

where L_k is the Kolmogorov length scale of the turbulent flow. If we interpret this relationship by taking L_k to be the small length scale of flow, this relation will let us determine the modified local burning velocity from the local reaction layer thickness. It is expected that the local δ^* would depend on the local small scale flow structure. The results from Part 1 of this proposal will be needed in this part of modeling. A functional relationship $\delta^* = \delta^*(u'^*)$ seems reasonable at this stage. To obtain the local u'^* that contains the small scale kinetic energy up to certain given scale, we use some ideas from large-eddy simulation (LES), where the effect of the large scales is directly computed and the small subgrid scales are modeled. In this case, we propose to use the Smagorinsky model [67],

$$(u'^*)^2 = \rho C_I \Delta^2 |\bar{S}|^2, \quad |\bar{S}|^2 = 2S_{i,j}S_{i,j}, \tag{21}$$

where $S_{i,j}$ is the large scale rate of strain tensor, which can be computed from the resolved large scale flow, Δ is the filter size that is proportional to the grid size, and C_I is to be determined through modeling. For example, the approach developed in [11] can used.

Given that information about the local flame thickness, the modified local burning velocity is therefore used in the G-equation, where the flow is chosen to have a Kolmogorov energy spectrum.

2.2.2 Effects of Mean Chemical Reaction Rate

In the case where the Zeldovich number $\beta >> 1$, the reaction rate is highly sensitive to the temperature so it is not reasonable to expect that $\omega^* = \omega_L$. In this case, we are mainly interested in how ω^* affects the local burning velocity S_L^*. The approach is to take S_L^*/S_L as in Eq. (18) and use the functional dependence of ω^*/ω and D^*/D on the small scale flow structure obtained from Part 1. Given detailed results from Part 1 of the proposal, we will be able to characterize S_L^*/S_L solely from the small scale flow structure and a large scale mean flow, with the small scale u'^* from a similar Smagorinsky model. This part of work is expected to be substantially more expensive.

2.3 Numerical Considerations

We have several different codes to solve the G-equation, with second-order upwind treatment of both the advection terms and the nonlinear propagation term [50]. A numerical concern of solutions to the G-equation is the behavior of G near the flame front represented by $G = 0$. It is hoped that the value of G at a point gives the distance to the front. The reinitialization procedure was introduced by Sussman, Smereka and Osher [69] and there are also alternative approaches [63, 79]. We plan to use the latter approach here (Huygens principle flowing). The coupling with a potentially highly varying S_L^* can introduce new phenomena, such as additional cusps and island formation. The robust nature of the G-equation is suitable for these situations.

2.4 Flow Configuration and Objectives

To compare our approach to this flame front propagation in flows with separate large and small scales, we choose the type of flows similar to those used by Haworth and Poinsot [33] as a benchmark problem. This flow configuration was also recently used by Bourlioux, Klein and Moser [11]. The problem involves the propagation of a flame in a two-dimensional channel and the initial flow is given in terms of some vorticity distribution with a prescribed turbulent spectrum. The flame is propagating from the left to the right and periodic boundary conditions are imposed on the top and bottom of the computational domain. We propose to take several steps to couple the flow to the flame propagation: (1) freeze an incompressible flow generated from some different vorticity distributions by choosing them randomly, with some given energy spectrum; (2) assume a constant density model and solve the Navier-Stokes equations with an initial vorticity distribution independently; (3) solve the low-Mach number system with a full coupling between the flame and the fluid flow. In all of these stages, the G-equation is solved with the large scale fluid flow and modified S_L^* to generate S_T, with physical parameters comparable to those in [33]. Eventually, a careful comparison of results with the DNS results in [33] will be made. If the results compare well with the DNS results, it will prove the value of our approach, since our approach is much less expensive than DNS calculations.

3 Buoyancy Effects in Front Propagation in a Hele-Shaw Cell

It is well known that buoyancy affects the propagation rates and shapes of premixed gas flames, and its effects on flame propagation have been studied for many years [20, 41]. An understanding of these effects is necessary to assess the hazards associated with accidental fires and explosions resulting from the leakage of gaseous fuels or liquid fuel vapors into air or other oxidizing atmospheres. However, a detailed understanding of this interaction exists only for certain very simple systems such as a rising flame in a cylindrical tube [40]. Also, the interaction between weakly turbulent flames and buoyant flow, which is relevant to many applications such as industrial furnaces, is not well understood.

Among the reasons why there is a lack of understanding of buoyancy effects on flame propagation, are (1) the large density ratio across the flame front (7 for a typical gaseous flame) which greatly complicates the flame/flow interaction [70]; and (2) the fluid property differences across the front which lead to large changes in the Reynolds and Grashof numbers.

To minimize the complicating influences of large thermal expansion, heat losses, and curvature/strain influences, Prof. Paul Ronney at the University of Southern California has conducted a series of experiments [65, 31, 57] that employ aqueous autocatalytic chemical reactions that produce propagating chemical fronts which are analogous to premixed gas flame fronts. These fronts have very low density changes (typically 0.03%), which greatly simplifies numerical simulations because the Boussinesq approximation can be used in the Navier-Stokes equations. In particular, with aqueous fronts the flow field is divergence-free and baroclinicity can be neglected. Another advantage of the aqueous fronts is that the temperature change across the front is very small (typically 1^o K) and thus the transport properties are nearly unchanged across the front. Consequently, aqueous chemical fronts are ideal for simulation of buoyancy effects on premixed flame propagation.

The Hele-Shaw flow occurs in the gap between two parallel flat plates whose spacing is much less than the dimensions of the plates themselves. Here the Reynolds number of the flow between the plates is well below the value for transition to turbulence. It is one of very few interesting three-dimensional flows that can be reduced to a lower dimensional problem through averaging the velocity and pressure over the third dimension. The flow itself exhibits a rich set of phenomena. For example, when a less-viscous fluid is forced into a more-viscous immiscible fluid, the interface between the two fluids may exhibit fingering [60]. This fingering may also occur without imposed flow if the plates are oriented vertically and the less-dense fluid is underneath the more-dense fluid, so that buoyancy-generated flow may occur.

In a test case of the experiments of Ronney [58], an apparatus having dimensions 20 cm $\times$ 20 cm $\times$ 0.1 cm was constructed and a front was initiated near the bottom center of the cell. A rising front was observed (as expected) and exhibited pronounced wrinkling or "fingering" (Figure 2). This fingering was unexpected because the viscosity difference between the reactants and products is very small (about 5%) and the interface between the products and reactants has very little if any surface tension (since the solutions are dilute and miscible). Thus, it is unclear what mechanism leads to the wavelength selection observed experimentally. When the entire cell is turned horizontally, no fingering is observed and the front remains stable. Thus, the objective of this proposed numerical study is to understand the mechanism responsible for this fingering. Of particular interest is the mechanism that selects the wavelength of the fingers. An understanding of this fingering is relevant to modeling of practical buoyancy-driven flames because the fingering affects the surface area of the front and thus its propagation rate. This in turn will affect, for example, whether the front will undergo a transition from deflagration to detonation.

3.1 Existing Models and Numerical Approaches

First of all, we describe the flame propagation model we propose to use. As discussed above, in many cases the aqueous chemical fronts are very thin relative to the flow scales and the front propagation is considered in the flamelet regime. In this case, the front can be represented by a surface of discontinuity which is convected by the flow field and propagates in the normal direction with a prescribed burning velocity. This front can be described by a collection of markers, or by a level set of a scalar field. In the latter case, the scalar field G is governed by the G-equation (19) shown in Part 2 of this proposal.

The burning velocity S is taken to be dependent on the flame stretch κ, which is a combination of the fluid velocity strain rate and the mean curvature of the front [70] and for weak flame stretch it is given by

$$S(\kappa) = S_L(1 - b\kappa + \cdots) \approx S_L e^{-b\kappa}. \tag{22}$$

Here S_L is the laminar burning velocity for unstretched fronts, b is a coefficient, sometimes called the Markstein number, determined from analysis of the laminar flame structure.

In the experiment, the fluid temperature experiences an increase right after the reaction takes place. The density therefore drops according to the equation of state. However, the presense of the walls in the cell implies that the higher temperature cannot be sustained due to the heat loss to the walls, and therefore the density will return to the original value for the reactant. This heat loss effect is expected to modify the front instability mechanism according to the stability analysis of Joulin and Sivashinsky [35]. In the following, we describe our work [77] on the case that ignores the heat loss effect, and then in Section 3.2 we propose an approach to the case with heat loss effect.

The basic assumption in modeling the Hele-Shaw flow is that the velocity is everywhere parallel to the plates and its spanwise distribution is parabolic. In this case, Darcy's law is often used to describe the flow field, rather than the more complicated three-dimensional Navier-Stokes equations. It has the form

$$\mathbf{u} = -\frac{w^2}{12\mu}\nabla(p + \rho y g), \tag{23}$$

and the two-dimensional flow is still incompressible. Here w is the gap width, y is the upward coordinate, g is the gravitational constant, and both the viscosity μ and the density ρ can have different constant values in both the product and reactant regions.

Across the chemical front, which is denoted by $\Gamma(t)$, certain jump conditions are required. By taking the divergence of Eq. (23), we know that the pressure satisfies the Laplace equation in both regions. We impose the jump conditions

$$[p] = 0, \quad [\frac{\partial p}{\partial n}] = g\Delta\rho\cos\theta, \qquad \mathbf{x} \in \Gamma, \tag{24}$$

where θ is the tangent angle of the front at a point on Γ. The first condition is based on the Laplace-Young condition and the assumption that there is no surface tension effect. The second condition is derived from the assumption that the normal fluid velocity is continuous across the front. We see that this jump is proportional to the density difference $\Delta\rho$, which is due to buoyancy effect.

Boundary integral formulations are very powerful in dealing with Hele-Shaw problems [24, 22, 34]. In this case there is a very simple representation. If we consider the flow in an infinite space, we can represent the pressure in terms of the front Γ via a single layer potential [30], with the addition of a hydrostatic term:

$$p(\mathbf{x}) = \frac{\Delta\rho g}{2\pi} \int_\Gamma \log|\mathbf{x}-\mathbf{y}| \cos\theta(\mathbf{y}) dS_{\mathbf{y}} - \rho_1 g y, \tag{25}$$

The fluid velocity away from the front can be obtained by taking the gradient of the pressure. At point $\mathbf{x}$ on the front, the local normal fluid velocity is

$$u_n = \mathbf{u}\cdot\mathbf{n} = -\frac{w^2 g\Delta\rho}{12\mu}\left[\frac{1}{2\pi}\int_\Gamma \frac{\partial}{\partial n_{\mathbf{x}}} \log|\mathbf{x}-\mathbf{y}| \cos\theta(\mathbf{y}) dS_{\mathbf{y}} + \frac{1}{2}\cos\theta(\mathbf{x})\right] \tag{26}$$

The combined normal velocity of the front is therefore $u_n + S$. To consider the effect of the bounded region, we can add an additional potential flow to correct the normal velocity on the boundary of the cell.

The numerical difficulty with this model is that the fingering is a physically unstable process. In this case, we choose to use the $\theta - L$ formulation [37, 34] to describe the front, because of the advantages it offers in the forms of the evolution equations. In this formulation, the tangent angle (θ) and the total arclength (L) of the front are tracked and the time evolutions are governed by

$$\theta_t = \frac{2\pi}{L}(V_\alpha + \theta_\alpha U) \tag{27}$$

$$L_t = -\int_0^{2\pi} \theta_\alpha V d\alpha. \tag{28}$$

Here α between 0 and 2π is a parameter for the front, V is the normal velocity and U is a specially chosen tangential velocity (which does not affect the front evolution) that maintains the equal arclength property of the front discretization. The advantage of this form is the better numerical stability achieved, which is very important to this problem where small perturbation to the front can grow in time.

In Figure 3, we show the calculated fronts that originate from a perturbed circle. We clearly see that some fingers have formed, resembling those observed in the experiments of Ronney [58]. We have found that the wavelength of the fingers is determined by the amount of curvature dependence (b) of the burning velocity. We also note that the fingers disappear when S_L is large enough. More detailed results are given in [77].

3.2 Proposed Work to Include Heat Loss Effects

The $\theta - L$ formulation is very accurate for interface dynamics and excels in dealing with evolving fronts connected with curvature effects. However, a major drawback is that topological changes of the front are difficult to handle. Nevertheless the previous work provides us with a very reliable understanding of the early stage of the fingering phenomenon. Next we propose to use the G-equation for the front dynamics where merging and splitting of fronts are easily dealt with. In our previous work [74, 75], the G-equation was employed in several premixed flame propagation problems. In the G-equation, a fluid velocity field for the whole domain is required and it is naturally available from the single layer potential above.

To include the heat loss effect, we need to study the transient aspect of the system. We propose to study numerically the Boussinesq approximation to the Euler-Darcy equations,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p - f\mathbf{u} + \beta\mathbf{g}(T - T_u) \tag{29}$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = -h(T - T_u), \tag{30}$$

with the velocity satisfying $\nabla \cdot \mathbf{u} = 0$. Here T is the temperature and T_u is the temperature of the walls, β is the thermal expansion coefficient, $f = 12\mu/w^2$ is the friction coefficient, and $\mathbf{g}$ is the gravity. The linear stability of a flat front was studied by Joulin and Sivashinsky [35] using the Euler-Darcy's equations. Here we propose several steps to approach these equations, combined with the G-equation formulation, to solve for the evolution of any arbitrary initial front.

First we can ignore the transient effects of the momentum equation and the pressure satisfies

$$\nabla^2 p = \beta \mathbf{g} \cdot \nabla T. \tag{31}$$

We note that T has a jump at the front and then decays smoothly to T_u due to the heat loss. Physically we can imagine that there is a singular line source along the front and a layer of smooth source distribution behind the front. Since this equation is linear, we can split it into two Poisson's equations. The solution to the first one is again given by the single layer potential, while the second one can be solved by a finite difference solver. However, since the source distribution is supported on a curved region which may be narrow compared to the box size of the problem, a high-resolution elliptic solver is required. For this purpose, we propose to use the immersed interface method developed by LeVeque and Li [39] in this project. This method is designed to represent curved boundaries where the sources may be contained accurately and is especially helpful in our problem where fingers are developing. The geometry of the layer is obtained by solving the G-equation, using second-order upwind approximations. To update the temperature, we solve Eq. (30) with a second-order implicit finite-difference method, since the coefficient h can be large and the system is therefore quite stiff.

We expect to understand two aspects of the phenomenon from the above proposed work: the modification effects of the fingering due to the heat loss, and the mechanism for the wavelength selection of the fingers. The heat loss coefficient is expected to play an important role. A potential practical application of this is to use the finger wavelength observed to estimate the fluid properties.

At the next stage we propose to consider the transient effect we neglected in the first step. In this case the flow field has an evolution by itself and we propose to extend the projection method mentioned in Part 1 to deal with this case. This will lead to an elliptic equation similar to the one discussed above and the elliptic solver developed in the first stage will be used again. It should be mentioned that we are not aware of any transient effect of the momentum equation discussed in the literature and it is probably a worthwhile effort.

The array sizes which arise in this problem are similar to those in Part 1. However, the nature of the fingering development may require much higher resolution. Another aspect that requires additional resolution is that the thickness of the heat loss layer can be very small when the coefficient h becomes large. This is an important regime in the parameter space that we want to explore.

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