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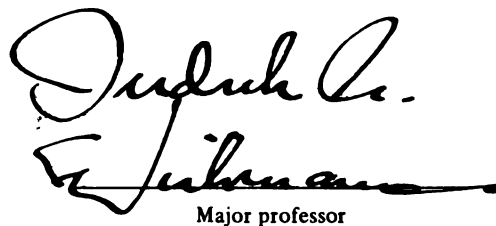
**FEATURES OF DIFFUSION FLAME BEHAVIOR NEAR  
COLD CHEMICALLY INERT SURFACES**

presented by

**BALACHANDAR VARATHARAJAN**

has been accepted towards fulfillment  
of the requirements for

**MASTER'S** degree in **MECHANICAL  
ENGINEERING**

  
Major professor

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**FEATURES OF DIFFUSION FLAME BEHAVIOR NEAR COLD  
CHEMICALLY INERT SURFACES**

**By**

**Balachandar Varatharajan**

**A THESIS**

**Submitted to  
Michigan State University  
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## ABSTRACT

### FEATURES OF DIFFUSION FLAME BEHAVIOR NEAR COLD CHEMICALLY INERT SURFACES

By

Balachandar Varatharajan

Features of diffusion flames near cold chemically inert surfaces are examined using a model problem, which takes two-dimensional diffusion and convection into account. The objective is to understand the structure of the region near the diffusion flame tip. Numerical simulations show that the mass fraction profiles exhibit distinct behavior in the mixing, triple flame, and the diffusion flame regions. It is also noted that mass fraction contours form a good approximation to the premixed flame arcs of the triple flame near the triple point. The stoichiometric premixed flame tip postulate for diffusion flame tips has been analyzed in detail. Numerical results show that this postulate is true for lifted flames while the behavior for attached flames is complicated. Finally a limiting case of the model problem with applications in flame spread theory is analyzed and a pseudo-exact solution is presented for the heat flux to the cold fuel.

**To my parents with love**

## ACKNOWLEDGMENTS

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# NOMENCLATURE

|           |                                                                         |
|-----------|-------------------------------------------------------------------------|
| C         | Constant that specifies loci of constant $Pe_p$                         |
| $C_p$     | Specific heat at constant pressure                                      |
| D         | Mass diffusivity                                                        |
| $D_a$     | Damköhler number, $D_a = (1/\alpha)AL^2Y_{OO}e^{-E/RT_f}$               |
| d         | Nozzle diameter                                                         |
| E         | Activation energy                                                       |
| g         | Difference between local solution for Z and $Z_\infty$                  |
| H         | Excess enthalpy, $H = \tau + y_O + y_F - 1$                             |
| h         | Difference between local solution for Z and $Z_0$                       |
| k         | Thermal conductivity                                                    |
| $\hat{L}$ | Half-width of the channel                                               |
| L         | Nondimensional width of the channel (see CHAPTER IV)                    |
| $l_d$     | Divider thickness                                                       |
| P         | Pre-exponential factor, $P = \frac{AL^2Y_{OO}}{\alpha_0}$               |
| Pe        | Peclet number, $Pe = Ul/\alpha$                                         |
| Q         | Flow rate, $\pi d^2/4$                                                  |
| q         | Heat flux, $q = \partial H/\partial \eta = \partial \tau/\partial \eta$ |
| R         | Universal Gas constant                                                  |

|            |                                                                       |
|------------|-----------------------------------------------------------------------|
| $r$        | Radius, $r = \sqrt{x^2 + y^2}$                                        |
| $S_L$      | Premixed flame speed                                                  |
| $Sc$       | Schmidt number                                                        |
| $T_0$      | Ambient (cold-wall) temperature                                       |
| $T_f$      | Flame temperature                                                     |
| $U$        | Oxidizer velocity                                                     |
| $u_0$      | Nozzle exit velocity                                                  |
| $v$        | Velocity in the y-direction                                           |
| $x$        | Horizontal coordinate                                                 |
| $y$        | Vertical coordinate                                                   |
| $Y_i$      | Mass fraction of species i, $i = O, F, P, I$                          |
| $y_i$      | Normalized mass fraction, $y_o = Y_O / Y_{OO}$ , $y_F = Y_F / Y_{FF}$ |
| $Z$        | Mixture fraction, $Z = (\phi y_F + 1 - y_O) / (\phi + 1)$             |
| $Z_f$      | Mixture fraction at DF arc, $Z_f = 1 / (\phi + 1)$                    |
| $Z_0$      | Mixture fraction near exit plane                                      |
| $Z_\infty$ | Mixture fraction at $y \rightarrow \infty$ (see Equation (21))        |

## Subscripts

|     |                                                                            |
|-----|----------------------------------------------------------------------------|
| $P$ | Perpendicular to the flame-tip plane (i.e., along the DF arc at its' tip.) |
| $q$ | Quench point                                                               |
| $t$ | Tangential plane                                                           |

## Greek

|                |                                                                                                 |
|----------------|-------------------------------------------------------------------------------------------------|
| $\alpha$       | Thermal diffusivity, $\alpha = \frac{k}{\rho C_p}$                                              |
| $\alpha_0$     | Enthalpy ratio, $\alpha_0 = 1 - T_0/T_f$                                                        |
| $\beta$        | Zeldovich number, $\beta = \alpha_o E/RT_f$                                                     |
| $\delta$       | Variable in Equation (11), $\delta = Y_I - Y_{IF}$                                              |
| $\Delta$       | Difference between inert species in the oxidizer and fuel stream,<br>$\Delta = Y_{IO} - Y_{IF}$ |
| $\eta$         | Normalized streamwise coordinate                                                                |
| $\theta$       | Angle (see Figure 25)                                                                           |
| $\lambda_i$    | Sensitivity coefficient                                                                         |
| $\mu$          | Function defined in Equation (20)                                                               |
| $\gamma$       | Stoichiometric coefficient                                                                      |
| $\xi$          | Normalized transverse coordinate                                                                |
| $\chi_i$       | Variable corresponding to 'i' (see section 3.1)                                                 |
| $\rho$         | Density                                                                                         |
| $\tau$         | Normalized temperature, $\tau = (T - T_0)/(T_f - T_0)$                                          |
| $\phi$         | Overall stoichiometric ratio, $\phi = \gamma Y_{FF}/Y_{OO}$                                     |
| $\hat{\omega}$ | Dimensional reactivity, $\hat{\omega} = \rho A Y_O Y_F e^{-\frac{E}{RT}}$                       |
| $\omega$       | Normalized reactivity, $\omega = y_O y_F e^{-\beta(1-\tau)/(1-\alpha_0(1-\tau))}$               |

## **Abbreviations**

|    |                                      |
|----|--------------------------------------|
| DF | Diffusion flame                      |
| FF | Fuel stream                          |
| PF | Premixed flame                       |
| P1 | Postulate                            |
| OO | Oxidizer stream                      |
| IF | Inert species in the fuel stream     |
| IO | Inert species in the oxidizer stream |

# INTRODUCTION

The behavior of diffusion flames (DFs) near cold chemically inert surfaces is not clearly understood. The combustion literature contains references to such problems that are being increasingly analyzed using the concept of tribrachial or “triple” flames. Triple flames are thus named because they are made up of a fuel rich and a fuel lean premixed flame arc, both of which are attached to a long trailing diffusion flame. When non-premixed fuel and oxidizer are blown into a channel, they undergo a mixing process. When the local temperature is high enough, they ignite, which results in a triple flame. The objective of this thesis is to analyze, using numerical and analytical techniques, the solution of a well-posed problem that will reveal the structure of such triple flames. This will in turn lead to a better understanding of DF behavior near cold chemically inert walls.

## Background

A knowledge of the structure of triple flames will enhance the fundamental understanding of at least the following physical problems: Flame spread over solid fuels, flame attachment to a cold wall between two streams of reactants - the splitter plate problem, flame attachment in a bunsen-burner, flame propagation in stratified air mixture, droplet ignition by a hot surface, and flame propagation in a combustion chamber. The structure of a typical triple flame is shown in Figure 1, which shows the fuel rich and fuel lean PF arcs along with the trailing DF arc. The point at which these three arcs meet is called a Triple Point (TP).

Initial efforts to understand this structure were mainly experimental. Later, with the

advent of high activation energy asymptotic methods, the efforts shifted to theoretical and numerical analysis. But the emergence of Direct Numerical Simulations(DNS) shifted the emphasis more towards the numerical methods. The following will be a brief review on the above efforts. This literature review is centered around the contributions of H. Phillips, De Ris, J. Dold, A. Liñán et al and I. Wichman[1-10].

Triple flames were first experimentally observed by H. Phillips [1] while analyzing a model for methane layers near the roofs of coal mine shafts. In that paper he assesses the likelihood of a roof layer of methane initiating a coal dust explosion by studying how the speed of the flame depended on the distribution of gas in the layer and the stoichiometric burning velocity of methane-air mixture. Using the principles of dimensional analysis, he designs a model which produced a propagating triple flame. Based on the experimental measurements he concludes that the speed of a flame depended only on the burning velocity of the stoichiometric mixture and is independent of the quantity of fuel and the concentration gradient at the interface. Though triple flames were photographed and aspects of it measured, there was no theoretical explanation given for such dependencies.

Triple flames also appear in the flame spread literature. The structure of diffusion flames near cold, chemically inert walls is of fundamental importance in the study of flame spread over solid fuels. A typical flame spread process is illustrated in Figure 2 where a diffusion flame propagates into an opposing flow of oxidizer. Near the leading edge of the spreading flame, the diffusion flame cannot survive because of the heat losses to the cold fuel and also to the sides. This small region should control the flame spread process because unlike premixed flames diffusion flames do not have propagation characteristics. Thus, if the flame is to have a spreading velocity, the leading edge should exhibit premixed

flame behavior. This mechanism is explained clearly by De Ris in his thesis [2] on flame spread as follows:

*“Near the cold wall there will be three flame fronts. As a cool reactant diffuses from its source to the flame, it will be mixed with a smaller amount of the opposite reactant which has diffused between the flame and the cold wall. When these reactants reach the ignition temperature, they will react along the secondary flame front until one of the reactants has been consumed. What remains of the other reactant will diffuse toward the main flame front.”*

In his model, however, he neglects such flames by assuming that the ignition temperature of the hot gases is lower than the vaporization temperature of the solid fuel. This forces the diffusion flame tip to lie on the surface of the fuel and thus eliminates the triple flame and any other flame structure there.

The first theoretical analysis of triple flame structure was by Dold [3]. Dold examines the structure of slowly varying triple flames under the assumption of low heat release and shows that the triple flame propagation speeds depend on the transverse mixture fraction gradient and are bounded above by the maximum adiabatic laminar flame speed. Hartley and Dold [4] later analyze the problem for rapidly varying flames, since the expansions given in Dold’s paper do not hold for large mixture fraction gradients and when the radius of curvature of the premixed flames is of the same order as the thickness of preheating regions of the PF. When they are of the same order, they find that the propagation speed is still positive. In a separate paper Dold shows that the propagation speeds become negative only when the radius of curvature is very small, as in strained flows, thereby predicting Bray et al’s numerical results which were to appear later. Dold also explains the use of triple flame theory to turbulent flame theory. In a non-premixed system, when the strain rate is very high, the diffusion flame sheet ruptures leaving a “hole” in the flame sheet. This

leads to two-dimensional laminar triple-flamelet theory. Such a model can be used to predict the dynamical response of a hole in a diffusion flame to a flow field.

A. Liñán [6] made a major contribution to diffusion flame structure by exploiting the high activation energy asymptotics to reveal the various regimes. Liñán initially restricted his analysis of diffusion flames to one-dimensional models, which do not result in triple flames but reveal fundamental features of diffusion flames like ignition and extinction limits. But Liñán and Crespo [7] later studied the asymptotic structure of unsteady, but one-dimensional diffusion flames formed by simultaneous mixing and chemical reaction of two reactant streams. Ignition occurs by means of a thermal-runaway process and subsequent combustion takes place due to a deflagration wave propagating from the ignition point until they cross a stoichiometric surface where a diffusion flame is created. To simplify analysis, Liñán and Crespo assume that upstream conduction and diffusion are negligible. The premixed flames cannot exist after the initial ignition period and they are extinguished leaving behind the reaction products, and the reactant in excess resulting in a diffusion flame separated by two equilibrium regions. As noted correctly by Dold, their simplifying assumption is only valid if the velocity of the reactants leaving the splitter plate is much greater than the stoichiometric adiabatic premixed flame speed.

Bray et al [5] analyzed the flame propagation in laminar mixing layers taking into account the two-dimensional nature of the triple flame problem. In this paper a theoretical model is presented for analysis of structure of triple flames in a strained mixing layer which arises in the counterflow configuration. Their numerical simulations give the structure and propagation velocities of triple flames for various strain rates. They show that when strain rate increases - caused by a reduction in Damkohler number - the propagation

velocity decreases, and at large strain rates the propagation velocities even become negative with an extinction front propagating along the diffusive interface rather than a front that initiates combustion.

Vervisch et al [8] analyzed the effect of heat release on triple flames in partially premixed flows. Their numerical simulations of laminar mixing layers with a uniform approaching field confirm the decrease in PF speed with increasing transverse mixture fraction gradient. Heat release also increases the triple flame speed by redirection of the flow in front of the flame. This article also presents some scaling laws that determine flame speed in terms of density change for small transverse mixture fraction gradient.

Most of the above work dealt with flames that were far away from cold walls and thus were not affected by physical boundaries. Wichman [9] studied the quenching of a diffusion flame near a cold wall in which the multi-dimensionality of the problem is taken into account. Using high activation energy asymptotic methods he shows that the functional form of the quenching distance is identical to that obtained by one-dimensional analysis except for a multiplicative factor. In a separate article [10], he analyzes the generic features of triple flame structure and speculates several possible flame shapes. In this thesis, the model problem examined by Wichman will be studied in detail to reveal the generic features.

## **Motivation**

Though triple flames as noted above were discovered in the early 1960s, their structure has yet to be sufficiently understood. The analysis of the structure is complicated because near the leading edge the governing equations exhibit elliptic behavior, thus making it difficult to apply the powerful analytical techniques that can be applied in the case of para-

bolic problems. The general belief that a clear understanding of the structure of the triple flame region may aid us in building better models describing several physical phenomena served as the basic motivating factor for this thesis. Towards this goal we shall analyze the structure of triple flames using the numerical results of an elliptic model with convection and two dimensional diffusion. First some of the features that have been analyzed by Wichman [9-10] will be established on a sound footing. This will reveal some of the generic features about the behavior of primary variables, like temperature and mass-fraction, and Schvab-Zeldovich variables, like mixture fraction and excess enthalpy, in the mixing region.

The engineering importance of determining the propagation speed of a triple flame served as the second motivating factor. A knowledge of this quantity will aid us in calculating the optimum speed at which fuel should be blown past a burner such that both blow-off and explosion can be prevented. Consequently many researchers have postulated stoichiometric premixed flame tips and constructed their experimental analyses and theoretical models on the consequences of this postulate. But there are instances in which this assumption might not hold. A partial explanation of the scope and limitations of this postulate will be given by analyzing a simplifying model problem and measuring the velocity into the triple point and comparing it with the stoichiometric PF speed.

In flame spread problems, the heat flux to the fuel is an important quantity since it aids in the selection of fuels. Some existing models predict an infinite heat flux to the solid fuel, which is unrealistic. A realistic estimate of this heat flux and its' engineering importance served as the third motivating factor. For this purpose, a limiting case of the model problem is considered and the exact solution to the excess enthalpy field is derived. An

expression for the heat flux to the fuel is derived using this solution, which depends on two parameters. Combining numerical results we are able to obtain a complete expression for the heat flux.

## **Outline**

The thesis is organized into five chapters. The first chapter explains the mathematical model along with the assumptions used.

The second chapter explains the generic and reaction independent statements that can be made using the above mathematical model and a finite difference solution. The convergence characteristics of the numerical code used are also presented in this chapter.

The velocity entering the triple point has been postulated to be equal to the premixed flame speed. A kinematic analysis of the mixture fraction field is performed and a formula is derived for the velocity into the triple point. This velocity is compared with the premixed flame speed to analyze the conditions under which this postulate holds.

The fourth chapter discusses a limiting case of the model described in Chapter 1. In this case the cold wall covers the whole channel and an exact solution is available for the symmetric flame. Using this solution a pseudo-exact expression for the heat flux to the fuel is derived.

The fifth chapter summarizes the major results and conclusions of this study.

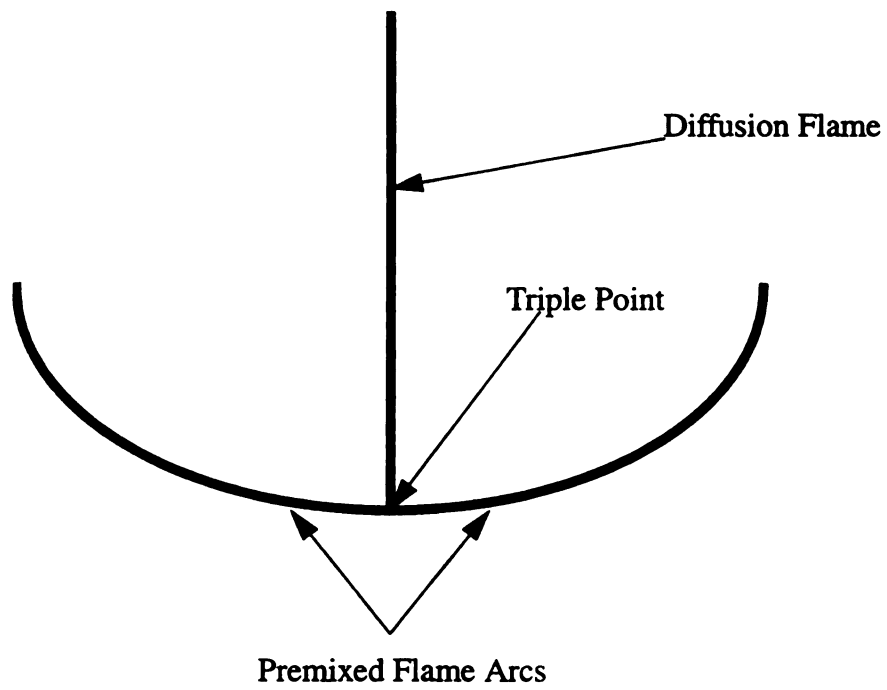


Figure 1 - A schematic representation of a triple flame

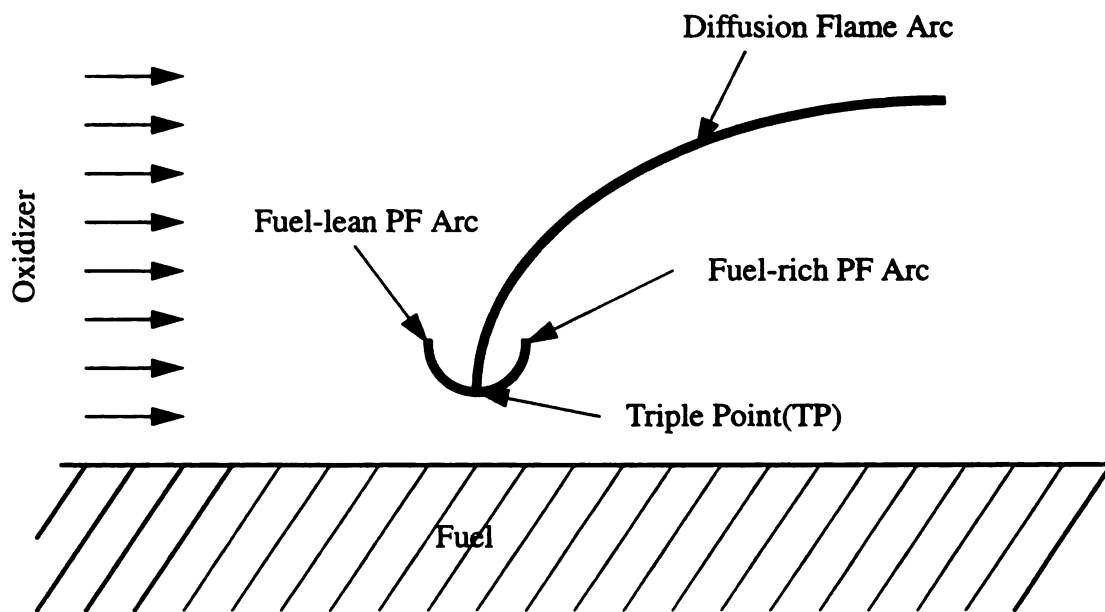


Figure 2 - Flame spreading over a liquid or solid fuel.

# **CHAPTER I**

## **The Model**

In this chapter, the mathematical model that will be examined in the succeeding chapters is formulated with the governing equations, assumptions and boundary conditions. While three limiting cases of the model will be examined in this thesis only the most general form will be discussed in this chapter.

### **1.1 Describing Equations**

Consider the case of a fuel and an oxidizer stream flowing past a divider into a channel as shown in Figure 3. We shall assume a non-premixed system, so that the fuel and oxidizer come into contact only after they flow past the divider. In a small region close to the divider, the fuel and oxidizer mix together and ignite when the temperature is sufficiently high, resulting in a triple flame consisting of two premixed flame arcs and a long thin trailing diffusion flame arc. This describes a typical splitter-plate problem which will be used for examining diffusion flame structure near cold walls.

The equations used to model the above problem are the conservation equations for a multi-component, chemically reacting system namely, the mass, momentum, energy and species conservation equations, which have been tabulated in reference [11]. The following assumptions will be applied to the above equations.

- The flow is steady, one-dimensional, inviscid and uniform throughout the flow field.  
The momentum equation with the above assumptions just states that the pressure will be constant in the domain.
- The body forces are absent. Subsequently there will be no buoyancy or vorticity in the flow.
- The radiative heat flux, Soret and Dufour terms are negligible in the energy equation.
- A one step irreversible reaction -  $F + \nu O \rightarrow (1 + \nu)P + \text{heat}$  - will be assumed. For the reaction rate a simple Arrhenius expression will be used.
- The overall specific heat capacity and the mass diffusivity are constant.
- The diffusion velocities obey Fick's law.
- The molecular weights of fuel and oxidizer are equal.
- The Lewis number, which is the ratio of thermal to mass diffusivity, is unity.

With the above assumptions the species and the energy equations can be written as follows.

$$\nu \frac{\partial Y_F}{\partial y} = D \nabla^2 Y_F - \frac{\hat{\omega}}{\rho}, \quad (1.1.1)$$

$$\nu \frac{\partial Y_O}{\partial y} = D \nabla^2 Y_O - \frac{\gamma \hat{\omega}}{\rho}, \quad (1.1.2)$$

$$\nu \frac{\partial T}{\partial y} = \alpha \nabla^2 T + \frac{q_F \hat{\omega}}{\rho c_p}, \quad (1.1.3)$$

where

$$\hat{\omega} = \rho A Y_O Y_F e^{-\frac{E}{RT}} \quad (1.1.4)$$

In the above equations  $\nu$  is the velocity in the streamwise direction,  $Y_F$  and  $Y_O$  represent

the mass fractions of the fuel and oxidizer respectively,  $T$  is the temperature,  $\gamma$  is the stoichiometric coefficient,  $\alpha$  is the thermal diffusivity,  $D$  is the mass diffusivity,  $\rho$  is the density,  $E$  is the activation energy,  $R$  is the Universal Gas Constant, and  $A$  is the frequency factor.

## 1.2 Boundary Conditions

The model will be complete only when the boundary conditions for the fuel and oxidizer mass fractions, and the temperature are specified. The porous lower walls of the channel are capable of admitting a convective and/or diffusive influx of the corresponding reactant. To the left of the divider there will be only oxidizer, and to the right there will be only fuel. In other words, the left side porous wall destroys any fuel that comes into contact with it and the right side porous wall destroys any oxidizer that comes into contact with it. This makes the respective mass fractions on the either sides of the divider approach their reservoir values.

The sides of the channel are also porous and they can admit only a diffusive influx of oxidizer or fuel. The mass fractions on the left and right walls are also maintained at their reservoir values.

Far downstream, the gradients of all variables in the flow direction vanish. In this region the problem is truly one-dimensional and only a diffusion flame exists in this region.

The divider surface will be assumed to be inert, so that the gradients of the mass fractions will be zero. Thus Dirichlet boundary conditions are specified on the porous walls

and Neumann conditions on the divider surface.

All the walls of the channel and the divider surface will be maintained at a temperature  $T_0$ . The equations and the boundary conditions in physical coordinates are shown in Figure 3.

### 1.3 Nondimensionalization

Since it is difficult to deal with the equations in the physical coordinates, they shall be nondimensionalized. The streamwise and transverse coordinates will be normalized by the half width  $L$  of the channel. The flow velocity will be normalized by the characteristic diffusion velocity  $D/L$ . The fuel and oxidizer mass fractions can be normalized by their corresponding reservoir values  $Y_{OO}$  and  $Y_{FF}$ . The temperature excess  $(T - T_0)$  will be normalized by the greatest possible temperature excess  $(T - T_f)$ , where  $T_f$  is the adiabatic flame temperature. When the above equations are normalized in the manner described above several nondimensional groups appear; the enthalpy ratio  $\alpha_0$ , which usually varies over a small range; the nondimensional activation energy also called as the Zeldovich number  $\beta$ . It depends on the value of  $\alpha_0$  and is usually assumed to be large; the Damköhler number  $D_a$ . It is the ratio of flow time to chemical reaction time.

It can be seen that the system of equations shown in Figure 3 is highly nonlinear. Instead of solving three nonlinear equations simultaneously it will be easier to use the Schvab-Zeldovich procedure to derive two coupling functions. This will reduce the number of nonlinear equations to be solved from three to one although, two more linear equa-

tions equations need to be solved. The first coupling function will be the mixture fraction variable, which involves only the mass fractions of the fuel and oxidizer. It is defined as follows:

$$Z = \frac{\phi y_F + 1 - y_O}{\phi + 1} = (1 - Z_f)y_F + Z_f(1 - y_O), \quad (1.3.1)$$

where  $Z_f$  is the value of the mixture fraction when  $y_F$  and  $y_O$  both equal zero and  $\phi$  is the overall stoichiometric ratio. The second coupling function will be the excess enthalpy coupling function, which involves the mass fractions of both fuel and oxidizer and also the temperature. It is defined as follows:

$$H = \tau + y_O + y_F - 1. \quad (1.3.2)$$

The conserved scalars  $Z$  and  $H$  result in two linear Helmholtz equations, which along with a nonlinear equation can be used to obtain the solution for the temperature and mass fraction fields. The complete system of equations along with the boundary conditions is shown in Figure 4 in terms of the two coupling functions.

## 1.4 Limiting Cases

We shall refer to the model described above as Model A. Two limiting cases of the above model will be used in this thesis.

### 1.4.1 Model B - Infinitesimal Divider

In this model, the thickness of the divider approaches zero. The boundary conditions on the three sides of the channel become Dirichlet in character. This model will be used in

CHAPTER II for examining the effects of divider and also in for the evaluation of the stoichiometric flame speed hypothesis. This model is discussed in CHAPTER III.

#### **1.4.2 Model C - Large Divider**

In this model, the thickness of the divider approaches the channel width and the convective flow is absent from the bottom of the divider. The governing equations reduce to Laplace equations for the coupling functions. This model is used to analyze the heat flux signatures. This model is discussed in CHAPTER IV.

### **1.5 Numerical Code**

The numerical code to the general problem (Model A) was developed by Dr. B. Ramadan. This code solves the model using finite differences and the SLOR iterative method. The input to the code will include the grid information, Damköhler number  $D_a$ , enthalpy ratio  $\alpha_0$ , activation energy  $\beta$ , convective flow  $Pe$ , stoichiometry  $\phi$ , and the relaxation parameter. The code solves for the mixture fraction  $Z$ , temperature  $\tau$ , and the excess enthalpy fields. From this the mass fraction fields can be calculated using relations equations (1.3.1) and (1.3.2).

In the succeeding chapters we shall use the numerical code to understand the features of diffusion flame behavior near cold walls.

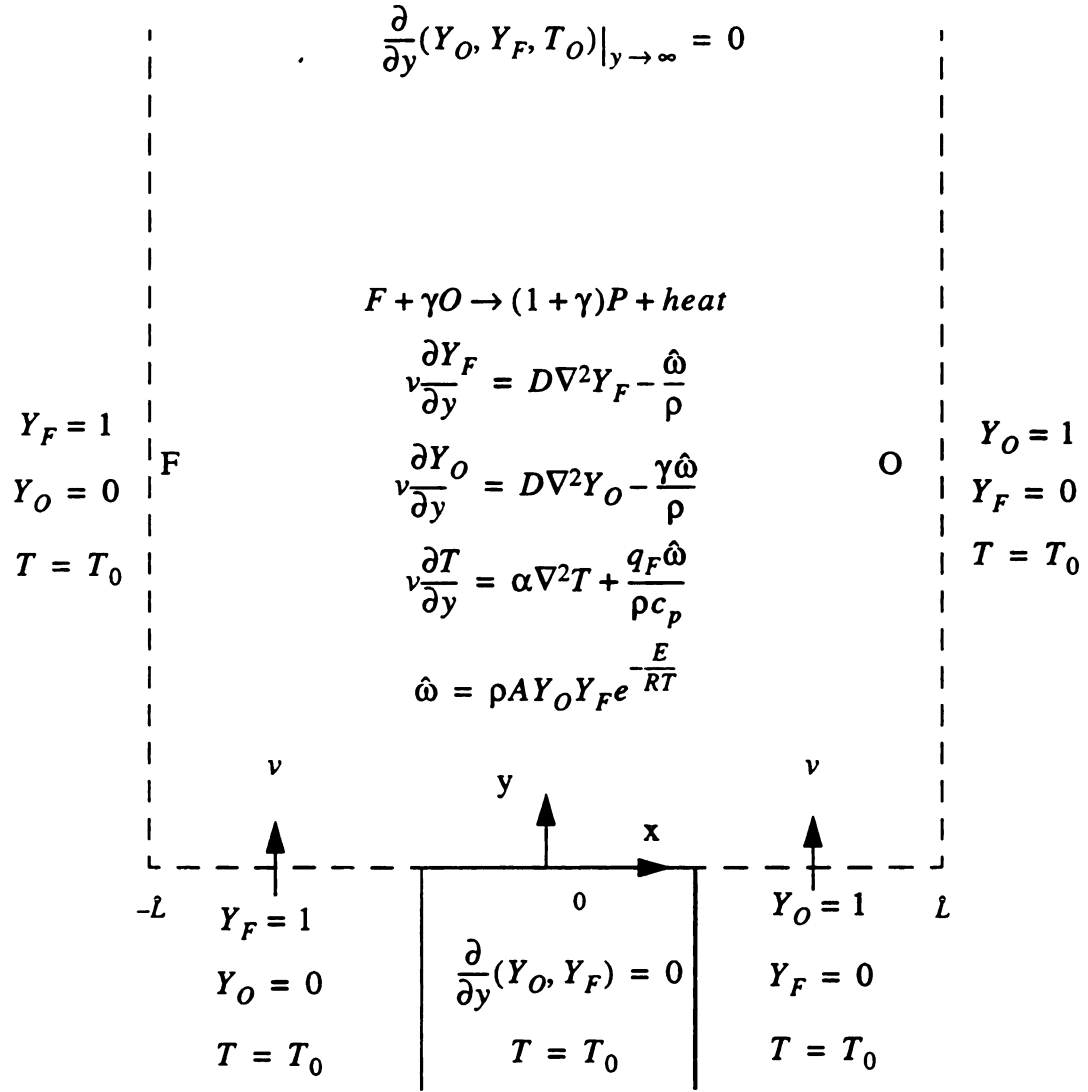
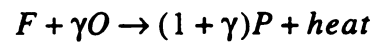


Figure 3 - Model in terms of physical coordinates

$$\frac{\partial}{\partial y}(y_F, y_O, \tau, Z)|_{\eta \rightarrow \infty} = 0$$



$$L(\circ) = Pe \frac{\partial(\circ)}{\partial \eta} - \nabla^2(\circ)$$

$$L(Z) = 0$$

$$L(H) = 0$$

$$L(\tau) = (1 + \phi) D_a \omega$$

$$L(y_F) = -D_a \omega$$

$$L(y_O) = -\phi D_a \omega$$

$$\omega = y_O y_F e^{-\beta(1-\tau)/(1-\alpha_0(1-\tau))}$$

$$Z = 1 \quad | \quad F$$

$$y_F = 1$$

$$y_O = 0$$

$$\tau = 0$$

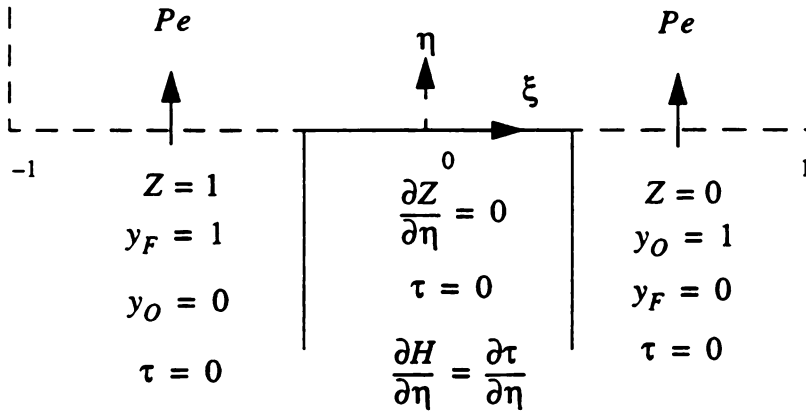
O

$$Z = 0$$

$$y_0 = 1$$

$$y_F = 0$$

$$\tau = 0$$



**Figure 4 - Model in terms of normalized variables**

## CHAPTER II

### Generic Statements

#### 2.1 Introduction

In this chapter, the model problem formulated in CHAPTER I (Model A) shall be analyzed theoretically and numerically in order to understand the generic features of triple flames.

In section 2.2 we shall study the solutions of the temperature, mass fractions, mixture fraction, excess enthalpy, and reactivity fields obtained using the numerical code for both the symmetric and unsymmetric flame configuration. Then the qualitative behavior of the mass fraction profiles, in the three regions formed when fuel and oxidizer are blown past the divider, will be analyzed.

In section 2.3 we shall identify the various parameters in the model and study their influence on the solution. A convergence analysis on the numerical code for the excess enthalpy field is also presented.

Then in section 2.4 we shall examine the behavior of the primary and Schvab-Zeldovich variables along the contours of constant  $Z$ ,  $y_O$ ,  $y_F$ , and  $\tau$ . This leads to some simple differential relations between these variables. Although these relations served only as a check on the numerical code, they are useful as a generic result and may serve as tools for arguments that might be developed in the future. These relations are listed in this thesis after numerical verification.

Most of the afore-mentioned differential equations are valid only when the excess enthalpy field is identically zero throughout the domain. This situation occurs when the divider is infinitesimally thin or when the assumption of an adiabatic divider is made. When the divider is isothermal and hence, cold, the excess enthalpy field is non-zero and the above relations do not hold. We shall try to understand the influence of the enthalpy field on the model problem in section 2.5. The enthalpy field is found to be negative on the surface of the divider. Physical intuition backed with theoretical analysis and numerical results will be used to establish this aspect.

Near the triple point, the fuel and oxidizer isoplexes have been hypothesized to coincide with the two arcs of triple flame. This hypothesis, if true, can lead to a variety of flame shapes as explained in [10]. The validity of this hypothesis shall be examined for both symmetric and unsymmetric flames section 2.6

Finally, the main conclusions of this study are listed in section 2.7.

## 2.2 Numerical Solution of the Model

The model problem shown in Chapter 1 was solved numerically for the mixture fraction, mass fractions, temperature and reactivity fields. The solution contours of  $Z$ ,  $\tau$ ,  $y_O$ ,  $y_F$  and  $H$  are shown in Figure 5 for a symmetric flame and in Figure 6 for an unsymmetric flame. We shall examine each of these contours separately.

The mixture fraction contours (top left) give the location of the diffusion flame. Depending on the stoichiometry, the diffusion flame lies along the various  $Z$ -contours. For a symmetric flame, the diffusion flame lies along the line  $Z = 1/2$ . For the unsymmetric

flame ( $\phi = 2$ ) shown in Figure 6 the diffusion flame lies along the line  $Z = 1/3$ . We note parenthetically that the value of  $Z$  varies from one on the fuel side to zero on the oxidizer side. Far from the exit plane the  $Z$ -contours are parallel, thus emphasizing the fact that the far-field problem is truly one-dimensional.

The reactivity contours (top right) show the location of the triple flame which is identified by two arcs of PF and a long trailing DF. The triple point is identified by the point of maximum reactivity. From this figure, we can see that the flame quenches at a certain height above the cold wall. For the unsymmetric flame configuration, the reactivity contours are shifted to one side or the other depending on the stoichiometry. Also, near the triple point, the mass fraction contours (bottom left) produce a characteristic shape identifying the triple flame. For the symmetric flame, the fuel and oxidizer mass fraction contours are a reflection about the axis  $\xi = 0$ . This can be explained in terms of the equations for the fuel and oxidizer mass fractions given in Chapter 1, which become identical when  $\gamma = 1$ . The mass fraction contours also become parallel in the far-field. The mass fraction contours for the unsymmetric configuration are no longer a reflection about the  $\xi = 0$  axis. The excess enthalpy contours (bottom right) show that there is a drop in the enthalpy values on the surface of the divider suggesting that the divider acts as a heat sink. The excess enthalpy field will be analyzed separately in Section 2.5.

Numerical results show that there exist three distinct regions where the above solutions show distinct behavior. As the fuel and oxidizer leave the exit plane, they undergo a mixing process; consequently, there is a mixing layer near the exit plane. In this region, the solution of the problem is irreducibly two-dimensional. In the triple flame region that follows the mixing layer, the problem is still two-dimensional with the chemical reaction.

But the diffusion flame region, which follows the triple flame region exhibits one-dimensional behavior. The three regions will be analyzed using the fuel and oxidizer mass fraction values at increasing distances from the divider.

### 2.2.1 Mixing Layer

In this layer, the non-premixed fuel and oxidizer undergo a mixing process. Hence, the gradients of fuel and oxidizer mass fractions in the  $\xi$ -direction are very high in this layer. The flame is not established until the fuel and oxidizer have mixed together to a certain degree, which depends on the chemical reaction time and hence on the Damköhler number. Figure 7 shows the oxidizer mass fraction values for a symmetric flame at increasing distances from the exit plane. The solid line and the dotted line correspond to the profiles in the mixing layer at different distances from the exit plane. We can see that the mass fraction values tend to approach the frozen flow distribution in the beginning of the mixing layer. At the exit plane ( $\eta = 0$ ) the gradients in the  $\xi$ -direction are maximum on the two sides of the divider. This is because of the boundary conditions imposed on the  $y_O$  field. These distinct maxima (M1 and M2) approach each other to merge into a single maximum (M3) in the mixing layer, slightly downstream of the exit plane. From the figure, we can also see that the peak of this maximum value drops with subsequent increased mixing. Thus the gradients undergo a process similar to relaxation in the mixing layer. After this, the triple flame region is formed and the mass fraction profiles exhibit a qualitatively different behavior.

### 2.2.2 Triple Flame Region

In this layer the fuel and oxidizer react establishing a propagating premixed flame. In Figure 7, the oxidizer mass fraction values and its gradient in the  $\xi$ -direction in the triple flame region are represented by dot-dashed lines. The  $y_O$  profile in the fuel-rich region has a local maximum (T1), which was absent in the mixing layer. The gradients of  $y_O$  show the presence of two extrema (one of which is a minimum - T2, while the other is a maximum - T3) in contrast to the single maximum observed in the latter half of the mixing layer. Also this is the only region in which the mass fraction gradients have opposite signs. Our simulations show that the distance between the extrema increases in the triple flame region. Thus these extrema should correspond to the fuel-rich and fuel-lean arcs of the triple flame. As we move further away from the exit plane we enter the diffusion flame region.

### 2.2.3 Diffusion Flame Region

In this region, the fuel and oxidizer mass fractions are zero on the fuel-lean and fuel-rich sides respectively. In Figure 7, the dashed lines represent the  $y_O$  profile and its gradient in the diffusion flame region. The  $y_O$  profiles do not exhibit the local maximum that was present in the triple flame region, while the gradients show the presence of a single inflection point (I) at the location of the diffusion flame. From the gradients of the fuel and oxidizer mass fractions at the inflexion point, we can obtain the fuel and oxidizer consumption rate at the DF. This region is not of much importance to us since the structure of laminar diffusion flames is well understood. We shall therefore focus our attention on the

mixing layer and the triple flame region.

## 2.3 Influence of Parameters on the Solution

We shall identify the major parameters in the model and examine their influence on the solution. The parameters in the model are: enthalpy ratio  $\alpha$ , normalized activation energy or Zeldovich number  $\beta$ , Damköhler number (or the pre-exponential factor), divider thickness  $l_d$ , and the flow rate  $Pe$ . The first three parameters appear in the Arrhenius reactivity term and can be classified as chemical parameters;  $l_d$  appears in the boundary condition on the exit plane; and  $Pe$  appears in the governing differential equation. We shall examine the effect of each of these parameters on the solution separately.

### 2.3.1 Effect of Chemical Parameters

The chemical parameters in the model are  $\alpha$ ,  $\beta$ , and  $D_a$ . The enthalpy ratio,  $\alpha = 1 - T_0/T_f$  varies over a narrow range - approximately from 0.7 to 0.9. These values emphasize the fact that the (cold) wall temperature is small compared to the maximum possible temperature in the flame. While  $\alpha$  influences the location of the flame with respect to the cold wall through the Damköhler number, it also influences the peak of the reactivity field. Our numerical simulations show that reactivity increases when  $\alpha$  is increased. The parameter  $\beta$  is the Zeldovich number. It varies approximately from 6 to 9. It influences the quench radius and also the peak of the reactivity term. Parameter  $\beta$  is also related to the thickness of the reaction zone of the diffusion flame. High activation energy

asymptotic methods have shown that the thickness of the reaction zone is of the order  $\beta^{-1}$ . As  $\beta$  decreases, the diffusion flame tends to follow the stoichiometric  $Z$  contour less closely. It is usually shifted to one side or the other depending on the global stoichiometry. This is discussed in [18].

The Damköhler number is  $D_a$ . It is usually defined as the ratio of flow time to chemical reaction time. It is related to the other parameters by the relation,

$$D_a = Pe^{-\beta/\alpha}, \quad (1)$$

where  $P$  is the pre-exponential factor. From equation (1) we can see that an increase in  $\beta$  leads to a decrease in  $D_a$  and an increase in  $\alpha$  leads to an increase in  $D_a$ . The flow velocity  $Pe$  also influences the value of the Damköhler number. When  $Pe$  is high, the flow time is small and the Damköhler number decreases. Damköhler number takes a wide range of values depending on the other parameters. It has a direct influence on the quench radius. When  $D_a$  is high, the chemical time is very small compared to the flow time. Thus the flame quenches closer to the wall. Results from asymptotic analysis (see [12]) show that the quench radius depends on  $D_a$  and  $\beta$  as  $r_q = a\sqrt{D/\beta^3}$ , where  $a$  is an  $O(1)$  constant. We refer the reader to CHAPTER IV for a discussion on the influence of chemical parameters on the heat flux to the cold wall.

### 2.3.2 Effect of $Pe$

While the chemical parameters influence the solution curves through the reactivity term, the parameters  $Pe$  and  $l_d$  affect the solutions through convective term in the govern-

ing equation and the boundary conditions respectively.

When  $Pe \rightarrow 0$ , the governing equations lose the convective term although the order of the differential equation is unchanged. Hence the limit is a regular perturbation limit even though some qualitative changes of behavior occur. On the other hand, when  $Pe \rightarrow \infty$  the problem becomes one-dimensional since the terms on the right hand side drop out. The order of the differential equation drops and the limit is a singular perturbation limit. Our numerical simulations show that when  $Pe = 0$ , the fuel and mass fraction contours assume a characteristic ‘onion’ shape near the triple point. Since triple flames require a convective flow to propagate into, in this case the triple flame region shrinks to a triple point. Figure 8 shows the characteristic ‘onion’ shape of the  $y_O, y_F$  contours.

When  $Pe$  is increased to  $O(1)$  values, the contours of fuel and oxidizer mass fractions show a characteristic ‘heart’ shape (see Figure 9). In this case the triple flames exist with their fuel-rich and fuel-lean PF arcs propagating against the flow. The heart shape formed by the mass fraction contours are believed to represent the two arcs of the triple flames. This hypothesis is examined in detail in Section 2.6.

The Peclet number  $Pe$  also influences the quench radius through the Damköhler number. They are related by the equation  $D_a = D_{a0}/Pe^2$ , where  $D_{a0}$  is the Damköhler number with zero convection. This relationship can be derived from the definition of  $D_a$  and by substituting  $t_{flow} = D/U^2$ , where  $D$  is the mass diffusivity and  $U$  is the dimensional velocity (note  $Pe = UL/\alpha$ ). Thus when  $Pe$  increases the flow time decreases and thus the Damköhler number also decreases. This will result in the flame quenching at a greater distance from the exit plane (or an increase of the quench radius). At a certain critical

value of  $Pe$ , the flame is very far from the exit plane and cannot sustain itself, leading to a phenomenon known as ‘blow-off’.

### 2.3.3 Effect of $l_d$

The divider thickness also influences the solution contours through the isothermal boundary condition enforced on the divider surface. The flame loses more heat to the cold wall when the divider is thicker. Hence, the divider thickness affects the location of the flame with respect to the exit plane, the length of the PF arcs of the triple flame, and the peak of the reactivity field. Figure 10 shows the reactivity contours for two different values of divider thicknesses (the dotted line corresponds to a thickness of 0.5 units and the solid line corresponds to a thickness of 0.1 units). It can be seen that when the divider is thick the flame quenches at a greater distance from the exit plane. The peak of the reactivity field drops as the divider gets thicker. This can be seen from Figure 11. In this figure, the maximum reactivity values are plotted against their corresponding  $\xi$  values. From Figure 11, we can also define a characteristic length of the triple flame, as the distance between the two zeros of the maximum reactivity reactivity profiles (see arrows in Figure 11). Hence, we can also note that when  $l_d$  is increased the characteristic length of the triple flame decreases. This is consistent with previous discussions in the literature on triple flames, which suggested that the characteristic triple flame shape and size were influenced by heat losses. The divider thickness also influences the mass fraction profiles. Numerical simulations indicate that the characteristic ‘onion’ or ‘heart’ shapes described in section 2.3.3 get wider as the divider thickness increases. The thickness of the mixing layer also increases with an increase in divider thickness. This can be seen from Figure 12, which

shows the mass fraction contours when the thickness of the divider is 0.1 units (solid line) and 0.5 units (dotted line). The mass fraction contours in the diffusion flame region are not influenced by the change in the divider thickness, suggesting that the diffusion flame region is less influenced by heat losses than the triple flame region. This conclusion is also relevant for the hypothesis we shall examine in section 2.6.

### 2.3.4 Convergence Analysis

A convergence analysis was performed on the excess enthalpy field because this particular boundary value problem was very sensitive to the size of the mesh used. The variation of  $H$  near the boundary was strong and hence precautions were necessary for accurate results. For our analysis, the mesh was gradually refined while maintaining the other parameters at constant values. Figure 13 shows the results of our analysis. We note that the magnitude of  $H$  on the divider surface increases as the mesh is refined even when the other parameters are kept at constant values. We also note that the slope of the curve decreases when the mesh size is below 0.1 units. In fact  $H$  varies by a factor of 1.27 when the mesh size is decreased from 0.15 units to 0.1 units (i.e. by a factor of 1.5). On the other hand,  $H$  varies only by a factor of 1.019 when the mesh size is decreased from 0.1 units to 0.025 units (i.e. by a factor of 4). In our numerical analysis, we used an average mesh size of 0.035 units. Hence, the mesh size used is fine enough to produce converged values of the excess enthalpy field.

## 2.4 Generic Differential Relations

We shall use two coupling functions for our analysis: mixture fraction  $Z$  and excess enthalpy  $H$ . From the definitions of these coupling functions, we have the following relations between  $Z, H$  and the primary variables:

$$Z = (1 - Z_f)y_F + (1 - y_O)Z_f, \quad (2)$$

$$H = y_O + y_F + \tau - 1. \quad (3)$$

Using equations (2) and (3), the fuel and oxidizer mass fractions can be expressed in terms of the other variables as

$$y_F = Z - Z_f(\tau - H), \quad (4)$$

$$y_O = 1 - Z - (1 - Z_f)(\tau - H). \quad (5)$$

We can use the above equations to examine the change in values of the variables along the oxidizer and fuel mass fraction contours. But initially let us assume that the excess enthalpy field is identically zero throughout the domain. This will occur when there is an adiabatic rather than an isothermal divider separating the fuel and oxidizer streams, or if the divider is infinitesimally thin. Under this assumption, using equation (4) the differential relationship  $dy_F = 0 = dZ - Z_f d\tau$  results, which is valid along the fuel isoplexes. Similarly using equation (2), we can write  $dZ = -Z_f dy_O$ . Thus we can write the following differential equations, which are valid on fuel isoplexes :

$$\frac{d\tau}{dZ} = \frac{1}{Z_f}, \quad (6)$$

and

$$\frac{dZ}{dy_O} = -Z_f. \quad (7)$$

These relationships are generic because they result solely from the definitions of the coupling functions. Applying this procedure to oxidizer, temperature and fuel mass fraction contours, we can obtain a set of differential relations on the corresponding contours similar to equations (6) and (7). These differential relations are listed in Table 1 in a compact form. These relations were used as a check on the numerical code. A sample numerical verification of these generic results for the symmetric flame is shown in Figure 14 and Figure 15, which show that  $d\tau/dZ$  and  $dZ/dy_O$  are constant and equal to the values given in Table 1 along the fuel isoplexes. Some more relations can be obtained by multiplying the two differential relations, but only the independent relations are listed below. All these relations are valid irrespective of the values of  $Z_f$ .

TABLE 1 Features of solution in the infinitesimal divider

|                           |                                                                               |                                       |
|---------------------------|-------------------------------------------------------------------------------|---------------------------------------|
| Oxidizer contours         | $\frac{d\tau}{dZ} = -\frac{1}{1-Z_f}$                                         | $\frac{dZ}{dy_F} = (1-Z_f)$           |
| Fuel contours             | $\frac{d\tau}{dZ} = \frac{1}{Z_f}$                                            | $\frac{dZ}{dy_O} = -Z_f$              |
| Temperature contours      | $\frac{dy_F}{dy_O} = -1$                                                      | $\frac{dy_F}{dZ} = 1$                 |
| Mixture fraction contours | $\frac{dy_F}{dy_O} = \frac{Z_f}{1-Z_f}$<br><br>-True even if $H$ is non zero. | $\frac{d\tau}{dy_F} = -\frac{1}{Z_f}$ |

## 2.5 Enthalpy Field and Exact Solution

In this section, we shall study the behavior of the excess enthalpy field. In Section 2.5.1 we shall explain some of the qualitative features of while in Section 2.5.2 we shall explain the methodology to obtain the exact solution to the excess enthalpy field.

### 2.5.1 Qualitative Features

The generic differential relations shown in TABLE 1 are valid when  $H = 0$ . The excess enthalpy field is non-zero when the isothermal boundary condition is imposed on the divider surface. Physically  $H \neq 0$  relates to the fact that heat is lost to the cold wall. Thus the gradient of  $H$  in the  $\eta$ -direction is positive on the divider surface since the heat flux is proportional to the negative of the enthalpy gradient on the divider surface. We observe that  $H$  is zero on the sides while both  $H$  and its gradient approach zero far downstream. Hence the value of  $H$  is negative on the surface of the divider as explained in [12]. We also note that according to its' definition  $H$  should be negative near a heat sink. To demonstrate this theoretically (see [12]), we note that on the surface of the divider,

$$H = y_O + y_F - 1, \quad (8)$$

since  $\tau = 0$ . Using this identity along with the fact that the sum of mass fractions of fuel, oxidizer, products and inert species should be unity, we get the following dimensional expression for  $H$  on the surface fo the divider.

$$H = -\frac{(Y_P + Y_I)}{Y_{OO}} + \left(\frac{1}{Y_{OO}} - 1\right) - Y_F \left(\frac{1}{Y_{OO}} - \frac{1}{Y_{FF}}\right). \quad (9)$$

Rewriting equation (9) we obtain,  $HY_{OO} = -(Y_P + Y_I - Y_{IO}) - y_F(Y_{IO} - Y_{IF})$ . From

this equation, we can prove that  $H$  is negative on the surface of the divider irrespective of the values of  $Y_{IF}$  and  $Y_{IO}$ , taking into consideration that  $Y_I$  is the solution of the boundary value problem given in Figure 3. From equation (9) we can see that there are three distinct cases. Case (i)  $Y_{IO} = Y_{IF}$ . The solution for the inert mass fraction field is  $Y_I = Y_{IO} = Y_{IF}$  throughout the domain. Thus  $H = -Y_P/Y_{OO}$ . Since the mass fraction values are always positive,  $H$  should be negative on the surface of the divider. Case (ii)  $Y_{IO} > Y_{IF}$ . In this case the solution for  $Y_I$  can be written as  $Y_I = Y_{IF} + \delta$ , where  $\delta$  is positive. Substituting this into equation (9), we obtain

$$HY_{OO} = -Y_P - \delta + \Delta(1 - y_F), \quad (10)$$

where  $\delta = Y_I - Y_{IF}$  and  $\Delta = Y_{IO} - Y_{IF}$ . Postulating the negativity of  $H$ , we get the following condition, which should be true on the divider surface.

$$\Delta(1 - y_F) \leq Y_P + \delta. \quad (11)$$

This equation has been numerically verified to be true. Figure 16 shows the two quantities on either side of the inequality plotted as a function of  $\xi$  on the divider surface. The veracity of equation (11) is obvious from the figure. Figure 17 shows the plots of the terms in equation (10) as a function of  $\xi$  on the divider surface. From this figure, we can see that the value of  $H$  is negative on the divider surface. We can also see that  $Y_P$  is maximum on the divider surface and it approaches zero at the divider ends. An interesting fact is that the location of the maximum of  $Y_P$  and the minimum of  $H$  coincide. This suggests that the dip in  $H$  occurs due to a drop in chemical enthalpy. The plots of  $\delta$  and  $\Delta y_F$  are self-explanatory. The third case corresponding to  $Y_{IF} > Y_{IO}$  can be analyzed in a manner simi-

lar to case (ii).

### 2.5.2 Exact Solution

The numerical solution for the excess enthalpy field is shown in Figure 18. Though  $H$  resembles a Dirac delta function, the area under the curve is not constant at all  $\eta = \text{constant}$  planes. Next, we shall develop an exact solution for the excess enthalpy field when  $\phi = 1$ .

The governing equation and boundary conditions for the excess enthalpy field are shown in Figure 19. Assuming that  $Pe$  is small  $Pe < O(1)$ , we can solve the equation for the  $H$ -field if the distribution of  $H$  or its gradient at the exit plane is known. But since this is coupled to the temperature field, this is usually unknown. Let us assume that  $H(\xi, 0) = f(\xi)$ . Expanding  $H$  in an asymptotic series, we get

$$H = H_0 + (Pe)H_1 + (Pe)^2H_2 + O(Pe^3). \quad (12)$$

Substituting this in the differential equation and solving for the highest order, we get a Laplace equation for  $H_0$  with the same boundary conditions as  $H$ . This equation can be solved if the function  $H_0(\xi, 0) = f(\xi)$  satisfies the equation

$$\frac{d^2 f}{d\xi^2} = -\lambda^2 f, \quad (13)$$

where  $\lambda$  is a constant. Under certain conditions, the function  $f(\xi)$  can be written as a Fourier series thus satisfying equation (13) (Note : equation (13) is satisfied by trigonometric functions). When this is possible, the solution for  $H_0$  can be written, after assuming separability, as

$$H_0 = f(\xi)e^{-\frac{\pi\eta}{L}}. \quad (14)$$

Thus the enthalpy field decays exponentially towards the far-field.

When  $Pe \neq 0$ , an exact solution can still be found for the symmetric flame. Assuming that  $H(\xi, \eta) = f(\xi)g(\eta)$ , the equation for  $H(\xi, \eta)$  can be separated with  $g(\eta)$  satisfying the differential equation

$$\frac{d^2 g}{d\eta^2} - Pe \frac{dg}{d\eta} - \lambda^2 g = 0. \quad (15)$$

Hence, the solution for  $H = H(\xi, \eta)$  can be written as

$$H = f(\xi)e^{\left(\frac{Pe - \sqrt{(Pe)^2 + 4\lambda^2}}{2}\right)\eta}, \quad (16)$$

where  $g(\eta)$  was obtained by solving equation (15). Thus the decay of  $H$  is exponential in the  $\eta$ -direction even in the presence of convective flow. Such exact solutions can also be found for the unsymmetric configuration, provided that the function  $f(\xi)$  can be represented in a Fourier series. The above procedure is exploited in Chapter 4, where an exact expression is given for the excess enthalpy field for both symmetric and unsymmetric configurations.

## 2.6 Triple Flame Shape

The triple flame is most reliably identified by the peaks in the reactivity field. However, it has been speculated (see [10]) that in some cases the fuel and oxidizer mass fraction contours near the triple point might coincide with the PF arcs of the triple flame. In this section, we shall examine this hypothesis in detail.

Figure 20 shows the reactivity and mass fraction contours near the triple point for a symmetric flame and Figure 22 for an unsymmetric flame. The PF wings of the triple flame are identified by the points of maximum reactivity along each  $x=\text{constant}$  plane (for a symmetric flame). From the figure, we can see that the PF arcs of the triple flame and the mass fraction contours lie very close to each other. Let  $\hat{n}_O$ ,  $\hat{n}_F$  and  $\hat{n}_r$  represent the unit vectors along the oxidizer, fuel and reactivity contours respectively. Mathematically we can say that if the postulate is correct, then on the fuel-lean side the cross-product of  $\hat{n}_F$  and  $\hat{n}_r$  should be approximately zero. Similarly the cross-product  $\hat{n}_O$  and  $\hat{n}_r$  should be approximately zero. Since the cross-product is proportional to the sine of the angle between the two contours, it is logical to expect the angle to be small if the postulate is correct. From Figure 20 and Figure 22, we can see that this is the case in the region near the triple point. But as we move away from the triple point, the angle increases and the postulate does not hold. This analysis has been repeated for the unsymmetric flame ( $\phi = 2$ ) in Figure 22. As the flame moves away from the symmetric flame configuration, one of the arcs of triple flame becomes more pronounced than the other. When  $\phi > 1$ , the fuel lean arc of the triple flame becomes more pronounced than the fuel-rich arc. Similarly the fuel-rich arc becomes more pronounced in the  $\phi < 1$  case. For the unsymmetric flame we can see from Figure 22 that the angle between  $\hat{n}_r$  and  $\hat{n}_F$  increases while the angle between  $\hat{n}_r$  and  $\hat{n}_O$  decreases, which suggests that the strong PF arc is approximated with better accuracy than the weak PF arcs by the mass fraction contours. We can expect this effect to be magnified when we consider very high or very low  $\phi$  values. These graphs

show that when  $\phi > 1$ , the fuel-lean arc is approximated very closely by the fuel mass fraction contours and when  $\phi < 1$ , the fuel-rich arc is approximated very closely by the oxidizer mass fraction contours.

In order to determine the inaccuracy in approximating the PF arcs by fuel and oxidizer mass fraction contours, the values of fuel and oxidizer mass fraction along the PF arcs are plotted in Figure 21. In this figure the fuel and oxidizer values at the points of maximum reactivity at each  $\xi = \text{constant}$  plane is plotted as a function of  $\xi$ . From the figure we can see that when  $\xi < 0$ , the fuel mass fraction values along the PF arc changes by a small amount. The same is true of the oxidizer mass fraction values when  $\xi > 0$ . In fact  $y_O$  varies from (see TABLE 2) 0.0048 at  $\xi = -0.6463$  (where the reactivity is almost zero,  $r=0.001$ ) to 0.0954 at  $\xi = 0.0083$  (where the reactivity is maximum,  $\omega = 28.423$ ). Thus the variation in  $y_O$  is very small compared with the high variation we observe from  $\xi = 0.0083$  to  $\xi = 0.9899$ . Since this is a symmetric flame, the same is true of the fuel mass fraction values. Thus we can conclude that, for the symmetric flame, contours of fuel and oxidizer mass fractions can approximate the two PF arcs of the triple flame in a fairly accurate manner.

For the unsymmetric flame the strong arc is approximated closely by the oxidizer mass fraction contours. From we can see that oxidizer mass fraction changes from 0.0046 at  $\xi = -0.5250$  (where the reactivity is 0.0001) to 0.0735 at  $\xi = 0.1612$  (where the reactivity is 40.9978). But for the weak PF arc, the data in TABLE 3 shows that  $y_F$  varies from 0.0848 at  $\xi = 0.1612$  ( where the reactivitiy is maximum,  $\omega = 40.9978$ ) to 0.0240 at  $\xi = 0.2824$  (where the reactivity is 17.9645) and to 0.0049 at  $\xi = 0.5856$  (where the

reactivity is 0.0473). Thus, in this case even the weak PF arc is approximated closely by the mass fraction contours. However, this may not be the case when we consider very high or very low  $\phi$  values. For these configurations, the angles between the contours might be too high, especially far from the triple point, to validate the use of mass fraction contours to represent triple flames. But the inaccuracy is somewhat diminished by the fact that the mass fraction contours are not dense (thus the gradient is not steep) in the region of approximation.

TABLE 2 Variation in  $y_O$  values along the strong PF arc

| Type                        | $\xi$   | $y_O$  | reactivity |
|-----------------------------|---------|--------|------------|
| $\phi = 1$<br>(symmetric)   | -0.6463 | 0.0048 | 0.0001     |
|                             | 0.0083  | 0.0954 | 28.423     |
| $\phi = 2$<br>(unsymmetric) | -0.5250 | 0.0046 | 0.0001     |
|                             | 0.1612  | 0.0735 | 40.9978    |

TABLE 3 Variation of  $y_F$  values along the weak PF arc

| Type                        | $\xi$  | $y_F$  | reactivity |
|-----------------------------|--------|--------|------------|
| $\phi = 2$<br>(unsymmetric) | 0.1612 | 0.0848 | 40.9978    |
|                             | 0.2824 | 0.0240 | 17.9645    |

TABLE 3 Variation of  $y_F$  values along the weak PF arc

| Type | $\xi$  | $y_F$  | reactivity |
|------|--------|--------|------------|
| .    | 0.5856 | 0.0049 | 0.0473     |

From the above discussion, we conclude that the strong PF arcs can be approximated by the appropriate mass fraction contours and it is incorrect to approximate the weak PF arc by the corresponding mass fraction contours especially for very high or very low  $\phi$  values without careful consideration.

## 2.7 Conclusions

In this chapter, we have examined some generic features of triple flames using the model problem formulated in CHAPTER I.

Our numerical results show the existence of three different regions, which exhibit distinct behavior. The mixing layer is characterized by high values of cross-stream mass fraction gradients, which reduce to lower values further downstream. In the triple flame region, the gradients of the mass fractions have opposite signs. In the diffusion flame region, which appears downstream, the mass fraction profiles exhibit one-dimensional behavior.

The various parameters in the model problem have been identified and their influence on the solution contours analyzed. The chemical parameters like  $\alpha$ ,  $\beta$ , and Damköhler number influence the quench radius and the maximum reactivity. The flow parameter  $Pe$  influences the mass fraction contours and also the quench radius through the Damköhler number. Characteristic ‘onion’ or ‘heart’ shapes result depending on the value of  $Pe$ . The

geometric parameter  $l_d$ , which is the thickness of the divider influences the quench radius, the length of the PF arc, the maximum reactivity, the width of the characteristic 'onion' and 'heart' shapes, and the size of the mixing layer.

Some generic differential relations can be derived from the definitions of the mixture fraction and excess enthalpy coupling functions under the assumption of an infinitesimal divider or adiabatic divider. These relations have been listed after numerical verification.

The excess enthalpy values on the divider surface have been shown to be negative. The profiles of the mass fractions of fuel, oxidizer, inert species and products have been analyzed on the surface of the divider. Some generic relations have also been verified. A methodology for deriving the exact solution to the excess enthalpy field has been explained. The resulting solution shows that the excess enthalpy field decays from the surface values in an exponential fashion even in the presence of a convective flow.

The accuracy in representing the PF arcs of the triple flame by using the fuel and oxidizer mass fraction contours has been examined for both symmetric and unsymmetric flames. Our results show that this is justified for the strong PF arcs. The mass fraction values along the weak PF arc of the triple flame for very high  $\phi$  or very low  $\phi$  values vary by a greater degree, which makes it inaccurate to represent them using mass fraction contours without careful consideration.

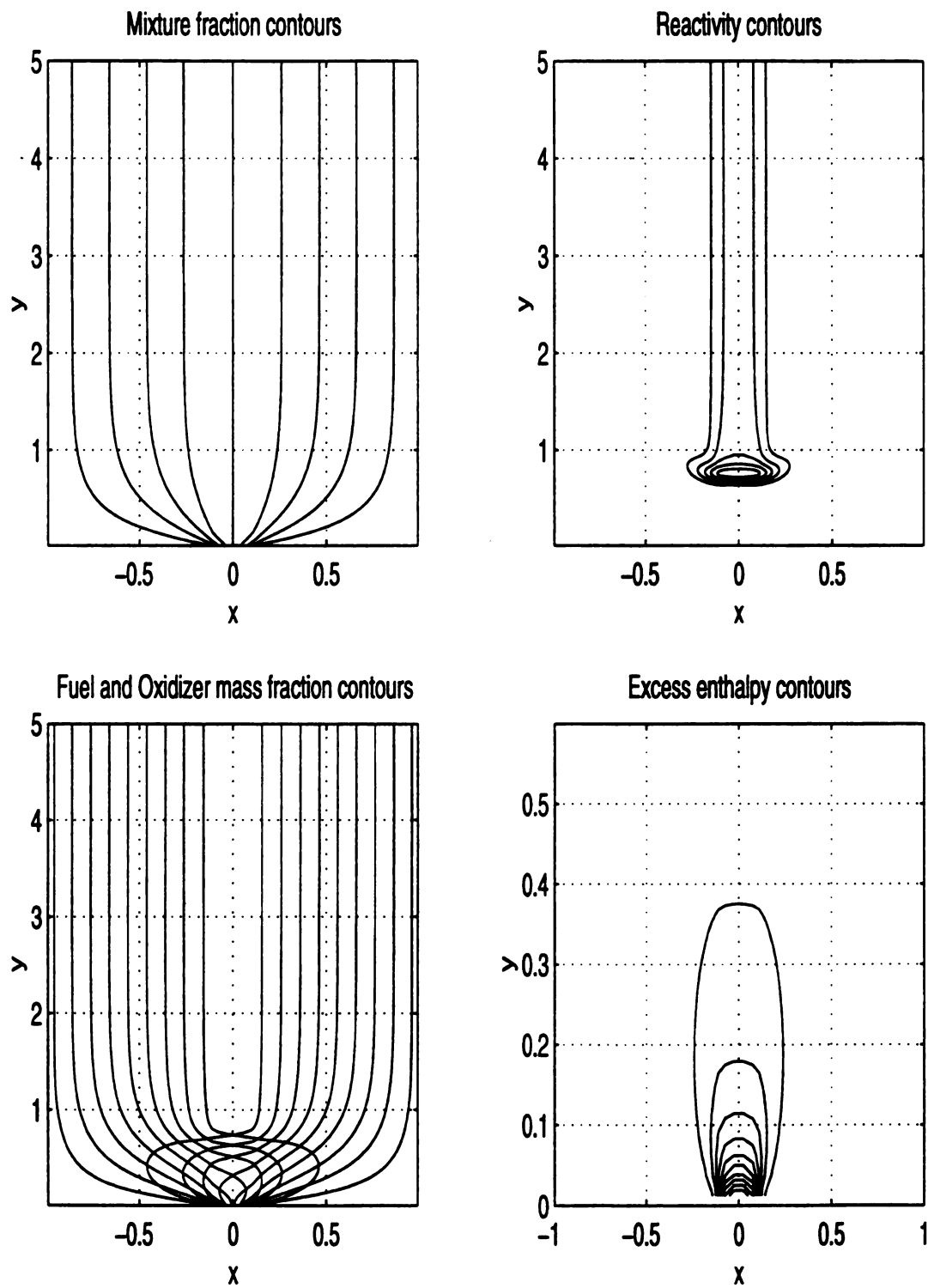


Figure 5 - Solution contours for a symmetric flame

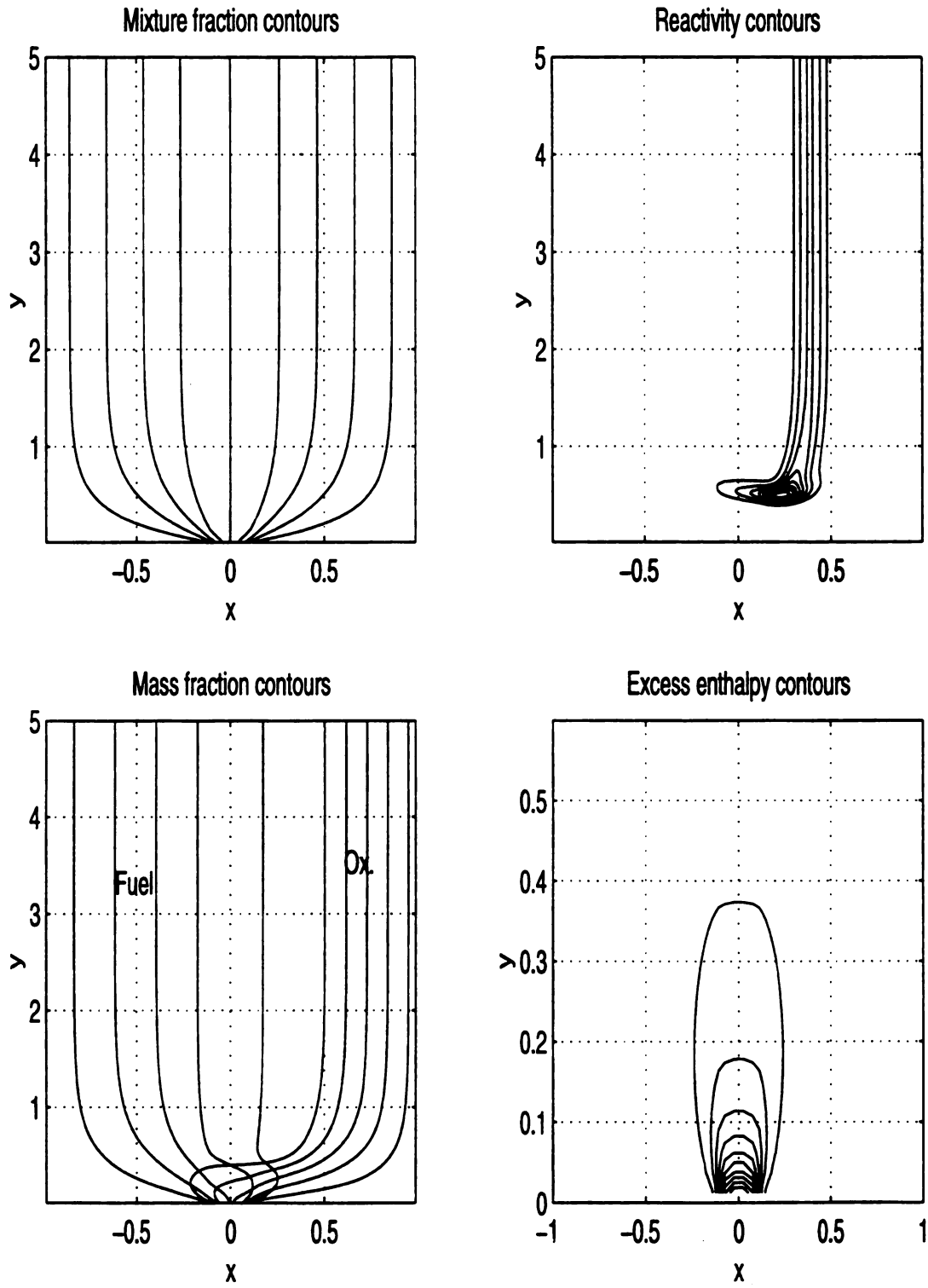


Figure 6 - Solution contours for an unsymmetric flame ( $\phi = 2$ ).

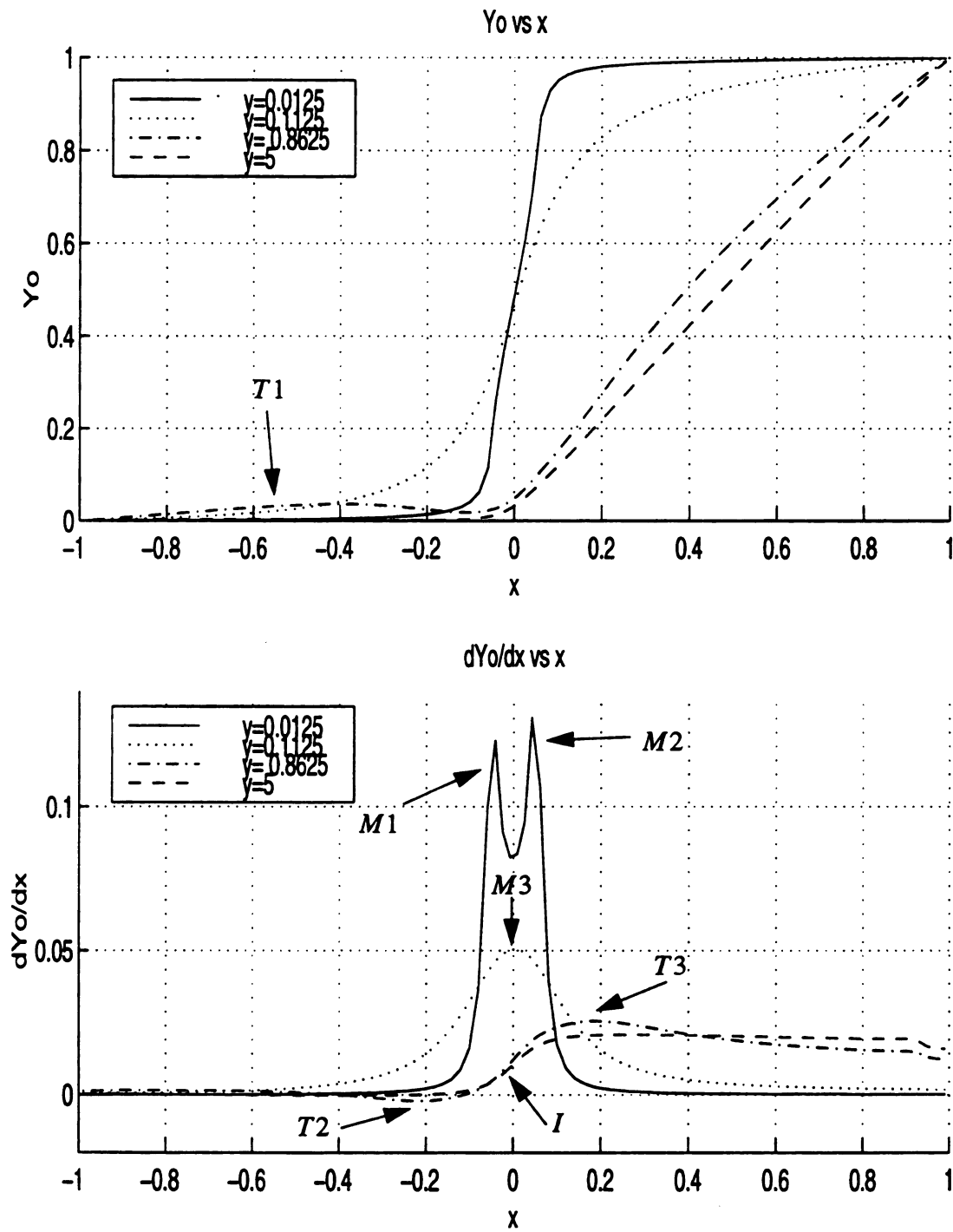


Figure 7 - Oxidizer mass fraction and its gradient in the  $\xi$ -direction vs  $\xi$

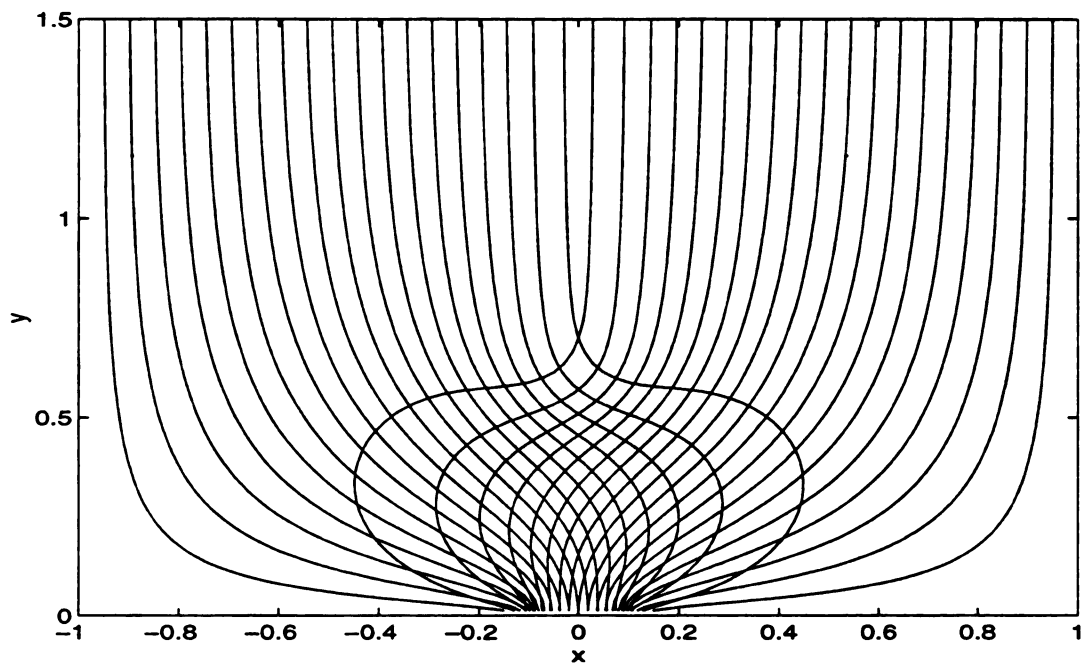


Figure 8 - Characteristic 'Onion' shape in the mass fraction contours

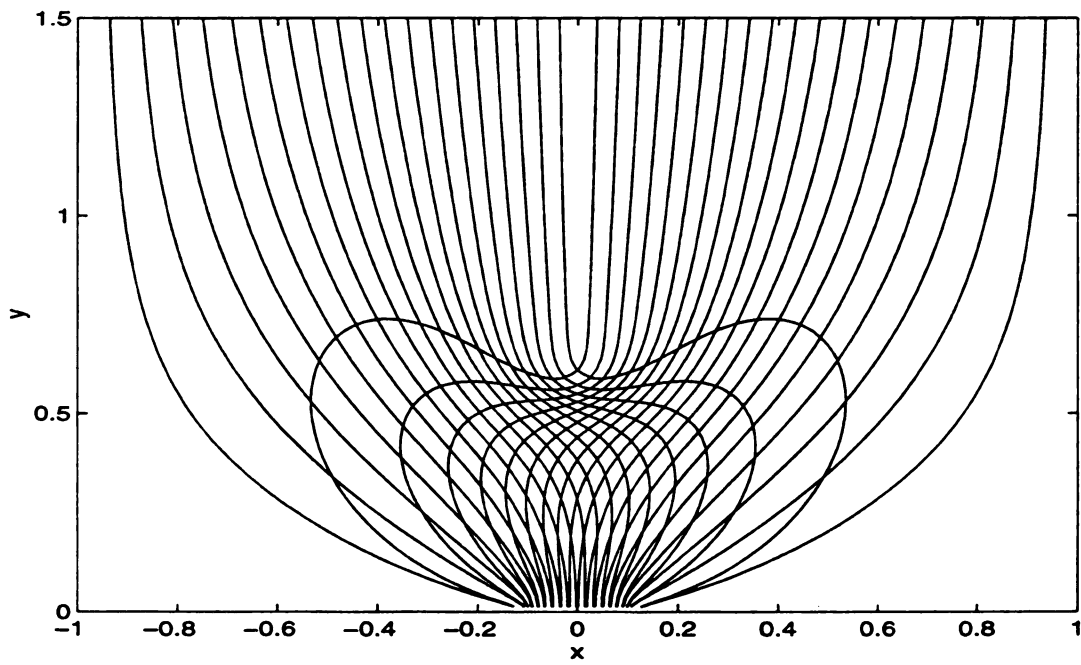


Figure 9 - Characteristic 'Heart' shape in the mass fraction contours

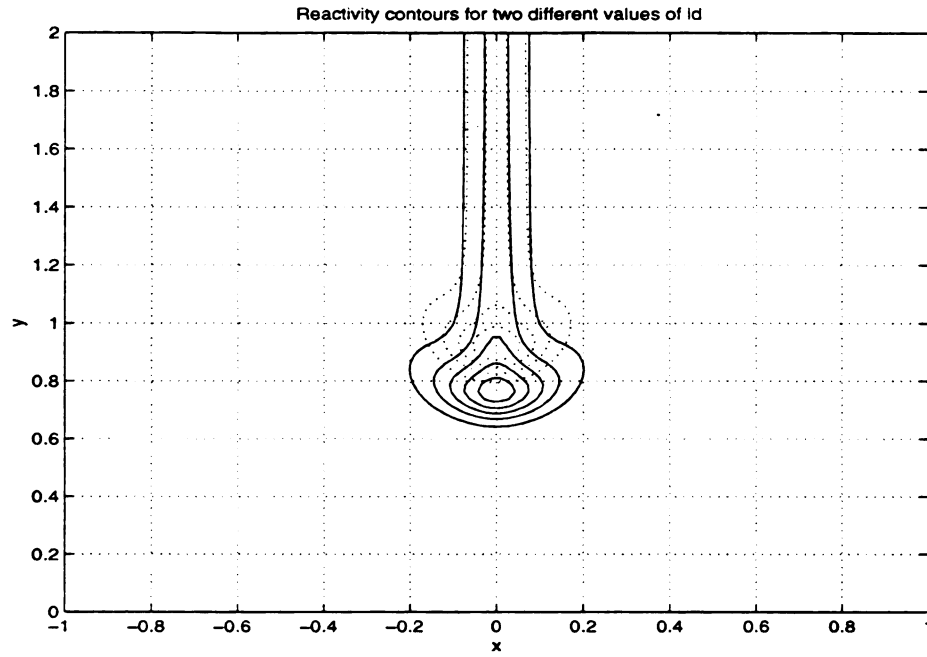


Figure 10 - - Reactivity contours for two different  $l_d$ .

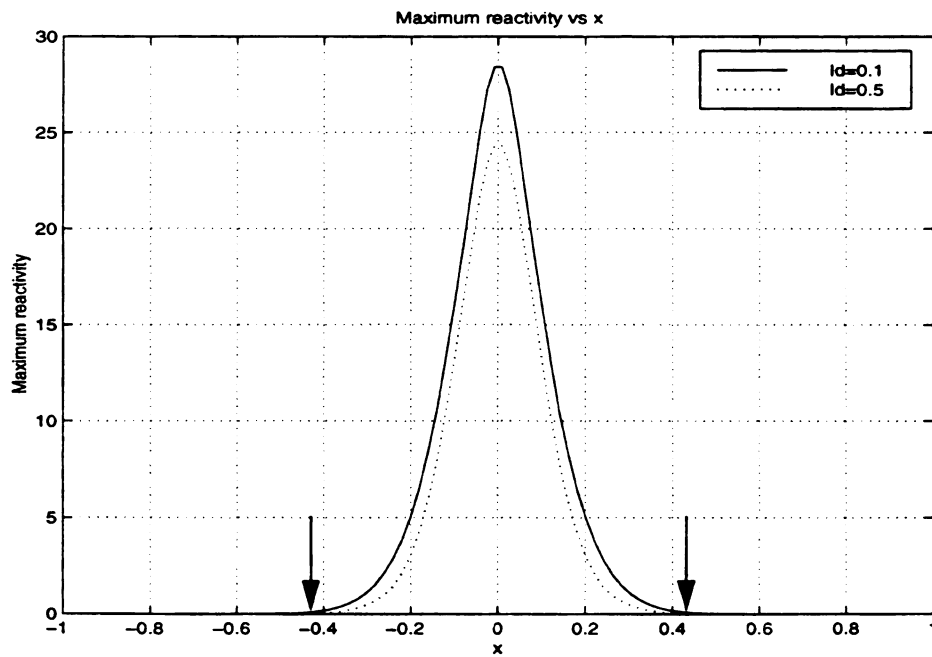


Figure 11 - Maximum reactivity values vs  $\xi$  for different  $l_d$

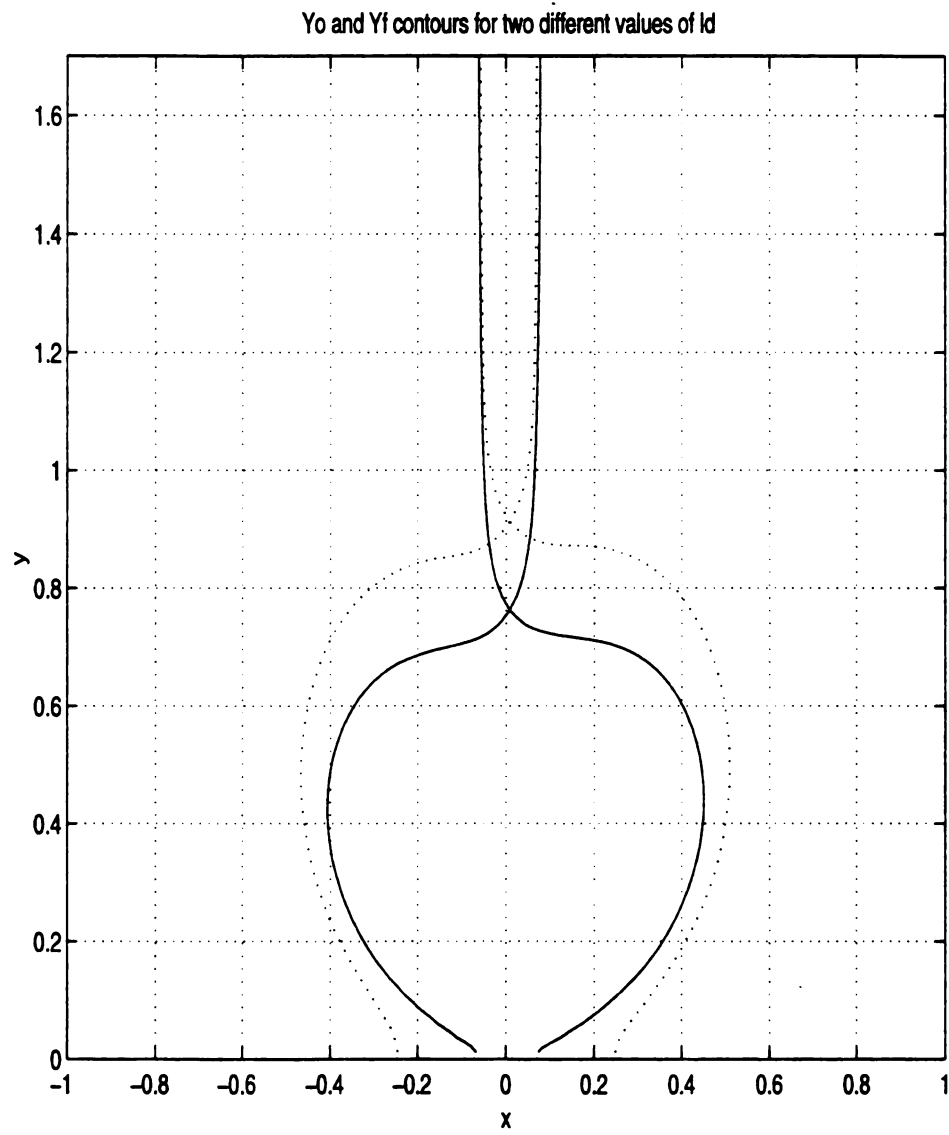


Figure 12 - Mass fraction contours for two different values of  $l_d$

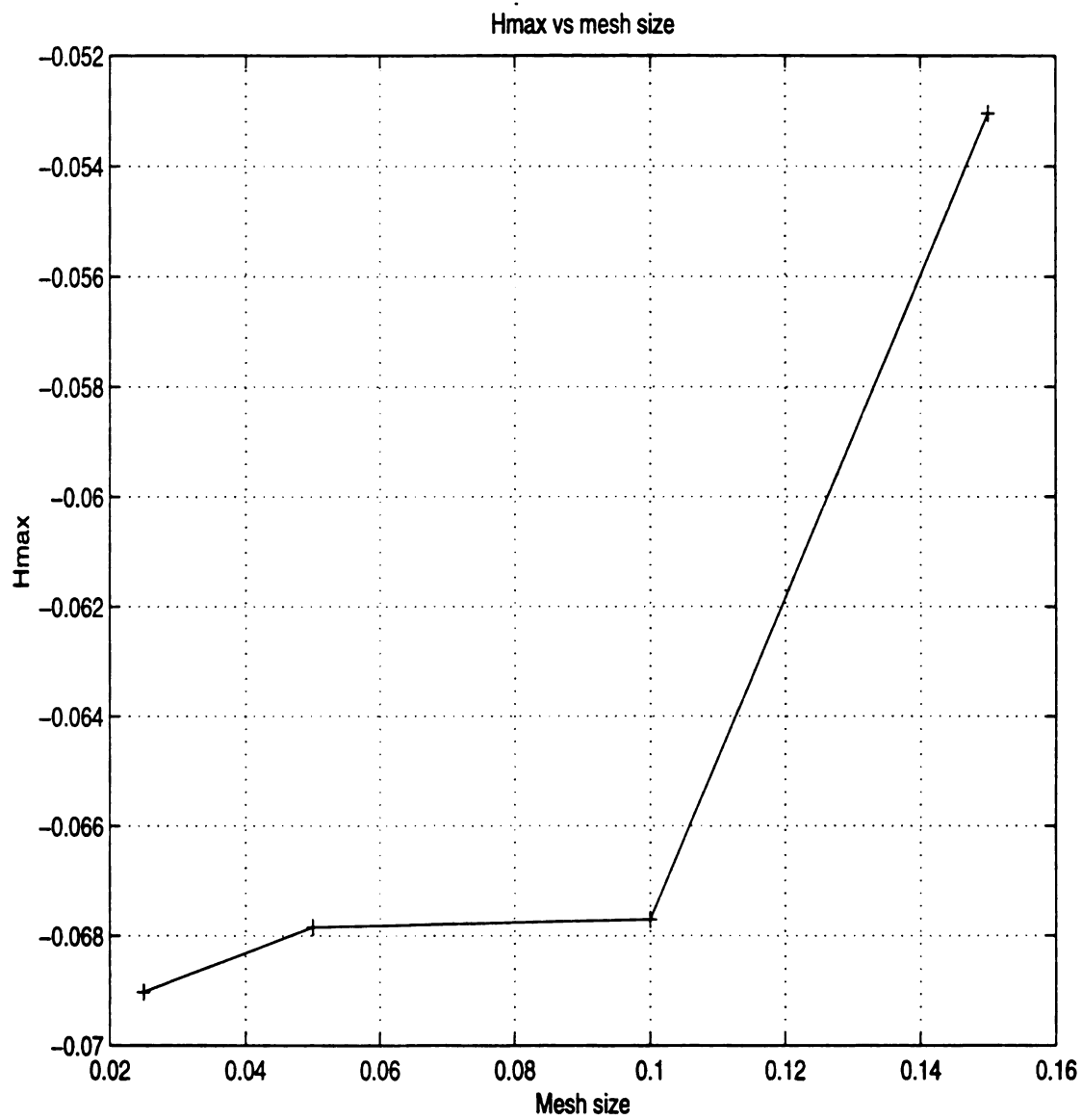


Figure 13 - Convergence analysis on the  $H$ -field

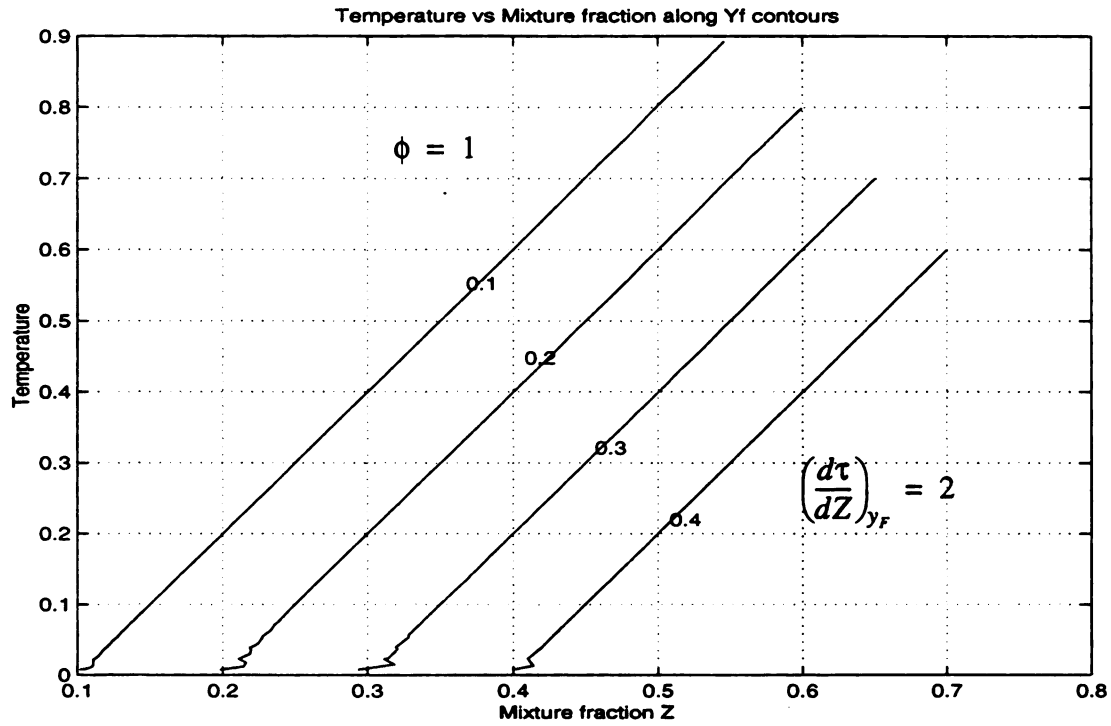


Figure 14 - Temperature  $\tau$  vs Mixture fraction  $Z$  along  $y_F$  contours

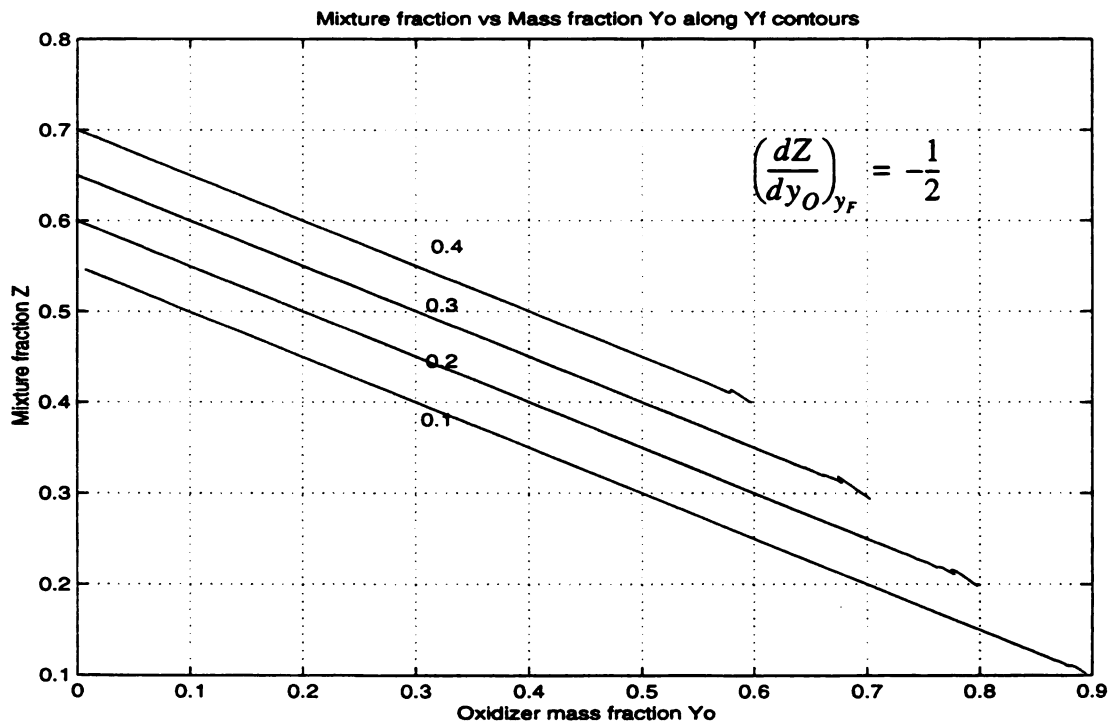


Figure 15 - Mixture fraction  $Z$  vs Ox. mass fraction  $y_O$  along  $y_F$  contours

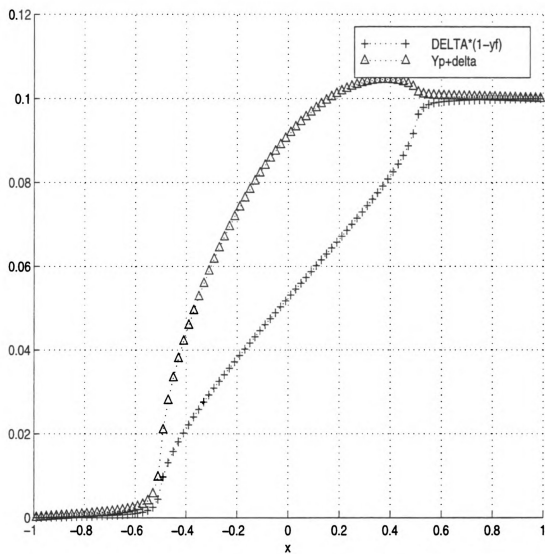


Figure 16 -  $\Delta(1 - y_f)$  and  $Y_p + \delta$  as a function of  $\xi$

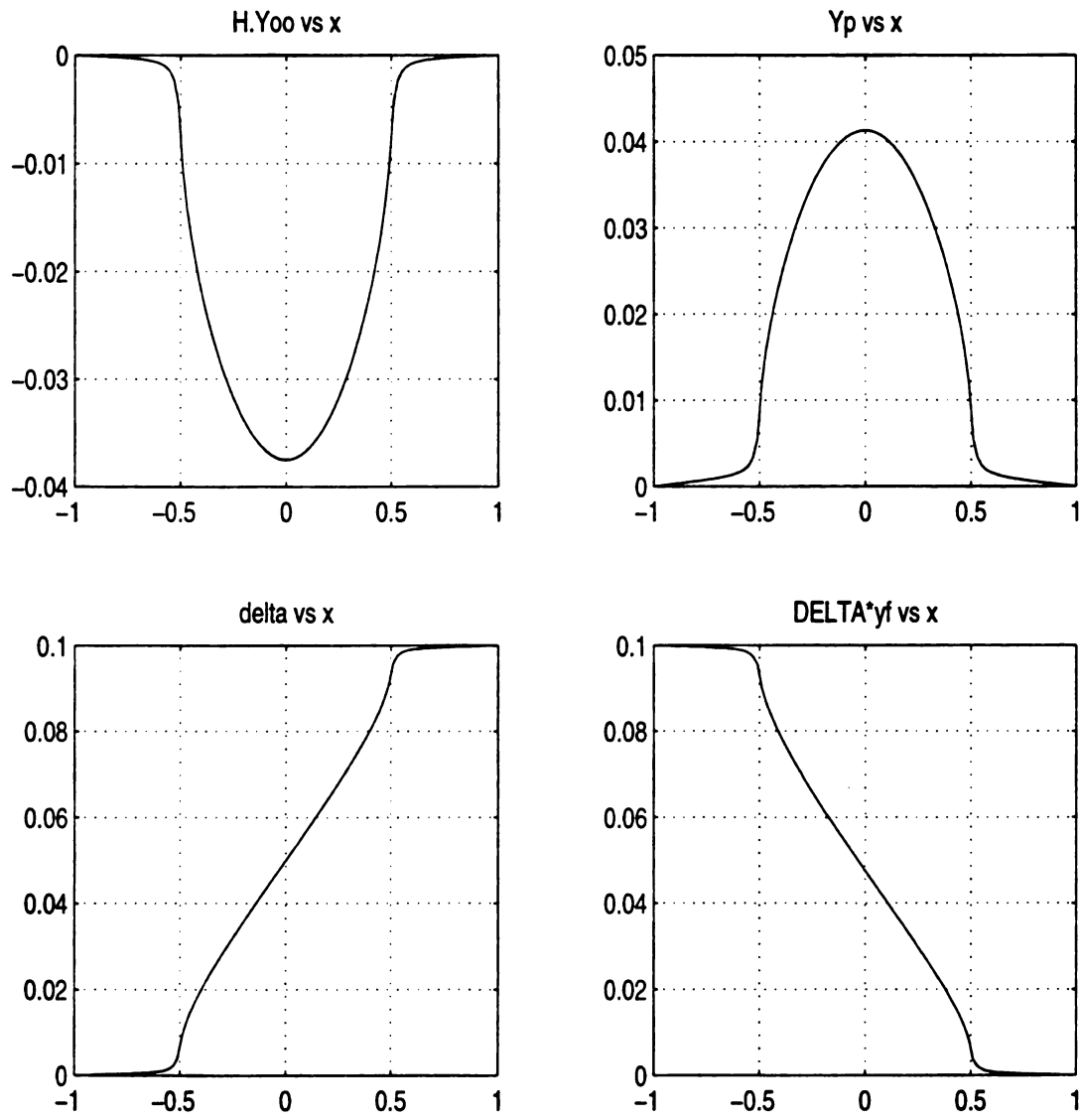


Figure 17 - The terms in equation (10) vs  $\xi$  on the divider surface

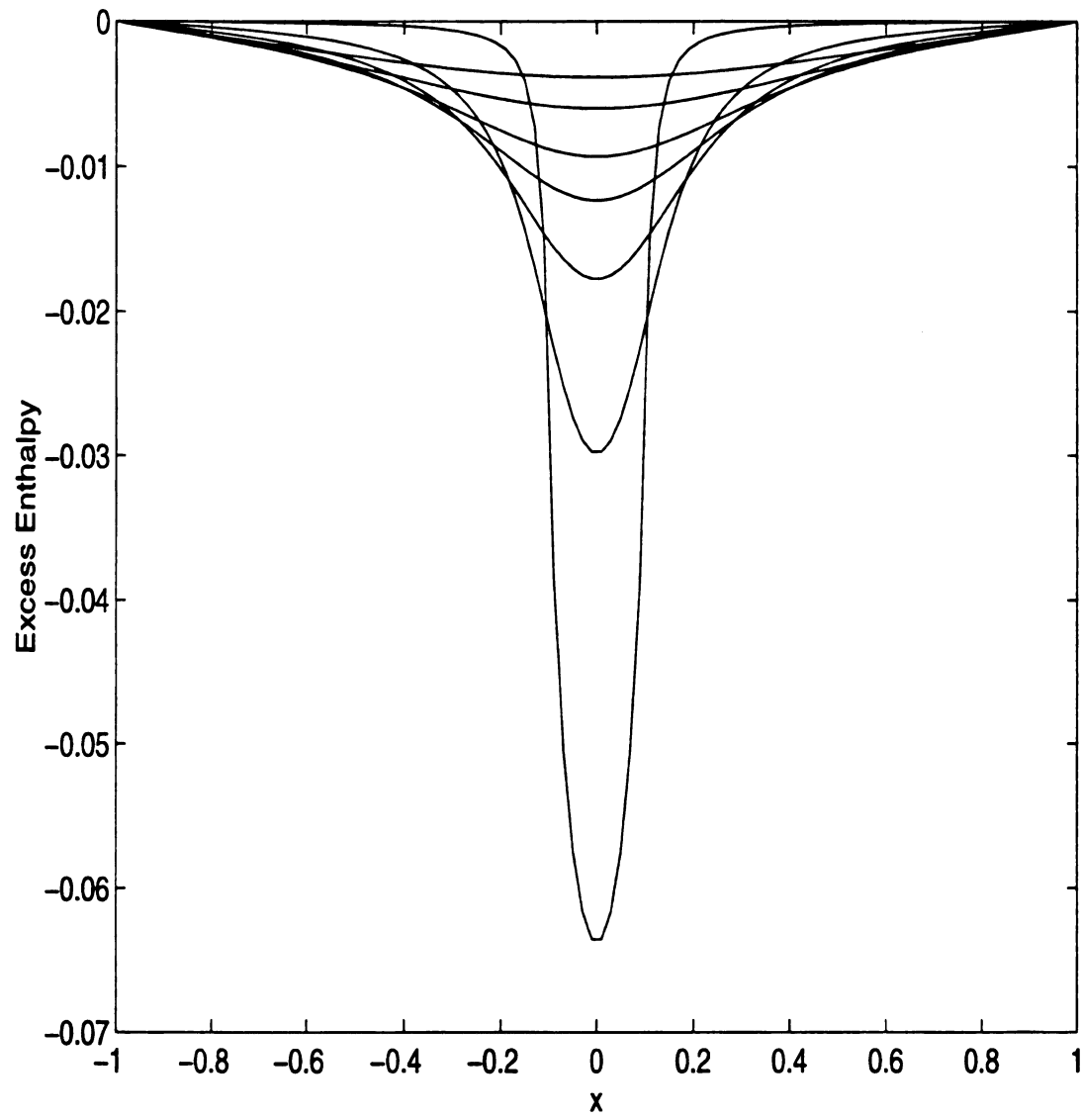


Figure 18 - The excess enthalpy values vs  $\xi$

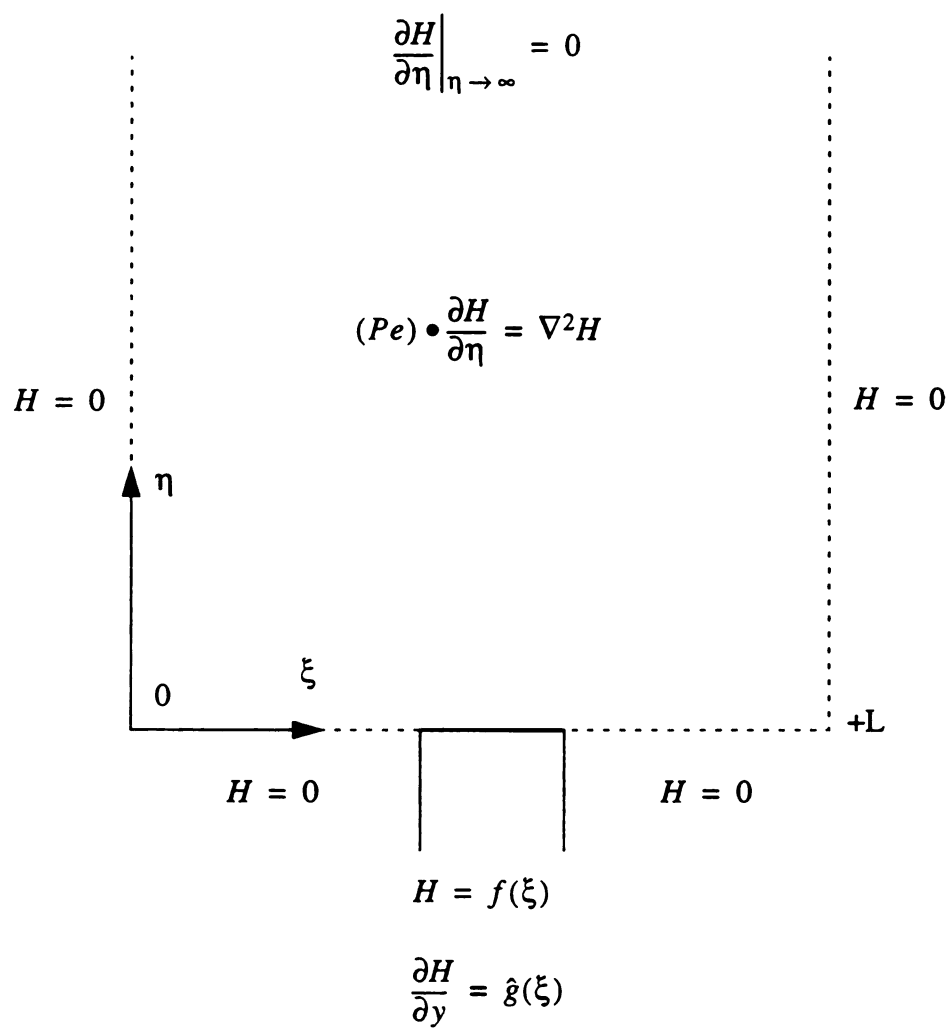


Figure 19 - Model for the excess enthalpy field

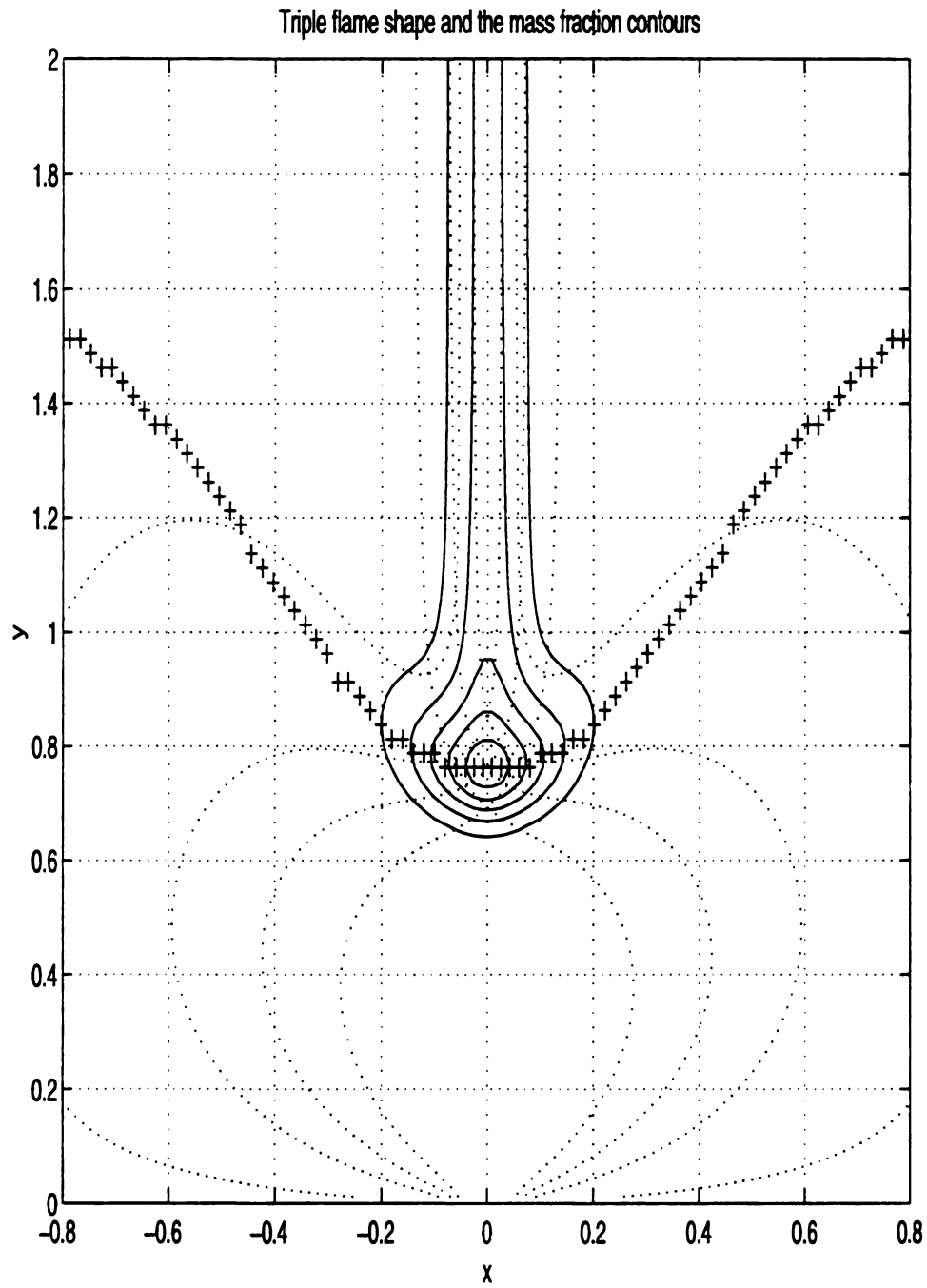


Figure 20 - Reactivity, mass fraction contours near the triple point

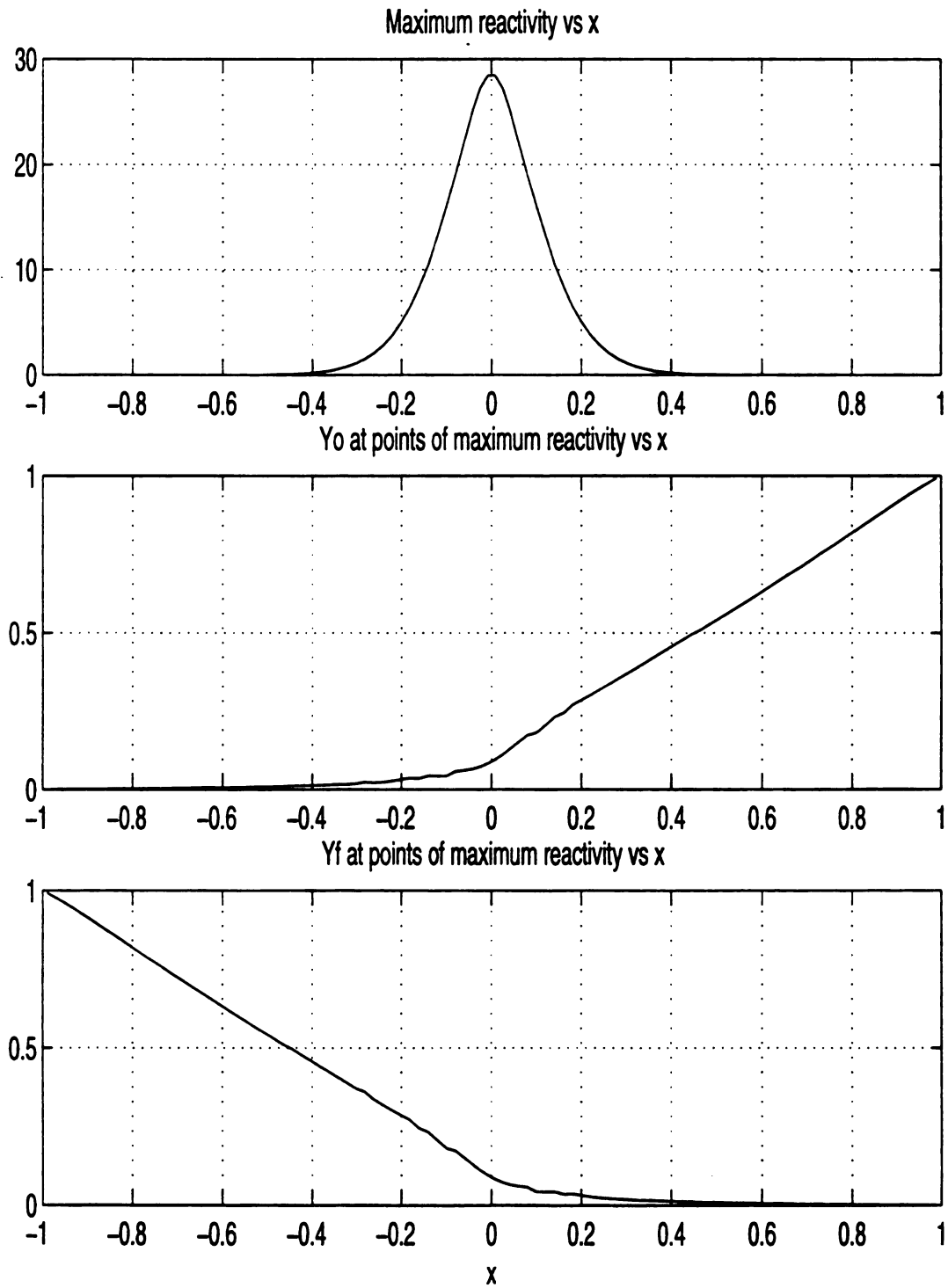


Figure 21 - Reactivity, fuel and ox. mass fraction values along PF arc

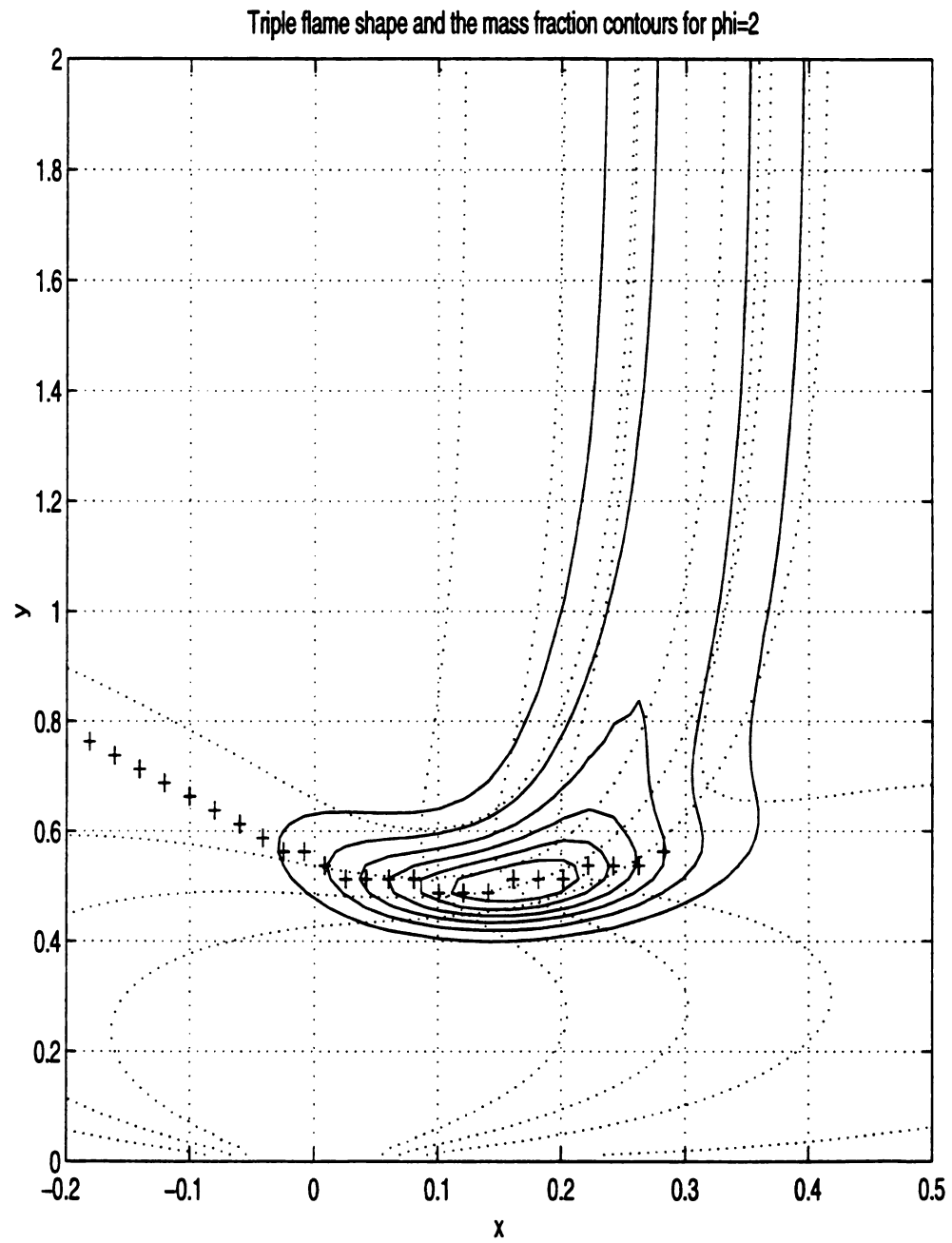


Figure 22 - Reactivity and mass fraction contours near the triple point

## CHAPTER III

### Stoichiometric Premixed Flame Speed

#### 3.1 Introduction

In this chapter we shall examine the extent to which a diffusion flame (DF) behaves as a stoichiometric premixed flame (PF). This question is relevant for discussions of flame spread and flame attachment in burners. It may have special relevance for laminar flamelet models of turbulence.

Numerous authors have, over many years, postulated stoichiometric PF tips - we call this postulate P1 - and constructed their experimental analyses and theoretical models on the consequences of postulate P1 [13] to [14]. We shall restrict P1 to zero heat loss flames, although later we shall relax this restriction and allow upstream heat losses as discussed in [16] and [17].

Under flow rates, stoichiometries, or distance from cold boundaries, the stoichiometric PF tip is an excellent modeling restriction. Nevertheless, we expect there are circumstances under which P1 is difficult to justify. The reason P1 becomes difficult to justify arises from the inherent deficiency of the stoichiometric PF concept. We now discuss this briefly.

It is known that the PF speed  $S_L$  depends on  $N$  variables  $\chi_i$ ,  $i = 1, \dots, N$  like stoichiometry, upstream heat losses, downstream heat losses, radiative heat losses, and so on. The sensitivity to each quantity is defined as  $\lambda_i = \bar{\chi}_i \partial S_L / \partial \chi_i$ , where  $\bar{\chi}_i$  is an average value

and  $\lambda_i$  is the  $i$ th sensitivity coefficient. If the  $\lambda_i$  is larger than all others, then it indicates that  $\chi_i$  is the dominant variable influencing flame speed in the  $\chi_i$ -range considered. Thus if  $\chi_1$  is the variable corresponding to stoichiometry coefficient and  $\chi_2, \dots, \chi_N$  are constant, with the  $\chi_i$  value corresponding to heat losses equal to zero, then P1 referred only to stoichiometry is logical. If, on the other hand,  $\chi_2, \dots, \chi_N$  are non-constant, and possibly non-zero, it is necessary to determine which has the largest influence. There may be cases in which stoichiometry is secondary while the heat losses dominate. For each problem, it is therefore necessary to construct an  $(N - 1)$  dimensional surface whose local maxima dictate the PF response. In our problem the DF lies very close to the stoichiometric surface, hence we expect near-stoichiometric PF propagation although heat losses, etc. will be important, perhaps even dominant near the lower surface. Consequently, we conclude that the definition “stoichiometric PF propagation” comprises many separate physical processes, some of which may be poorly understood or defined.

Our goal herein is to provide a partial explanation of the scope and limitations of P1 and, more broadly, to begin to develop a method for examining such questions in more complicated problems. For this purpose, we shall examine a model problem that contains elements we believe are important for theoretically studying P1. The model is analyzed in section 2.

### 3.2 The Model

We shall use Model B for our analysis. The configuration we shall employ is shown in

Figure 23 along with the normalized equations and boundary conditions. The cold sides admit a diffusive influx of fuel and oxidizer, whereas the lower walls, which are also cold and porous may also admit a convective influx of fuel and oxidizer. The convective flow is inviscid, hence the constant-property hypothesis produces a uniform, non-accelerating gas flow. Although this flow seems at first to be unrealistic, we have ample evidence from our two-dimensional, variable-property, confined-flow Navier-Stokes simulations that the velocity field in the vicinity of the flame tip is remarkably similar to that assumed in Figure 23. Figure 24 shows the velocity field for a typical case. In these numerical solutions, the inlet flow is of Poiseuille form at the exit plane. Despite this, it appears that thermal expansion and also buoyancy combine to produce a slug flow near the flame tip. Thus the slug flow hypothesis is justified.

The simplifications that we shall employ in our analysis are the following: The flame will be steady and the reaction will occur in one irreversible step, viz.  $F + \gamma O = (1 + \gamma)P + \text{heat}$  (mass basis). The gas properties are constant, the gas flow rates from both the reservoirs are identical, and the fuel and oxidizer Lewis numbers are unity. There is no fluid viscosity, there is no misalignment of pressure and density gradients (indeed there are no gradients of either quantity), there is no gravity: hence, there is no vorticity in the flow. The velocity distributions of Figure 24 support these restrictions in the vicinity of flame tip. In contrast to the model of Figure 24, we shall not examine the case of a finite thickness divider plate. Our divider, which is infinitesimally thin, has the sole purpose of separating the incident reactant streams from one another. Also in contrast to the numerical model, the inlet flow at the divider exit plane has temperature  $T_0$  (see Figure 23). We shall restrict ourselves to the case of a very high Zeldovich number,  $\beta \rightarrow \infty$ ,

hence the DF will lie very nearly along the mixture fraction arc,  $Z = Z_f$ . In actuality, the reactivity peak of the DF is displaced to one side or another of the arc  $Z_f$ , as discussed in [18] and verified in the detailed numerical integrations of [19].

In order to clarify our subsequent discussions, we shall examine some features of the model here. With reference to Figure 25, we define the contour  $Z = Z_f$  as the arc '0 $\infty$ '. From Figure 23, an infinitesimally thin divider renders the  $Z$  - value nonunique at the origin. The DF quenches at point 'q', which we identify as the flame tip. Point 'i' along the DF identifies the inflection point, where the DF curvature reverses. The angle  $\theta_p$  identifies the tangent to  $Z = Z_f$  at point 'q'; it also defines the flow component  $Pe_p$  entering the PF arc. The angle  $\theta_q$  defines the quench point 'q' in its absolute relation to the origin, with  $\xi_q = r_q \cos \theta_q$ ,  $\eta_q = r_q \sin \theta_q$  and  $r_q = \sqrt{\xi_q^2 + \eta_q^2}$ . The angle  $\theta_t$  defines the minimum (or maximum, when  $Z_f > 1/2$ ) angle that can connect the origin to the line  $Z = Z_f$  through a point of tangency; this point is identified as 't'. When the stoichiometry places the DF along the symmetry plane, where  $Z_f = 1/2$ , the points 'q', 'i', 't' coincide and  $Pe = Pe_p = Pe_{0q}$ .

If, however,  $Z_f$  is not equal to 1/2, the mass flux components  $Pe_{0q} \neq Pe_p$ . When point 'q' is between the origin and point 't',  $Pe_{0q} > Pe_p$  and  $Pe_{0q}$  approaches  $Pe_p$  from above. As point 'q' approaches the origin, we have  $Pe_p \rightarrow Pe_{0q} \rightarrow Pe$ . When point 'q' is between point 't' and ' $\infty$ ',  $Pe_{0q} < Pe_p$  and  $Pe_{0q}$  approaches  $Pe_p$  from below. As point 'q' approaches ' $\infty$ ', we have  $Pe_{0q} \rightarrow Pe_p \rightarrow Pe$  with  $Pe_{0q} < Pe_p < Pe$ . These behav-

iors, which occur on either side of  $Z = Z_f = 1/2$ , are qualitatively illustrated in Figure 26. Note that when  $Z_f = 1/2$ , all three lines coincide with the one marked as  $Pe$ . From the preceding definitions, illustrated in Figure 25, we can easily derive the following relations:

$$\frac{Pe_{0q}}{Pe} = \frac{\eta_q}{r_q}, \quad (17)$$

$$\frac{Pe_p}{Pe} = \frac{-\left(\frac{\partial Z}{\partial \xi}\right)_q}{\sqrt{\left(\frac{\partial Z}{\partial \xi}\right)_q^2 + \left(\frac{\partial Z}{\partial \eta}\right)_q^2}}. \quad (18)$$

We shall employ these identities in our subsequent analysis. Eq. (18) is derived by considering the flame arc  $Z = Z_f$ , along which  $dZ = 0$ , giving  $d\eta/d\xi = \tan\theta_p = -(\partial Z/\partial \xi)/(\partial Z/\partial \eta)$ . This identity, coupled with  $Pe_p/Pe = \sin\theta_p$ , leads directly to Eq. (18).

### 3.3 Analysis and Results

This section is subdivided into four subsections. In section 3.3.1 we obtain the exact solution for the mixture fraction field. In section 3.3.2, the qualitative nature of the loci of constant  $Pe_p/Pe$  given by Eq. (18) is examined. In section 3.3.3, we study various features of the solution that may be deduced from a comparison of Eqs. (17) and (18). In section 3.3.4 we shall compare the kinematic flame speed formula, Eq. (18), and the premixed flame speed evaluated with and without heat losses.

### 3.3.1 Exact solution for $Z(x,y)$

The boundary value problem for  $Z$  can be solved exactly by the method of separation of variables,

$$Z(\xi, \eta) = \frac{1-\xi}{2} + \sum_{n=1}^{\infty} \frac{\sin(n\pi\xi)}{n\pi} \exp\left[\frac{Pe - \sqrt{Pe^2 + (2n\pi)^2}}{2}\eta\right]. \quad (19)$$

When  $Pe \rightarrow 0$ , a closed form solution exists, viz,

$$Z(\xi, \eta) = \frac{1}{2} - \frac{1}{\pi} \operatorname{atan} \mu(\xi, \eta), \quad \text{where } \mu(\xi, \eta) = \frac{\tan \frac{\pi\xi}{2}}{\tanh \frac{\pi\eta}{2}}. \quad (20)$$

When  $\eta \rightarrow \infty$ , the above equations reduce to the one-dimensional solution,

$$Z_{\infty} = \frac{1-\xi}{2}. \quad (21)$$

All of the above equations will be used in the following analysis.

### 3.3.2 Loci of Constant $Pe_p/Pe$

These loci are examined by using Eq. (20) for  $Z(\xi, \eta)$  which produces a simple, qualitatively accurate expression for  $Pe_p/Pe$  that is valid for non-zero  $Pe$ . After some calculation, we find from Eq. (18) that

$$\frac{Pe_p}{Pe} = \frac{1}{\sqrt{C^2 + 1}}, \quad \text{where } C \equiv \frac{\sin \pi\xi}{\sinh \pi\eta}. \quad (22)$$

The curves of constant  $Pe_p/Pe$ , which are curves of constant  $C$ , are illustrated in Figure

27. Since  $C^2$  is always positive, we must have  $Pe_p/Pe < 1$  throughout the domain. Also

shown in Figure 27 are representative  $Z$  - contours, which intersect with an infinite number of  $Pe_p/Pe$  constant curves. Since there is no independent means provided herein for deciding which intersection gives point 'q', a separate and independent quenching calculation must be performed. This would specify  $\xi_q$  and  $\eta_q$ , which would give  $Pe_p/Pe$  from Eqs. (18) and (20). Along the  $Z_f$  arc, shown in Figure 26, we see that  $Pe_p/Pe$  approaches unity near the exit plane and also in the far field. In between, other positive values between zero and unity can be attained. The response is different for the symmetric flame along the centerline ( $Z = Z_f = 1/2$ ). Here, the value of  $C$  must always be zero, hence  $Pe_p/Pe = 1$ . The flow entering the symmetric flame tip never changes, consequently the case clearly illustrates that quantities other than the flame speed stoichiometry influence flame response. Note that when  $Z_f = 1/2$ , the maxima of temperature and reactivity lie on the line  $Z = Z_f$ . There is no lateral displacement of either the reactivity or the temperature maxima.

In section 3.3.3, we shall determine the extent to which freely propagating PF can describe the DF flame tip as  $C$  increases along a given  $Z = Z_f$  line from near-zero values to large values.

### 3.3.3 General Solution Features:

We form the difference of Eqs. (17) and (18) to find

$$\frac{Pe_{0q}}{Pe} - \frac{Pe_p}{Pe} = \frac{\eta_q}{r_q} + \frac{1}{\sqrt{\left(\frac{\partial Z}{\partial \eta}\right)_q^2 + \left(\frac{\partial Z}{\partial \xi}\right)_q^2 + 1}}, \quad (23)$$

from which we wish to deduce some features of the flame tip behavior. We examine two limiting cases, one for flame tips very far from the exit plane, the other for flame tips very near to the exit plane.

In the first case, the general solution for  $Z(\xi, \eta)$  from Eq. (19) approaches the value  $Z = Z_\infty = (1 - \xi)/2$ . Hence, we write  $Z(\xi, \eta) = (1 - \xi)/2 - g(\xi, \eta)$ , where  $g(\xi, \eta)$  is the negative value of the summation in Eq. (19) and may be interpreted as a correction to the far-field profile given by  $Z_\infty$ . Function,  $g(\xi, \eta)$  vanishes as  $\eta$  approaches infinity. The nature of  $g$  and  $\partial g/\partial \xi$  is shown in Figure 28, which has been computed using the exact solution. The top figure shows the function  $g(\xi, \eta)$  for large  $\eta$  and the bottom figure shows the gradient  $\partial g/\partial \xi$  at large  $\eta$ . Clearly,  $g$  is an odd function of  $\xi$  about the  $\xi$ -axis, whereas  $\partial g/\partial \xi$  is even. From the figure we can also see that as  $\eta$  increases both  $g$  and  $\partial g/\partial \xi$  approach zero. The arrows in the figure show the direction of increasing  $\eta$ . Substitution into Eq. (23) gives, after neglecting cubic terms in  $g_\xi$  and  $g_\eta$ , the approximate result

$$\left(1 - \frac{\eta_q}{r_q}\right) - \left(\frac{Pe_P}{Pe} - \frac{Pe_{0q}}{Pe}\right) = \frac{2g_\eta^2}{1 + 2g_\xi + 2g_\eta^2} \quad (24)$$

Far from the lower wall,  $g_\xi$  is small and hence the right hand side of Eq. (8) is just  $2g_\eta^2/(1 + 2g_\eta^2)$ , which is positive. Also, if we are above point 't', we have  $Pe_{0q} \rightarrow Pe_P$  from below (and vice-versa if we are below point 't'). For the right hand side to be positive,  $Pe_{0q}$  should approach  $Pe_P$  faster than  $\xi_q$  approaches  $r_q$ . Hence, the quenching distance is a relatively more sensitive quantity than the flow direction into the flame tip,

which suggests that flame chemistry is more important than the details of the flow field near the flame tip, even when it is far from the cold surface. In other words, the precise orientation of the flow streamlines entering the flame tip, whether along the directions defining  $Pe_P$  or  $Pe_{0q}$ , is less important than the position at which quenching of the flame tip occurs. The latter may dictate the former, not vice-versa.

In the second limiting case, the flame tip is very close to the cold wall. When  $\xi$  and  $\eta$  approach zero, we can write Eq. (20) as  $Z_0 = 1/2 - (1/\pi) \text{atan}(\xi/\eta)$ . Near the surface, we write  $h(x,y)$  such that  $Z = Z_0 + h(\xi, \eta)$ , where  $h(\xi, \eta)$  is given by

$$h = \sum_{n=1}^{\infty} \frac{\sin n\pi\xi}{n\pi} \left( \exp\left(\left(\frac{Pe - \sqrt{Pe^2 + (2n\pi)^2}}{2}\right)\eta\right) - \exp(-n\pi\eta) \right), \quad (25)$$

which accounts for the correction to  $Z_0$  from the convective flow. This expression for

$$h(\xi, \eta) \text{ reduces to } h = (Pe/2) \sum_{n=1}^{\infty} (1/n\pi) \sin(n\pi\xi) \exp(-n\pi\eta) + O(Pe^2) \text{ as } Pe \rightarrow 0.$$

Using this, we can evaluate Eq. (23) to find

$$\frac{Pe_{0q}}{Pe} - \frac{Pe_P}{Pe} = \pi r_q h_\eta \sin\theta_q \cos\theta_q \left( 1 + \frac{h_\xi}{h_\eta} \tan\theta_q \right), \quad (26)$$

where the behavior of the derivatives of  $h$  is described in Table 1 (below). Consequently,  $h_\xi$  is an odd function of  $\xi$  whereas  $h_\eta$  is an even function of  $\xi$ . The second term in parentheses is always negative but should be smaller than unity since we expect  $Pe_{0q} > Pe_P$  close to the cold wall, see Figure 26. We note also that the product  $h_\eta \cos\theta_q$  is always zero or positive.

Very close to the exit plane, it is obvious from Eq. (25) that once again the flame

chemistry dictates the solution. The flame chemistry dictates through  $r_q$ . The differences between  $Pe_{0q}$  and  $Pe_p$  follow from considerations of flow field and therefore are of secondary importance compared to flame chemistry. We note, in agreement with the first limiting case, that we can solve for  $Pe_p/Pe$  at point 'q' once  $Z(\xi, \eta)$  is known. Hence intersections of the loci of constant  $Pe_p/Pe$  and  $Z = Z_f$  can be obtained.

Table 4: Behavior of  $h_\xi$  and  $h_\eta$

|                     |              |              |                                |
|---------------------|--------------|--------------|--------------------------------|
| $\tan \theta_q > 0$ | $Z_\eta > 0$ | $h_\eta > 0$ | $0 < \theta < \frac{\pi}{2}$   |
| $\tan \theta_q < 0$ | $Z_\eta < 0$ | $h_\eta < 0$ | $\frac{\pi}{2} < \theta < \pi$ |
|                     | $Z_\xi < 0$  | $h_\xi < 0$  | $-1 < \xi < 0$                 |
|                     | $Z_\xi < 0$  | $h_\xi < 0$  | $0 < \xi < 1$                  |

### 3.3.4 Flame Speed Comparison

In this section, the component of flow velocity entering the triple point is compared with the adiabatic premixed flame speed. The point 'q' is obtained by means of a numerical solution of the model shown in Figure 23. This numerical code gives the mixture fraction, fuel and oxidizer mass fractions, temperature and the reactivity field for the entire domain. The point of maximum reactivity provides the location of point 'q'. Once this is known, the flame speed  $Pe_p/Pe$  can be calculated using the numerical solution for the  $Z$ -

field. The adiabatic premixed flame speed is given by,

$$Pe_{pf} = a \sqrt{\frac{D_a}{\beta^3}} \quad (27)$$

where  $a$  is an  $O(1)$  constant generally taken to be 2.

A numerical experiment was conducted to compare the two quantities. The value of  $\beta$  was kept fixed at a value of 8 and the Damköhler number was increased from a minimum value of 1000 to a maximum value of about 30,000. Physically, this amounts to changing only the pre-exponential factor  $A$  in our one-step reaction. The results are shown in Figure 29. This comparison was repeated for different values of  $Z_f$ . From Figure 29 there exists a linear correlation between the adiabatic and kinematic flame speed, until a limiting Damköhler number is reached. The correlation breaks down thereafter since  $Pe_p/Pe$  approaches a constant value. In this range, there is no longer a single value of  $Pe_p$  for a given PF speed. Figure 30 also shows the quench radii for the corresponding Damköhler numbers (or the PF speed values). When the value of  $C$  is low, which corresponds to a large quench radius, the adiabatic PF speed and the kinematic flame speed are proportional to one another. When  $C$  is large, the quench radius is small and the correlation breaks down. When the above procedure was repeated for different  $Z_f$ , it was seen that the range of Damköhler numbers for which the correlation holds decreases as the flame moves away from the symmetric flame configuration.

An empirical expression for the PF speed with heat losses has been discussed in [16] and [17], and can be written in terms of our dimensionless variables as

$$\frac{Pe_{loss}}{Pe_{pf}} = \exp\left[\frac{-\beta(1-\tau_f)}{2(1-\alpha(1-\tau_f))}\right], \quad (28)$$

where  $\tau_f$  is the temperature at the point of maximum reactivity. We determined that there was **no** correlation between the velocity obtained using Eq. (28) and  $Pe_p$ . This might be due to the empirical nature of the above expression.

We note an important feature of attached flames. The bottom figure in Figure 31 shows that when the flame is close to the wall, the PF arc on the side closest to the lower wall of the triple flame aligns itself perpendicular to the opposing flow. This does not happen when the flame is well-lifted, see the top figure in Figure 31. Our preceding analysis breaks down when this happens because the value of  $Pe_p$ , which is based on the mixture fraction contours, does not represent the propagation velocity of a diffusion flame tip. A more exact velocity may be one that is based on the alignment toward the oncoming flow of the appropriate PF reactivity contours.

### 3.4 Discussion and Conclusions

The stoichiometric PF postulate for diffusion flame tips near cold chemically inert surfaces has been examined using the model problem of Figure 23. Our examination shows that the component of flow velocity into the quench point correlates with the adiabatic PF speed when the flame is well-lifted or weakly attached. When the flame quenches closer to the cold wall, the flame response is quite complicated. This can be attributed to the realignment of the PF arc in a direction perpendicular to the opposing flow.

A reinterpretation of these results in terms of section 3.3 is possible. For the lifted

flame, the details of the flow direction are less important than the chemical response, as discussed below Eq. (24). Here, we may justifiably employ the flow velocity in the plane of the DF at its tip  $Pe_p$ . This conclusion is in agreement with most previous results for “free” flames [13] to [15] and [20] to [22], although in these studies no detailed study of this question is made: it is assumed a priori that the relevant flow is  $Pe_p$ . Such assumptions have also been made in [23] and [24], which deal with flame holding. For the attached flame closed to the cold wall, however, the situation differs. In accordance with section 3.3, the flame chemistry is more important to flame survival than the details of the flow direction. However, the flow direction is important and our results suggest that it is not the flow along the DF axis,  $Pe_p$ , but rather the flow  $Pe$  into the PF arc closest to the cold surface that is physically relevant. Hence, the attachment seems to occur through the influence of the near-wall PF arc. For  $0 < Z_f < 1/2$ , this is the oxidizer side PF arc, whereas for  $1/2 < Z_f < 1$  the fuel-side PF arc controls flame-tip attachment.

This conclusion has implications for real-flame attachment, where the flame chemistry occurs over many steps and where differences in the diffusivities of the various species - including radicals like H, OH, etc. - strongly influence the flame response. The overall stoichiometry  $\phi$  will specify the attachment PF, whether on the fuel or oxidizer side. The chemistry of a fuel-rich PF differs from the chemistry of a fuel lean PF, however. Thus, the Lewis numbers of different constituents (say  $Le_H$  for the rich PF and  $Le_{OH}$  for the lean PF) will assume prominence, depending on the side which attaches to the structure.\* Consequently DF tip attachment will be a complicated process dictated by global stoichiometry, flame chemistry, heat losses and mass diffusion of the controlling radicals and principal

species. For an accurate description, the heat losses cannot be fictitious. Radiative losses from the flame zone can be accounted for by a gas-phase loss term [25], although the importance of this quantity in comparison with losses from the cold surface is not obvious. Finally, our examination of two previous theories of flame attachment, which propose a stoichiometric mixture at flame tip with a common value of the fuel mass fraction, suggests that this hypothesis is not strictly true. Large percentage variations may occur in the species mass fractions near the flame tip, rendering the specification of some constant, universal value  $Y_F^+$  (as in [15]) quite suspect. Consequently, flame attachment is a more subtle mechanism than simple stoichiometric PF attachment, and further study of the flame structure near the quenching tip is warranted

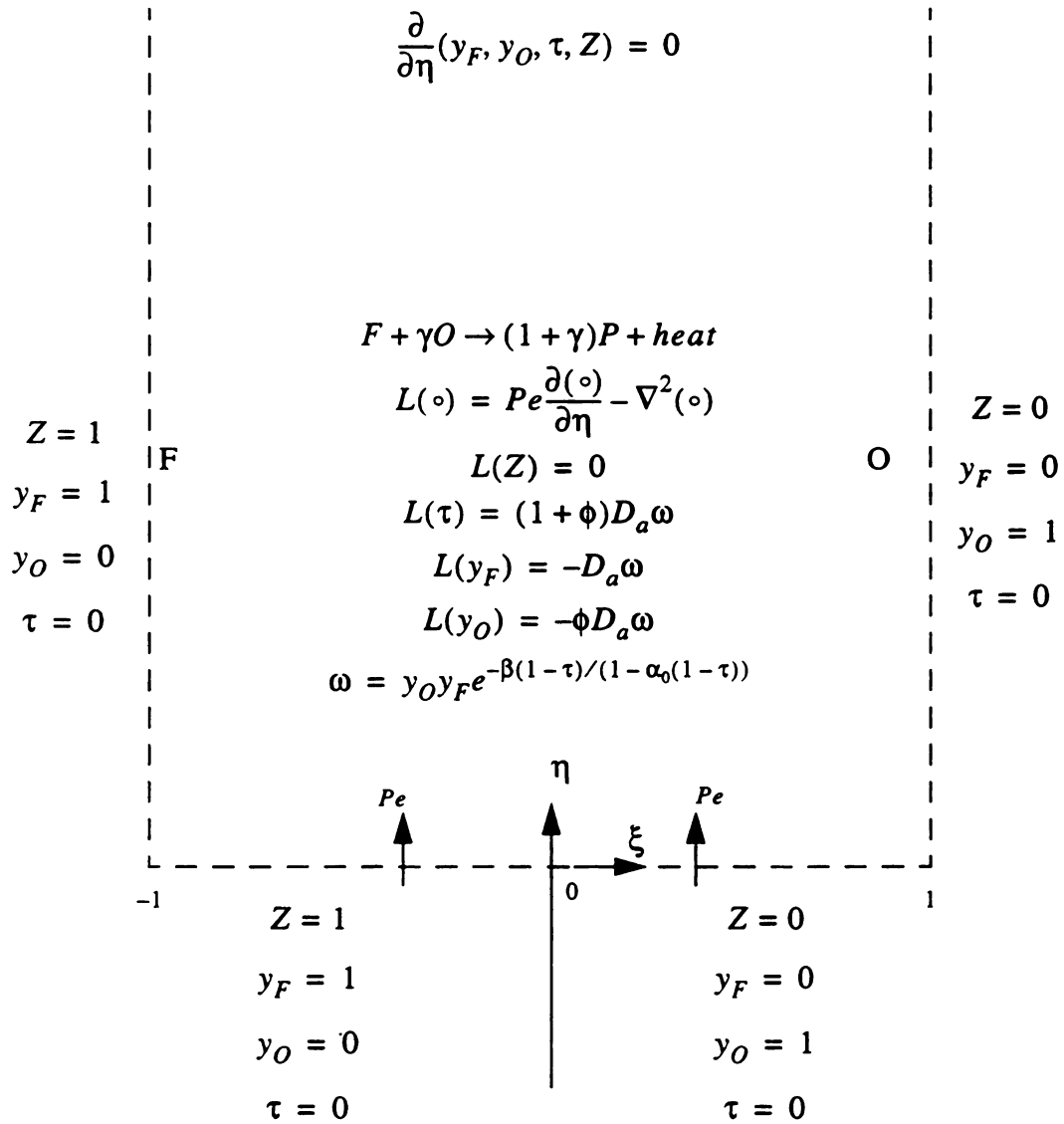


Figure 23 - Model with the infinitesimal divider (Model B)

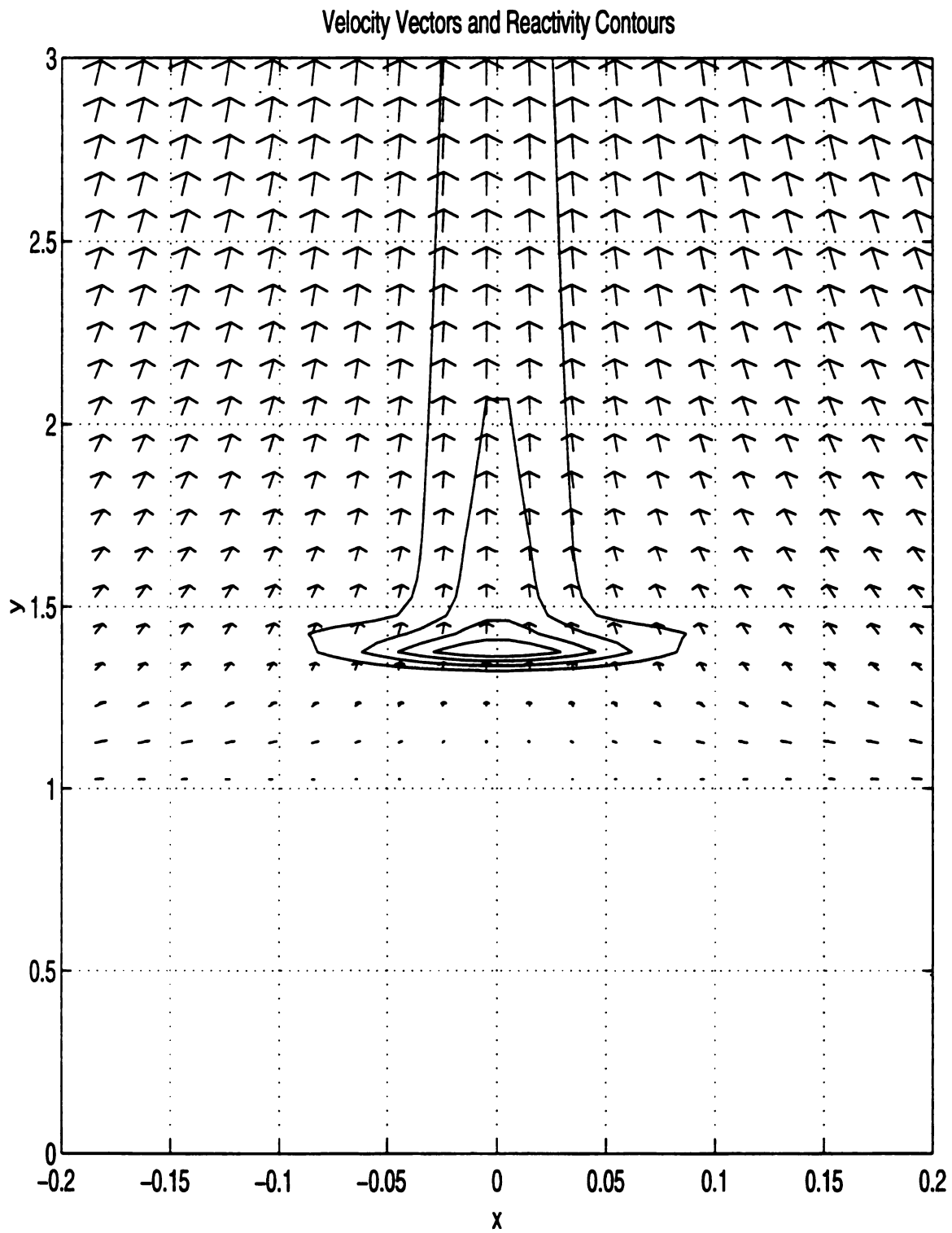


Figure 24 - The velocity vectors near the flame tip

**Figure 25 - Definitions of flame shape parameters**

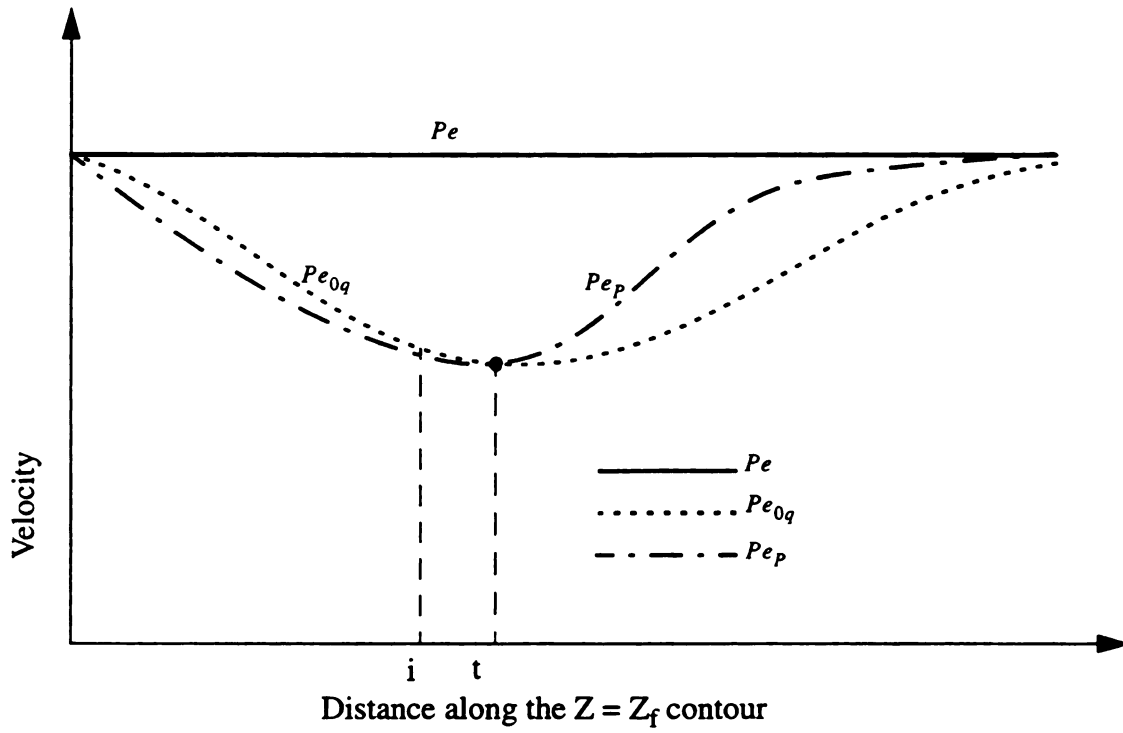


Figure 26 - Behavior of  $Pe_p$ ,  $Pe$  and  $Pe_{0q}$  along a  $Z = Z_f$  contour

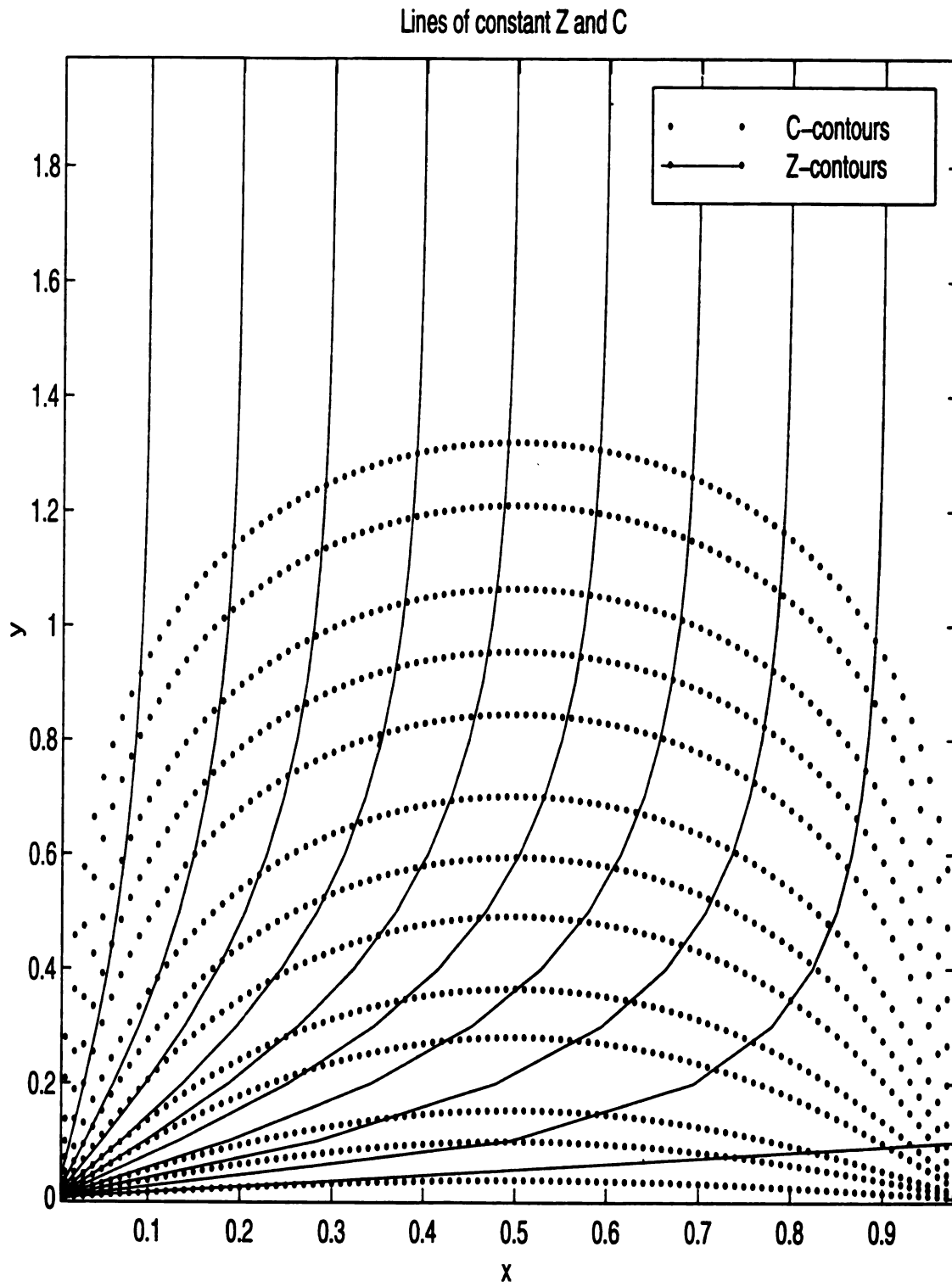


Figure 27 - Lines of constant Z and constant  $Pe_P$

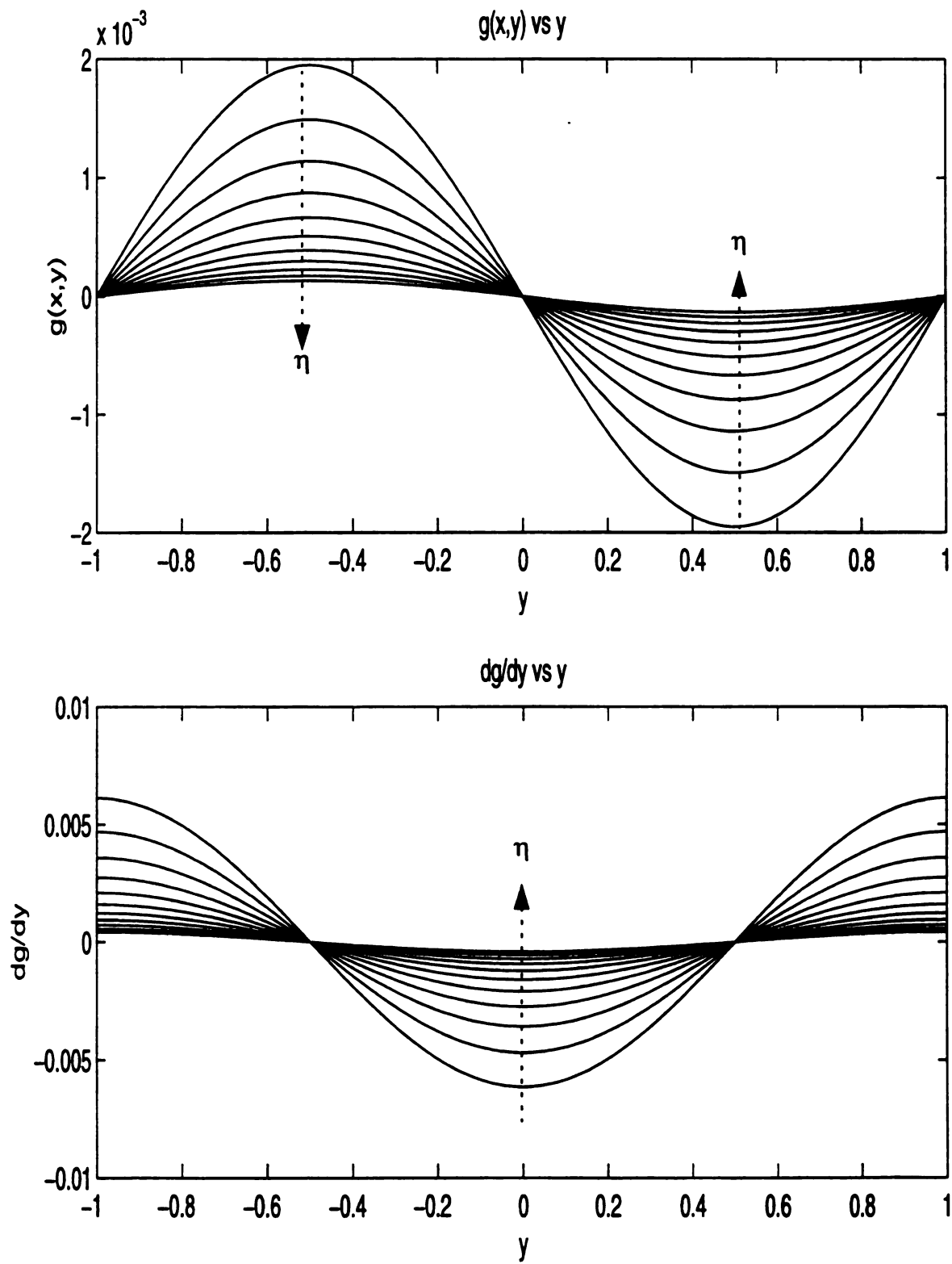


Figure 28 - Variation of  $g$  and  $dg/d\eta$  with  $\xi$

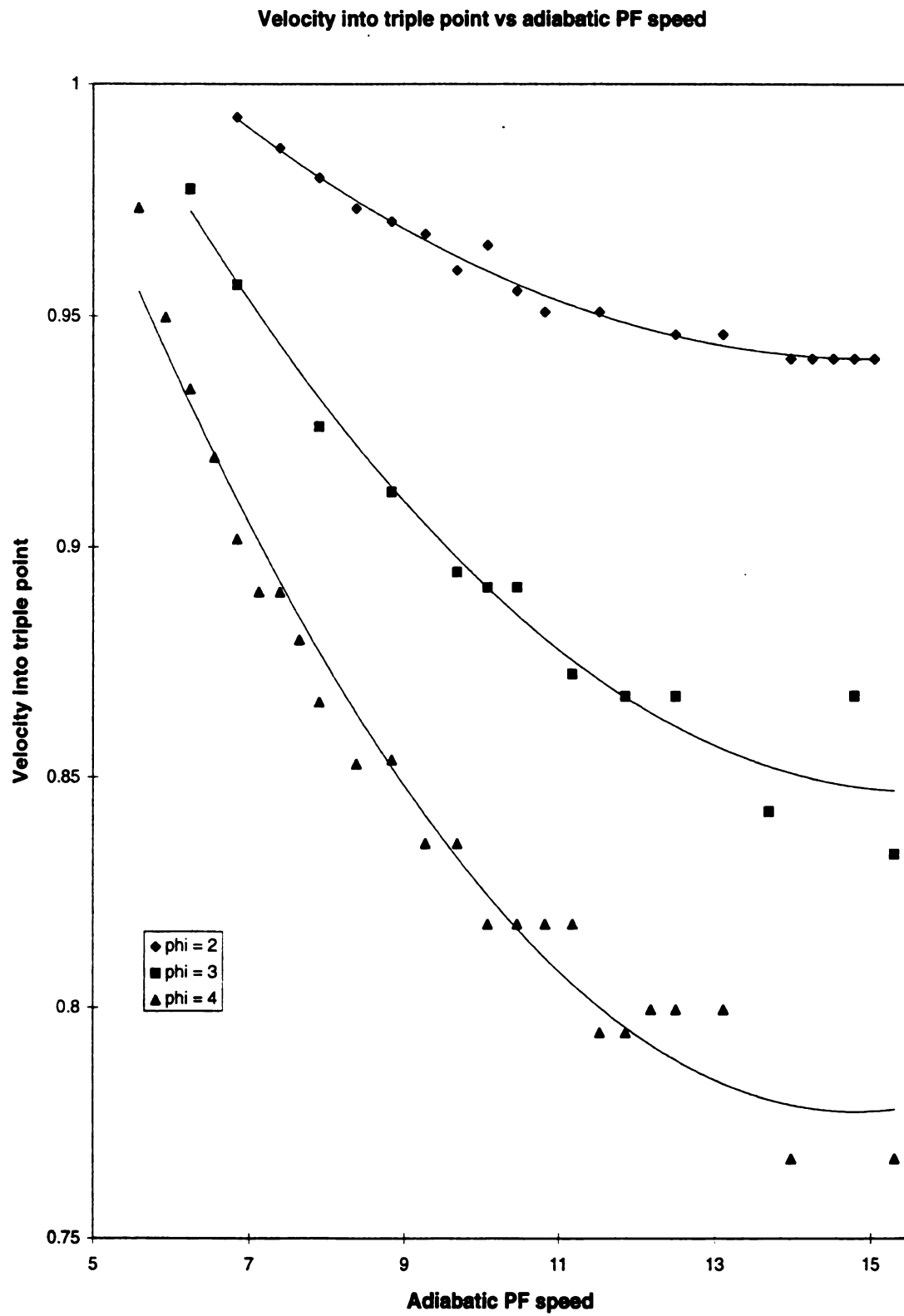


Figure 29 - Flow velocity  $Pe_p$  vs adiabatic PF speed  $Pe_{PF}$

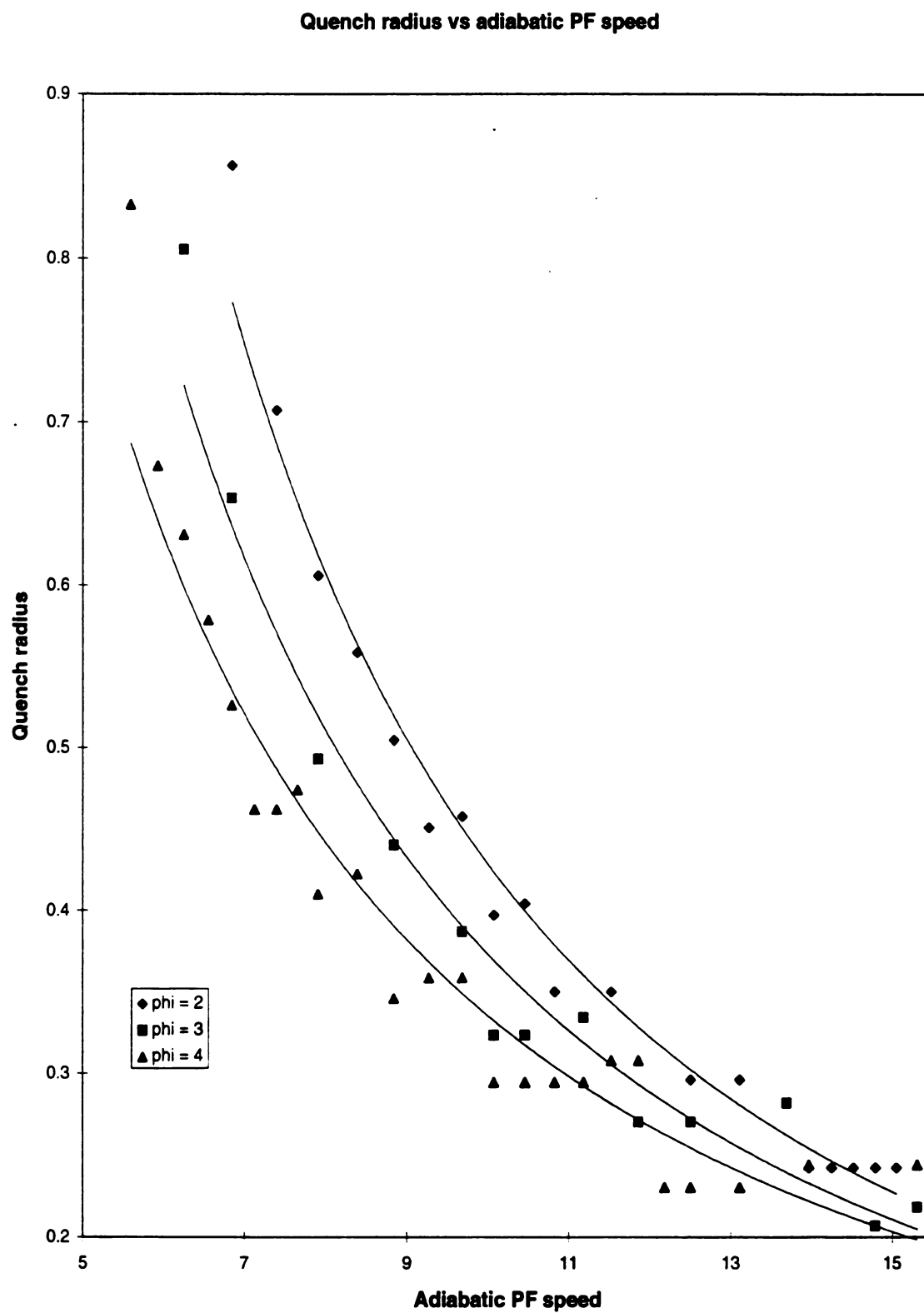


Figure 30 - Quench radius vs adiabatic PF speed  $Pe_{PF}$

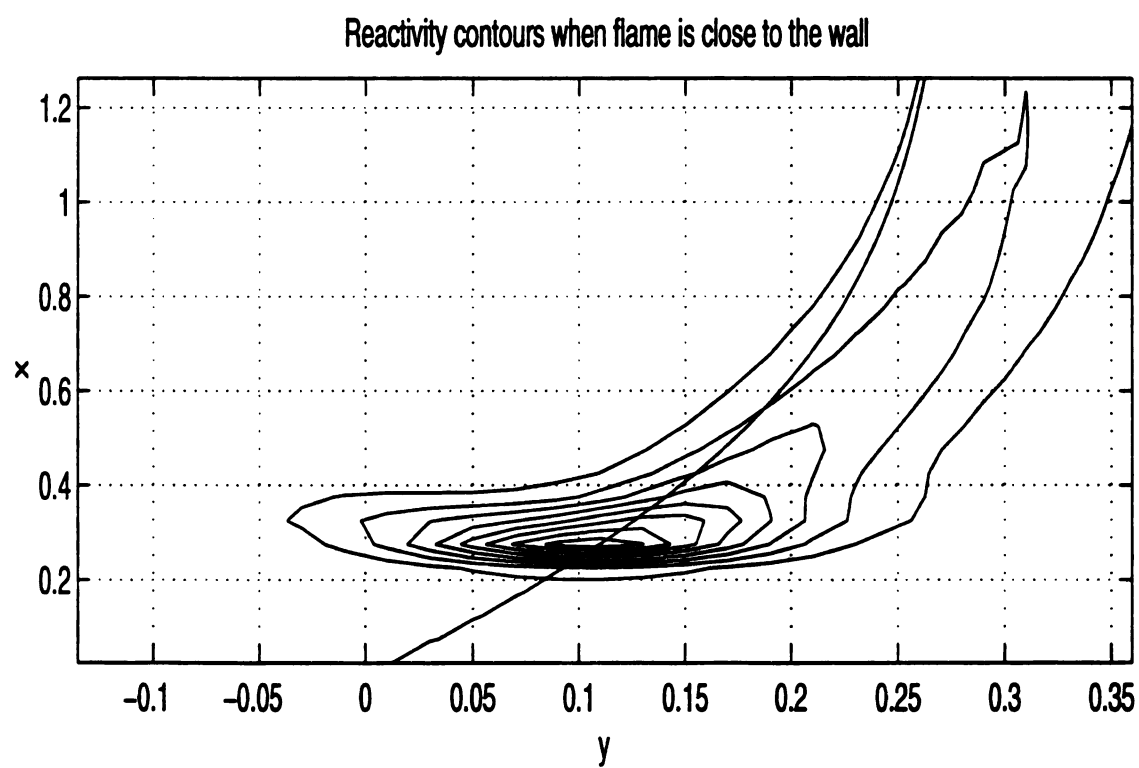
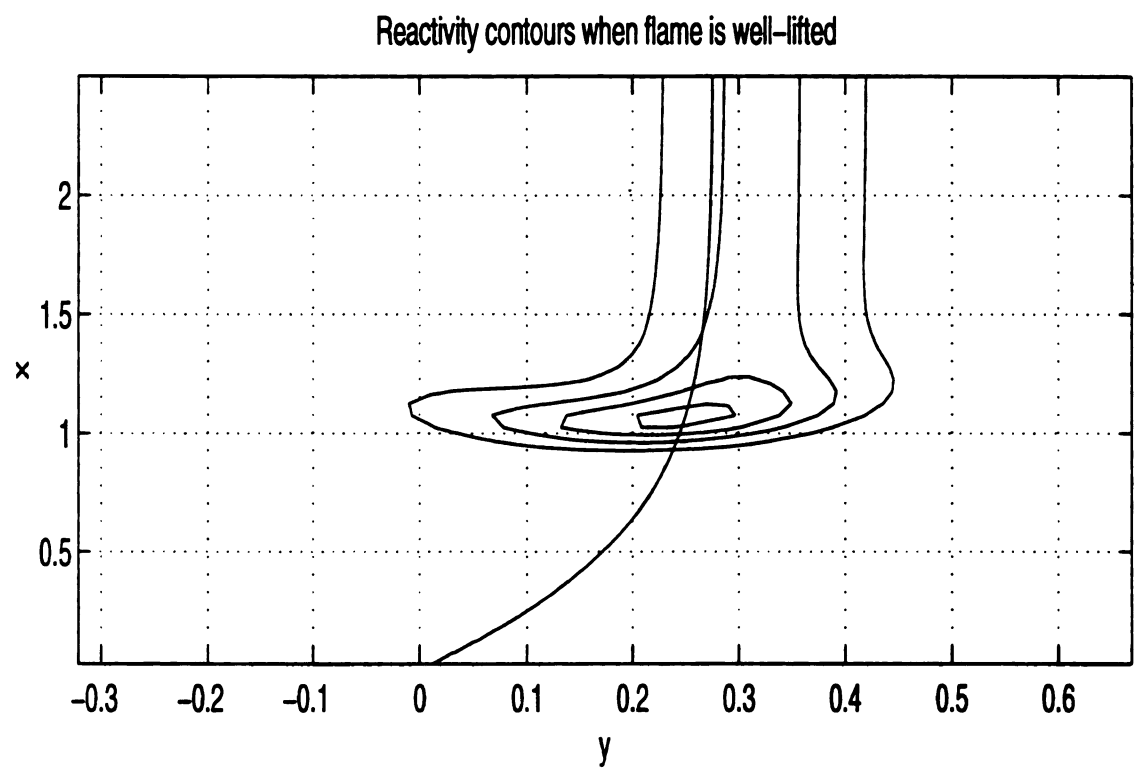


Figure 31 - Reactivity contours for two values of quench radius

## CHAPTER IV

### Heat Flux Distribution Along the Surface Beneath the Flame Tip

#### 4.1 Introduction

Triple flames may occur near the leading edge of a flame spreading over a solid or a liquid fuel. The study of flame spread over solid and liquid fuels has been analyzed by a number of researchers. A review of flame spread over solid fuels is given by Wichman [27]. The earlier researchers generally neglected the existence of the triple flame region by assuming that the vaporizing temperature of the solid fuel is greater than the ignition temperature. These models lead to flames that touch the fuel surface since there is no “cold wall” to quench the flame. In addition, the heat flux is of boundary layer form, with an  $x^{-1/2}$  singularity at the tip of the flame (i.e. at the attachment point). The heat flux obtained with a Burke-Schumann infinite-rate analysis is shown in Figure 32. The results of the numerical code is also shown in the above figure. The dashed lines represent the results of the numerical code while the continuous lines represent the theoretical heat flux. It can be seen that there is a significant difference at the center, where the heat flux approaches infinity. The figure also shows that the agreement is better when the value of  $\beta$  in the numerical code is increased. The theoretical heat flux was multiplied by a factor for comparing the two results. Thus this analysis precludes the calculation of realistic heat fluxes and also the existence of triple flames. This afore-mentioned vaporization tempera-

ture assumption will not be made here since it is generally believed that the triple flame region is very important for the flame spread process. Since the flame spreads by conducting heat upstream, and also to the fuel, the knowledge of the heat flux distribution along the solid fuel will be of fundamental importance in understanding the process of flame spread.

In this chapter, a flame spread model problem will be analyzed. The objective is to examine the region near the flame tip and to calculate the heat flux to the solid fuel. For this purpose, a simplified model problem, which has pseudo-exact solutions, will be formulated. From this pseudo-exact solution, the heat flux to the solid fuel can be calculated. Section 4.2 briefly explains the mathematical model of a typical flame spread problem, which will form the basis of the simplified model that will be discussed in section 4.3. The exact solution to this model will be discussed in section 4.4. This is followed by the analysis of the dependence of these parameters in section 4.5 and section 4.6. Section 4.7 discusses the conclusions of this study.

## 4.2 Flame Spread Model

A mathematical model of the opposed flow flame spread is shown in Figure 33. Oxidizer (or air) flows from left to right over the fuel surface. Under favourable conditions, the solid fuel vaporizes or gasifies at a surface temperature  $T_v$  and mixes with the oxidizer above establishing a spreading diffusion flame. This process can be modeled using species and energy conservation equations for the gas phase and the energy equation for the solid phase [2]. These are:

Gas phase;

$$(U_f + u(y)) \frac{\partial Y_i}{\partial x} = D_g \nabla^2 Y_i - \frac{v_i \omega}{\rho_g}, \quad i = O, F, \quad (29)$$

$$(U_f + u(y)) \frac{\partial T_g}{\partial x} = \alpha_g \nabla^2 T_g + \frac{q \omega}{\rho_g c_{pg}}, \quad (30)$$

where the reactivity  $\omega$  is given by

$$\omega = A_g \rho_g Y_O^m Y_F^n e^{-\frac{E}{RT}}. \quad (31)$$

Solid phase;

$$U_f \frac{\partial T_s}{\partial x} = \alpha_s \nabla^2 T_s. \quad (32)$$

The boundary conditions at the four outer surfaces are shown in Figure 33. At the fuel-oxidizer interface, the boundary conditions are complicated. We shall assume that the flame “attaches” at a distance ‘ $l$ ’ upstream of the vaporizing fuel. That is, the flame contour can be extrapolated along an arc to a terminus located at the surface of the fuel. Thus three distinct regions can be identified. The region upstream of the spreading flame is denoted by  $v_1$ . The region  $v_2$  lies between the attachment point and the point at which the fuel starts to vaporize and  $v_3$  is the fuel vaporizing region. On surface  $v_1$  the fuel and oxidizer mass fraction gradients will be zero since there is no vaporization or absorption respectively. Also, the heat flux from the gas equals the heat flux into the solid (NOTE: The fuel and gas transverse coordinates point in opposite directions). These conditions can be expressed as follows:

Surface  $v_1$ ;

$$\frac{\partial Y_O}{\partial y_s} = \frac{\partial Y_F}{\partial y_g} = \lambda_g \frac{\partial T_g}{\partial y_g} + \lambda_s \frac{\partial T_s}{\partial y_s} = 0 \text{ and } T_g = T_s. \quad (33)$$

On surface  $v_2$  all the above conditions will hold. We shall also assume that there is no oxidizer on the fuel surface. These conditions can be expressed as :

Surface  $v_2$ ;

$$\frac{\partial Y_O}{\partial y_s} = \frac{\partial Y_F}{\partial y_g} = \lambda_g \frac{\partial T_g}{\partial y_g} + \lambda_s \frac{\partial T_s}{\partial y_s} = 0 ; T_g = T_s ; Y_O = 0. \quad (34)$$

On the vaporizing fuel surface  $v_3$ , the fuel is convected and diffused normally from the surface and the net heat flux at the surface should be equal to the latent heat of vaporization. These conditions are given below.

Surface  $v_3$ ;

$$\frac{\partial Y_O}{\partial y_g} = 0 ; \frac{\partial Y_F}{\partial y_g} = \frac{m}{\rho_g D_g} (Y_F - 1) ; mL_v = \lambda_g \frac{\partial T_g}{\partial y_g} + \lambda_s \frac{\partial T_s}{\partial y_s} ; T_g = T_s = T_v. \quad (35)$$

The continuity of the variables at the surface will be enforced by matching their values at the surface.

The above model problem can be expressed in a normalized form. The mass fractions shall be normalized by their “reservoir” values and the gas and solid phase temperatures can be normalized by the greatest temperature difference. Thus the non-dimensional gas and solid phase temperatures are  $\tau = (T_g - T_\infty)/(T_f - T_\infty)$  and  $\sigma = (T_s - T_\infty)/(T_f - T_\infty)$ . The normalized equations and boundary conditions are shown in Figure 34.

The above model problem is difficult to solve analytically. But the equations are sim-

pler for the conserved scalar  $Z$ . Assuming Oseen-flow, with  $\varepsilon + u(\eta) = 1$ , the resulting equations for the  $Z$  field can be solved using the Wiener - Hopf method. The solution for  $Z$  is given below :

$$\frac{Z}{Z_f} = \frac{\operatorname{erfc}\left(\left(\frac{\sqrt{\xi^2 + \eta^2} - \xi}{2}\right)^{1/2}\right)}{\operatorname{erfc}(\sqrt{l})}. \quad (36)$$

Using the above equation, the lines of constant  $Z$  can be plotted. The above solution for  $Z$  will be used in formulating a simplified problem that will be used in the analysis that follows.

### 4.3 Flame Tip Model

From equation (36) we see that an expansion for the mixture fraction field near the flame tip near  $\xi = -l$ ,  $\eta = 0$  produces an expansion of the form

$$Z = Z_f + \text{constant} \cdot \xi + O(\xi^2, \eta^2, \xi\eta). \quad (37)$$

Hence, near the flame tip, the mixture fraction varies only linearly with the spatial coordinate  $\xi$  (not  $\eta$ , which enters in the higher order terms). For this reason, we feel justified in introducing a model problem in which the flame tip (and indeed, the rest of the flame also) is perpendicular to the fuel surface beneath. In addition, and consistent with this view, we suppose that the boundary conditions on either lateral side of this small region are also independent of  $\eta$ . These conditions are imposed at locations  $\xi = -l \pm \delta$  (see Figure 34). Thus, we replace the upstream and downstream boundary condition planes with fictitious “walls” located at  $\xi/\delta = -1$  and  $\xi/\delta = 1$ , where  $\delta$  is the characteristic size of the

domain in which  $Z = Z(\xi)$ . In the lowest approximation these walls can permit only the separate influx of fuel or oxidizer, not both simultaneously. Also in the simplest case, we eliminate from the governing equations the convective term. Hence under the supposition that near the surface the streamwise velocities are very small, the equations for the conserved scalars reduce to Laplace's equation.

We now specify the boundary conditions on this open rectangular domain. On the lower surface, the gradients of the fuel and oxidizer mass fractions will be zero, which follows directly from the model problem of equations (29) to (36). For the energy equation, instead of imposing the condition given earlier, we eliminate the solid phase problem by assuming that the non-dimensional gasification temperature  $\tau_v$  is negligible. Since we assume that the fuel does not vaporize in the region of interest, the temperature along the fuel surface should be significantly lower than the vaporization temperature. But  $\tau_v$  itself is around 0.15 which is small compared with unity. Hence we employ  $\tau = 0$  along the entire lower surface.

On the left and right side "walls", we shall impose reservoir conditions for the oxidizer and fuel mass fractions, assuming that the "wall" placed on the left side will consume any fuel that comes into contact with it and the "wall" on the right will consume any oxidizer it touches. This is again not exactly true for the physical problem, but it also introduces a level of simplicity into the analysis that renders it tractable. Since  $\delta$  is the characteristic diffusion length, we can assume that the left and right side walls are far from the point of heat release to justify a  $\tau = 0$  boundary condition on the left and right side "walls". This condition obviously ensures consistency with the temperature boundary condition on the

lower surface.

From the exact solution for  $Z$ , we can see, as discussed above, that the lines of constant  $Z$  intersect the fuel surface at right angles. Hence, inside the region of interest, we can assume that the lines of constant  $Z$  will almost be vertical. Thus, in the vertical “far field”, we suppose that the  $\eta$ -dependance is still suppressed and that our model problem becomes one-dimensional leading to the stipulation that the gradients in the  $y$  direction approach zero. Hence, we suppose that as  $\eta \rightarrow \infty$  the gradients of the variables in the  $\eta$ -direction will vanish because there is no longer a region of flame-tip quenching. With the above conditions, the model that we shall use to examine the heat flux will be as shown in Figure 35.

#### 4.4 Exact Solution and Heat Flux Calculations

To obtain the heat flux at the wall, the temperature field should be solved. Since this is a non-linear equation, we shall obtain the heat flux using the enthalpy field, whose gradient at the fuel surface will be equal to the temperature gradient since  $H = \tau + y_O + y_F - 1$  and  $\partial H / \partial \eta = \partial \tau / \partial \eta$  at the fuel surface. The model for the excess enthalpy field is shown in Figure 36. In this figure, the coordinate system has been moved to the bottom left corner of the domain by a translation. Let us also define the length of the divider as ‘L’ for purposes of generality. This model can be solved by separation of variables IF the distribution of the excess enthalpy function or the distribution of its gradient at the exit plane is known. Generally,  $H = f(\xi)$  is not known, since  $y_O$  and  $y_F$  are not specified. Neither is

$\partial H / \partial \eta$  known, since  $\partial \tau / \partial \eta$  is not specified. However, we can also solve for  $H$  IF we consider that the vertical  $H$ -gradient is known. Consequently, this leads to two types of model problems, the Dirichlet and Neumann problems. The exact solution for the Dirichlet problem is,

$$H = \sum_{n=1}^{\infty} a_n e^{-\frac{n\pi\eta}{L}} \sin\left(\frac{n\pi\xi}{L}\right), \quad (38)$$

where

$$a_n = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{n\pi\xi}{L}\right) d\xi. \quad (39)$$

Similarly, if the gradient of  $H$  is known, the coefficients will be given by

$$a_n = -\frac{2}{n\pi} \int_0^L g(x) \sin\left(\frac{n\pi\xi}{L}\right) dx \quad (40)$$

In the above equations, for purposes of generality, we have used  $L$  to represent the nondimensional length of the domain. This is different from the physical length  $\hat{L}$  used in CHAPTER I. It is obvious that  $f(\xi)$  or  $g(\xi)$  should be known to obtain the solution  $H(\xi, \eta)$  to the enthalpy field. Since we consider the heat flux at the surface as our principal unknown, we shall use the Dirichlet problem.

The excess enthalpy function  $H$  is related to the primary variables as  $H = \tau + y_O + y_F - 1$ . The boundary condition  $f(\xi)$  can be obtained only by solving the non-linear mass fraction and temperature fields. Since theoretical solutions are not available, numerical results must be used to obtain  $f(\xi)$ . By theoretical considerations it is clear that the function  $f(\xi)$  is dependent on stoichiometry, Damköhler number (or the pre-exponential factor), Zeldovich number and the enthalpy ratio. The form of  $f(\xi)$  for a

symmetric flame ( $\phi = 1$ ) from a numerical solution is shown in Figure 37 for fixed values of the Damköhler number (or the pre-exponential factor), enthalpy ratio  $\alpha$ , and Zeldovich number  $\beta$ , since these are the only four non-dimensional parameters. As can be seen in this figure, for a symmetric flame, the function  $f(\xi)$  can be approximated very closely as

$$H(\xi, 0) = H_c \sin\left(\frac{n\pi\xi}{L}\right) = f(\xi), \quad (41)$$

where  $H_c$  is the amplitude of  $f(\xi)$ , which will depend on the parameters introduced into the non-linear reactivity term. When equation (41) is substituted into equation (39), the solution for the H field is obtained as

$$H = H_c \sin\left(\frac{\pi\xi}{L}\right) e^{-\frac{\pi\eta}{L}}. \quad (42)$$

The comparison between the above equation (42) and the numerical result is shown in Figure 38. We note that the approximation is very good. The maximum error is within 4 percent. However, equation (42) is as accurate as the boundary condition. The heat flux to the cold wall is given by

$$q = \left. \frac{\partial \tau}{\partial \eta} \right|_{\eta=0} = \left. \frac{\partial H}{\partial \eta} \right|_{\eta=0}. \quad (43)$$

When equation (42) is substituted into the above equation, the expression for the heat flux to the cold wall is,

$$q = -\frac{\pi}{L} H_c \sin\left(\frac{\pi\xi}{L}\right). \quad (44)$$

The comparison between equation (44) and the numerical value of the heat flux is shown

in Figure 39. The error in the approximation is plotted in Figure 40. We can see that the maximum error about four percent.

For an unsymmetric flame, however, the functional form of  $f(\xi)$  is complicated (see Figure 41). It was found from the numerical results that  $f(\xi)$  could be expressed in general as a function of two unknowns. These are  $H_c$  and a characteristic length  $s$ , which are both functions of the parameters  $\alpha$ ,  $\beta$ ,  $D_a$  and  $Z_f$  in the reactivity term. Physically  $s$  is the distance from the origin to the minimum of  $f(\xi)$ . Thus  $H(\xi, 0) = f(\xi)$  can be approximately expressed as,

$$H = \left\{ \begin{array}{l} H_c \sin\left(\frac{\pi\xi}{2s}\right) \quad 0 < \xi < s \\ H_c \sin\left(\frac{\pi(\xi - 2s + L)}{2(L-s)}\right) \quad s < \xi < L \end{array} \right\} \quad (45)$$

The agreement between this approximation and the numerical result is shown in Figure 41. We see that it is an excellent prescription. When this  $f(\xi)$  is substituted into equation (39), the solution  $H(\xi, \eta)$  can be expressed an infinite summation,

$$H = \sum_{n=1}^{\infty} \frac{8n}{\pi} H_c \cos\left(\frac{n\pi s}{L}\right) \left( \frac{s^2}{L^2 - (2ns)^2} - \frac{(L-s)^2}{L^2 - (2n(L-s))^2} \right) e^{-\frac{n\pi\eta}{L}} \sin\left(\frac{n\pi\xi}{L}\right), \quad (46)$$

The above series is convergent as  $n \rightarrow \infty$ , since

$$\lim_{n \rightarrow \infty} n \left( \frac{s^2}{L^2 - (2ns)^2} - \frac{(L-s)^2}{L^2 - (2n(L-s))^2} \right) = 0. \quad (47)$$

The comparison between equation (46) and the numerical result is shown in Figure 42.

For the symmetric flame,  $s = 0$ . Using equation (46) the expression for the heat flux to the fuel becomes

$$q = \sum_{n=1}^{\infty} -\frac{8n^2}{L} H_c \cos\left(\frac{n\pi s}{L}\right) \left( \frac{s^2}{L^2 - (2ns)^2} - \frac{(L-s)^2}{L^2 - (2n(L-s))^2} \right) \sin\left(\frac{n\pi \xi}{L}\right). \quad (48)$$

This series is also convergent, since

$$\lim_{n \rightarrow \infty} n^2 \left( \frac{s^2}{L^2 - (2ns)^2} - \frac{(L-s)^2}{L^2 - (2n(L-s))^2} \right) = 0. \quad (49)$$

Obviously,  $H_c$  and  $s$  should be known to calculate the heat flux completely. The agreement between the symmetric heat flux and the flux calculated using the numerical code is shown in Figure 39. The error in the approximation as seen from Figure 40 is less than ten percent. Since the expression for the heat flux is exact, the error is mainly in the approximation to the distribution of  $H$  at the surface. To visualize the form of the heat flux, equation (48) is plotted for fictitious values of  $H_c$  and  $s$  in Figure 45. In this figure the value of  $H_c$  was kept constant while the value of  $s$  was varied. From the figure we can see that the maximum flux transferred to the fuel surface depends upon  $s$ , which is the location of the maximum of  $f(\xi)$ . The dependance of  $H_c$  and  $s$  on the four basic parameters will be examined in the next section using the numerical code developed by B. Ramadan. This will enable to us to understand the dependance of the heat flux on the four parameters  $\alpha$ ,  $\beta$ ,  $D_a$  and  $Z_f$ .

## 4.5 $H_c$ Dependence

The minimum value of  $H(\xi, \eta)$  in the entire domain is represented by  $H_c$ . Since  $H(\xi, \eta)$  satisfies the Laplace equation, the minimum value should occur on the boundary.

The dependence of  $H$  on the four parameters occurs because of the boundary condition at  $\eta = 0$ , where it is coupled to the non-linear temperature and mass fraction fields. These parameters occur in the Arrhenius reaction rate term. However, five parameters occur in the reaction term, namely the enthalpy ratio  $\alpha$ , the normalized activation energy or Zeldovich number  $\beta$ , the stoichiometry  $\phi$  or  $Z_f$ , the Damkohler number  $D_a$ , and the pre-exponential factor  $P$ . Four of these parameters can be related by means of a single relation,

$$D_a = P e^{-\beta/\alpha}. \quad (50)$$

Thus, there are four independent parameters, which can be used to determine  $H_c$  and  $s$ . For our convenience, we shall choose these four parameters to be  $\alpha$ ,  $\beta$ ,  $\phi$  and  $P$ . Next, we shall analyze the dependence of  $H_c$  on these four parameters with the assistance of the numerical code.

Parameter  $\alpha = 1 - T_o/T_f$  is essentially the enthalpy ratio. It varies over a fairly narrow range. In most practical situations, we can neglect the dependence of  $H_c$  on  $\alpha$ . For examining the dependence of  $H_c$  and  $s$  on  $\alpha$ , we shall keep the other parameters constant and vary  $\alpha$  from a minimum value of 0.7 to a maximum value of 0.8. In our numerical code, the net effect of changing the value of  $\alpha$  alone is a change in the value of the pre-exponential factor. To remove this variation, the Damköhler number was also varied in such a manner that the variation in the pre-exponential factor is offset and the only parameter that changes is  $\alpha$ . In each case the value of  $H_c$  is calculated. The dependence of  $H_c$  on  $\alpha$  is shown in Figure 46. This relationship can be approximated by a linear relationship

of the form  $H_c = a\alpha + b$ . We refer the reader to Table 5 for values of  $a$  and  $b$ .

The normalized activation energy  $\beta$  usually varies from 6-10. Figure 47 shows the variation in  $H_c$  with  $\beta$ . In our numerical experiment, the other parameters were kept constant (this includes changing the value of  $D_a$  to keep the pre-exponential factor constant) and the value of  $\beta$  was varied from a minimum value of 7 to a maximum value of 9. In this range the relationship can also be approximated linearly as seen from Table 5.

The dependence of  $H_c$  on  $\phi$  is shown in Figure 48. For performing this test, the value of  $\phi$  was varied from a minimum value of 0.6 to a maximum value of 5 while the other parameters were kept constant. Difficulties with the convergence of the numerical code forced us to exclude the highly nonsymmetric configurations that result when  $\phi$  takes very low and very high values. In the range considered this relationship is best approximated by a logarithmic relationship shown in Table 5.

The variation of  $H_c$  with  $D_a$  is shown in Figure 49. Keeping the other parameters constant, the value of  $D_a$  was varied from a minimum of 8000 to a maximum of 20000. The relationship can be approximated as shown in Table 5. Our tests reveal that this relationship is valid even when values of  $D_a$  outside this range are considered.

Thus we have analyzed the dependence of  $H_c$  on the four parameters separately. It is possible to write a single expression that includes the dependence on all the four parameters as follows:

$$H_c(\alpha, \beta, \phi, D_a) = H_c(\alpha_0, \beta_0, \phi_0, D_{a0}) + \left(\frac{\partial H_c}{\partial \alpha}\right)_0(\alpha - \alpha_0) + \left(\frac{\partial H_c}{\partial \beta}\right)_0(\beta - \beta_0) \quad (51)$$

$$+ \left(\frac{\partial H_c}{\partial \phi}\right)_0(\phi - \phi_0) + \left(\frac{\partial H_c}{\partial D_a}\right)_0(\sqrt{D_a} - \sqrt{D_{a0}})$$

The values of  $\alpha_0$ ,  $\beta_0$ ,  $\phi_0$ , and  $D_{a0}$  have to be chosen in such a way that the intercept  $H_c(\alpha_0, \beta_0, \phi_0, D_{a0})$  is the same when we consider each of these separately. Our calculations show that one possible combination of the reference values would result in the following equation for the dependence of  $H_c$  on the four parameters:

$$H_c = -0.406 + 0.19(\beta - 7.86) - 1.27(\alpha - 0.8) - 2.21 \times 10^{-3}(\sqrt{D_a} - \sqrt{17338}) - 0.08(\phi - 4.83) \quad (52)$$

Table 5  $H_c$  Dependence

|                   |                                               |
|-------------------|-----------------------------------------------|
| $H_c$ vs $\alpha$ | $H_c = -1.27\alpha + 0.61$                    |
| $H_c$ vs $\beta$  | $H_c = 0.19\beta - 1.9$                       |
| $H_c$ vs $D_a$    | $H_c = -2.2 \times 10^{-3}\sqrt{D_a} - 0.115$ |
| $H_c$ vs $\phi$   | $H_c = -0.08 \ln \phi - 0.28$                 |

## 4.6 $s$ Dependence

As explained above,  $s$  is the distance from the origin to the plane at which the minimum of  $f(\xi)$  occurs. The location of this plane has some physical significance. At the exit plane the coupling function  $H$  is related to the other variables by the relation

$H = y_O + y_F - 1$  since  $\tau = 0$ . Differentiating this with respect to  $\xi$  gives

$$\frac{dH}{d\xi} = \frac{dy_O}{d\xi} + \frac{dy_F}{d\xi} = \frac{df}{d\xi} \quad (53)$$

From the coupling function  $Z$ , we obtain

$$(\phi + 1) \frac{dZ}{d\xi} = \phi \frac{dy_F}{d\xi} - \frac{dy_O}{d\xi} \quad (54)$$

When the exact solution for  $Z$  is substituted in the above equation,

$$\phi \frac{dy_F}{d\xi} - \frac{dy_O}{d\xi} = -\left(\frac{\phi + 1}{L}\right) \quad (55)$$

Solving equations (53) and (55) for  $dy_F/d\xi$  and  $dy_O/d\xi$ , we get

$$\frac{dy_F}{d\xi} = \frac{\frac{df}{d\xi}}{1 + \phi} - \frac{1}{L} \quad (56)$$

$$\frac{dy_O}{d\xi} = \frac{\phi}{\phi + 1} \frac{df}{d\xi} + \frac{1}{L} \quad (57)$$

At  $\xi = s$ , the value of  $H = H_c$  and  $dH/d\xi = 0$ . Thus the gradients of the fuel and oxidizer mass fractions become  $(dy_F/d\xi)_{\xi=s} = -1/L$ , and  $(dy_O/d\xi)_{\xi=s} = 1/L$ . The value of the gradient at  $\xi = s$  is thus equal to the gradients that would result if the flow is frozen. Thus the maximum heat flux occurs at a point where the gradients of the fuel and oxidizer mass fraction become equal to the frozen flow values. The gradients are also equal in magnitude. The numerical simulations also indicate that when  $\xi = s$ , the values of the fuel and oxidizer mass fractions are almost equal.

The value of  $s$  increases as the flame moves away from the symmetric configuration.

While the exact dependance of  $s$  on the parameters will be the subject of our analysis, we

note an interesting behavior with regard to the reactivity contours. Our numerical simulations show that as the flame moves away from the center, one of the arcs of the triple flame becomes more pronounced than the other.

Our objective is to analyze the dependence of  $s$  on the four basic parameters. This was done using the numerical code. The parameters were varied within the ranges specified in section 4.5. Unlike  $H_c$ ,  $s$  varies linearly with all the four parameters in the range considered. But we can expect a logarithmic dependence of  $s$  on  $\phi$  if the values of  $\phi$  close to zero were considered. This is shown in Figure 54, where the variation of  $s$  with  $\phi$  is plotted with the expected trendline assuming that  $s$  approaches zero as  $\phi$  approaches zero. The difficulty in obtaining numerical convergence for very low values of  $\phi$  forced us to adopt a linear relationship in the range considered. The curve-fit equations are shown in Table 6.

Table 6 Dependence of  $s$  on the four parameters

|                 |                         |
|-----------------|-------------------------|
| $s$ vs $\alpha$ | $s = 0.4\alpha + 0.78$  |
| $s$ vs $\beta$  | $s = -0.07\beta + 1.64$ |
| $s$ vs $D_a$    | $s = 3e-06 D_a + 1.05$  |
| $s$ vs $\phi$   | $s = 0.056\phi + 0.95$  |

We can also write a single expression relating  $s$  to the four basic parameters as follows.

$$s(\alpha, \beta, \phi, D_a) = s(\alpha_0, \beta_0, \phi_0, D_{a0}) + \left(\frac{\partial s}{\partial \alpha}\right)_0 (\alpha - \alpha_0) + \left(\frac{\partial s}{\partial \beta}\right)_0 (\beta - \beta_0) \\ + \left(\frac{\partial s}{\partial \phi}\right)_0 (\phi - \phi_0) + \left(\frac{\partial s}{\partial D_a}\right)_0 (D_a - D_{a0}). \quad (58)$$

Similar to the expression for  $H_c$  we can determine the reference values  $\alpha_0$ ,  $\beta_0$ ,  $\phi_0$  and  $D_{a0}$  such that the intercept has the same value when each parameter is considered separately. One such combination of the reference values results in the following equation:

$$s = 1.1 + 0.4(\alpha - 0.8) - 0.07(\beta - 7.7) + 3 \times 10^{-6}(D_a - 16666.7) + 0.056(\phi - 2.68). \quad (59)$$

While some equations form a good approximation even outside the range considered, it must be emphasized that the above equations, in general, are accurate only in the range indicated.

## 4.7 Conclusion

In this chapter we have analyzed a flame spread model with the objective of calculating the heat flux distribution to the solid fuel beneath the flame tip. Towards this objective a simple model problem has been formulated and the excess enthalpy field has been solved exactly. Our analysis shows that we can approximate the heat flux to the solid fuel by means of an infinite summation with the help of two parameters that depend on the enthalpy ratio, the normalized activation energy, the Damköhler number (or the pre-exponential factor) and the stoichiometry. Approximate expressions that correlate this dependence have been given. Our expression for heat flux shows that the magnitude of heat flux also depends on the location of maximum of  $f(\xi)$ . The larger is the value of  $s$ , the greater is the heat flux. The complete solution for the excess enthalpy field is also presented.

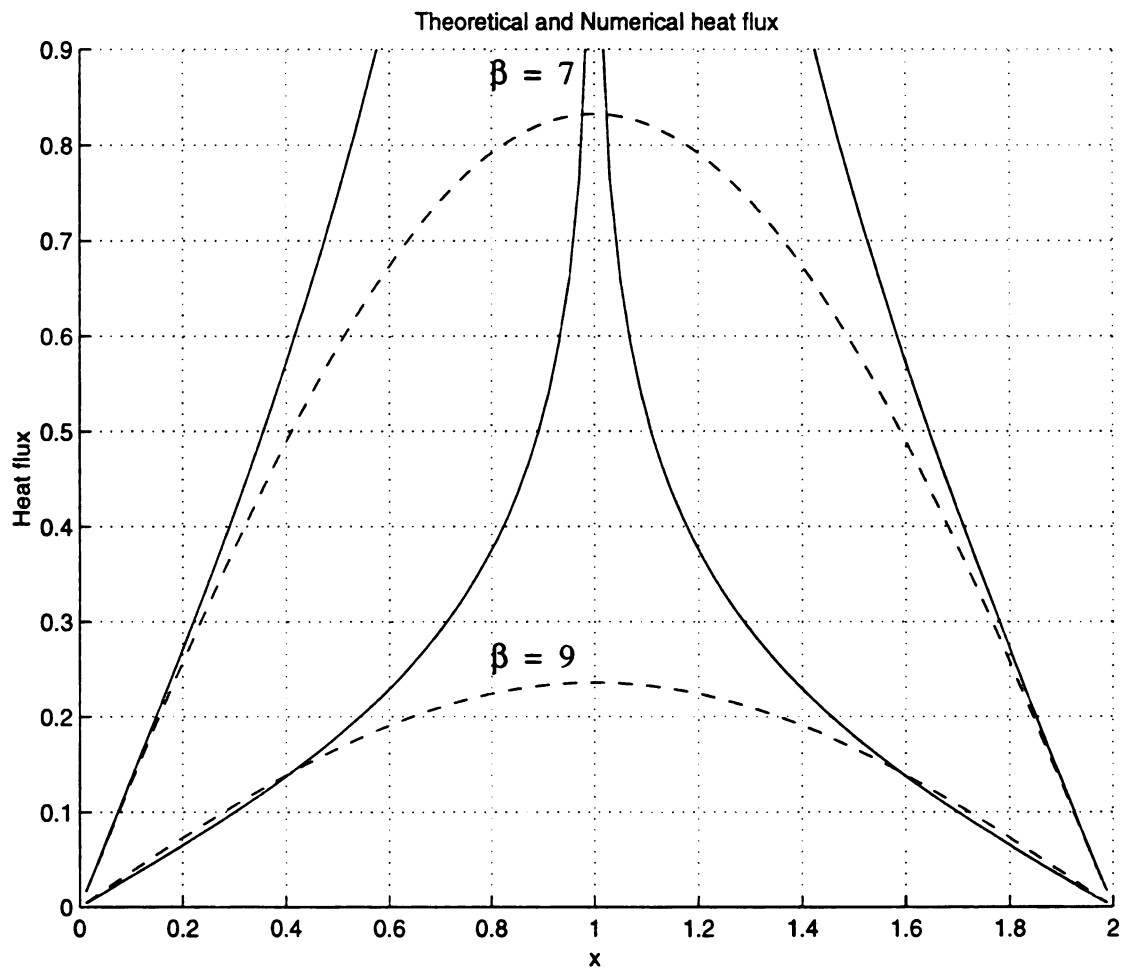


Figure 32 - Infinite and finite heat flux

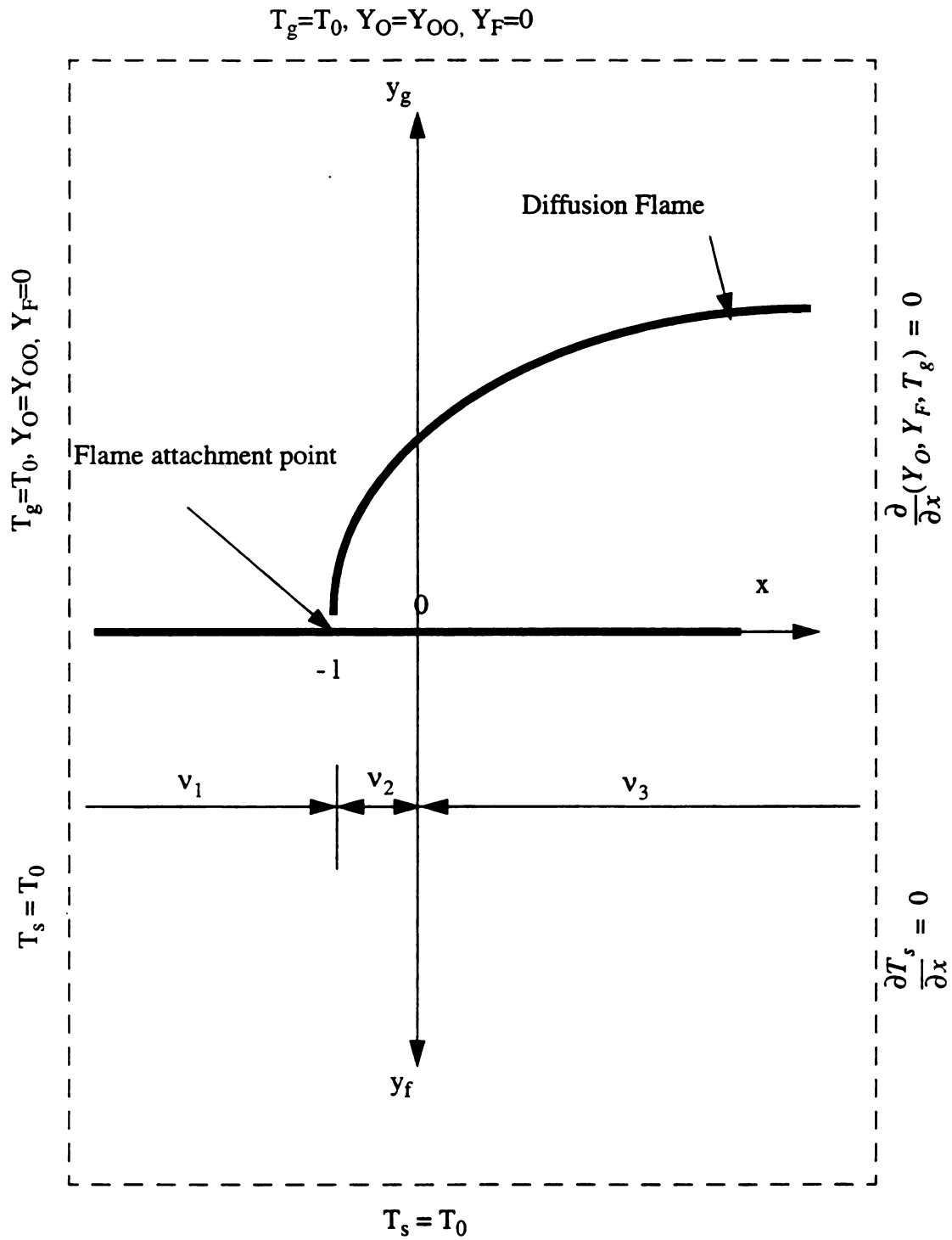


Figure 33 - Mathematical model of flame spread in physical variables



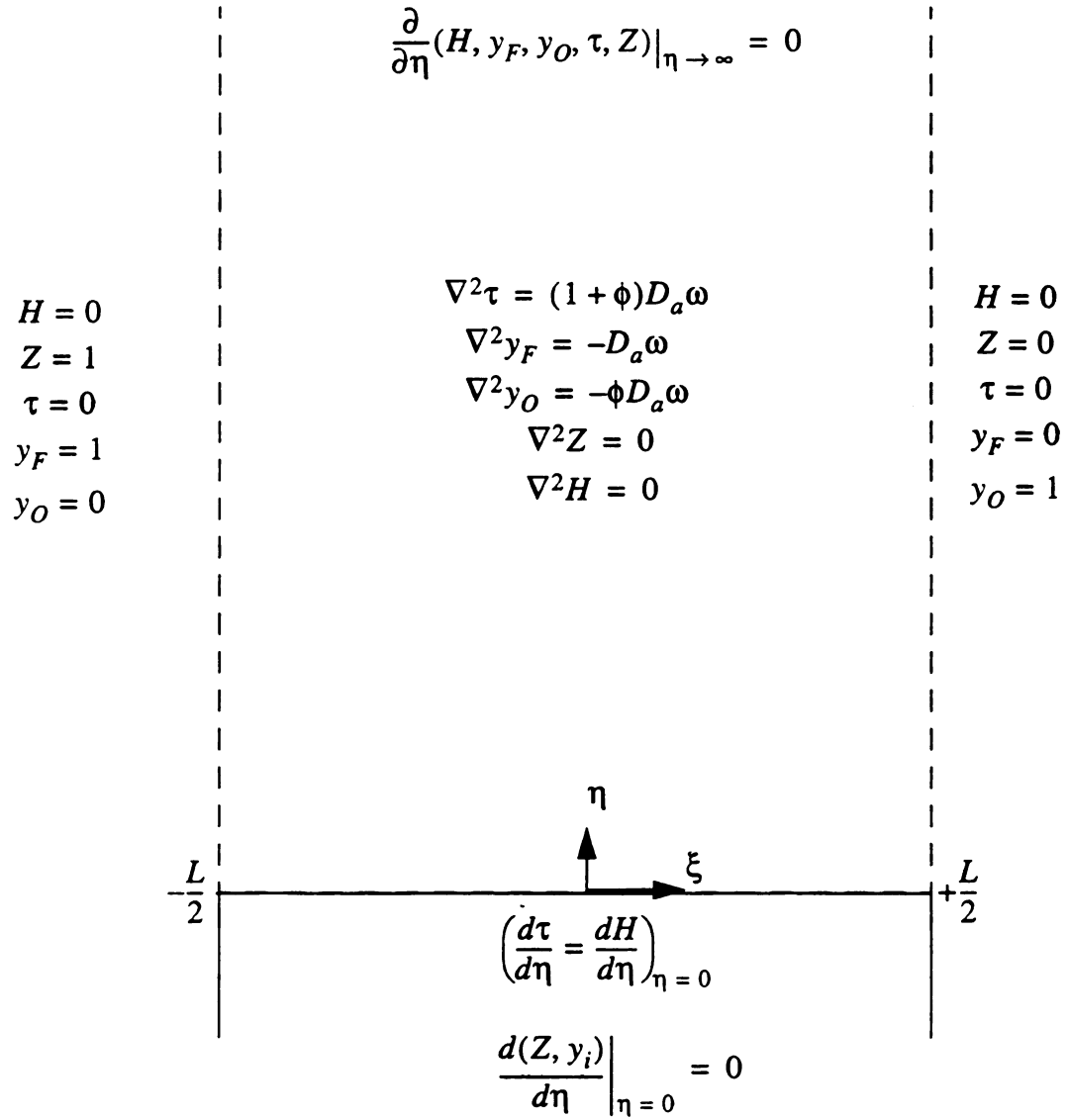


Figure 35 - Simplified model problem near the flame tip

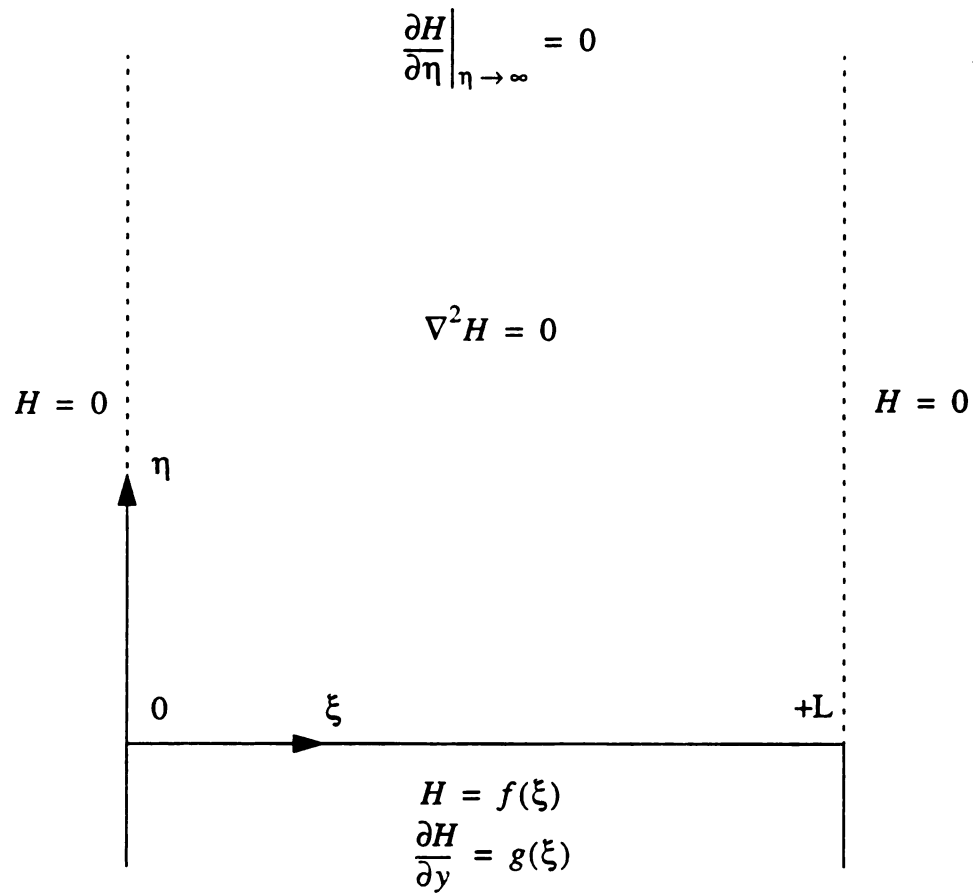


Figure 36 - Model for the excess enthalpy field

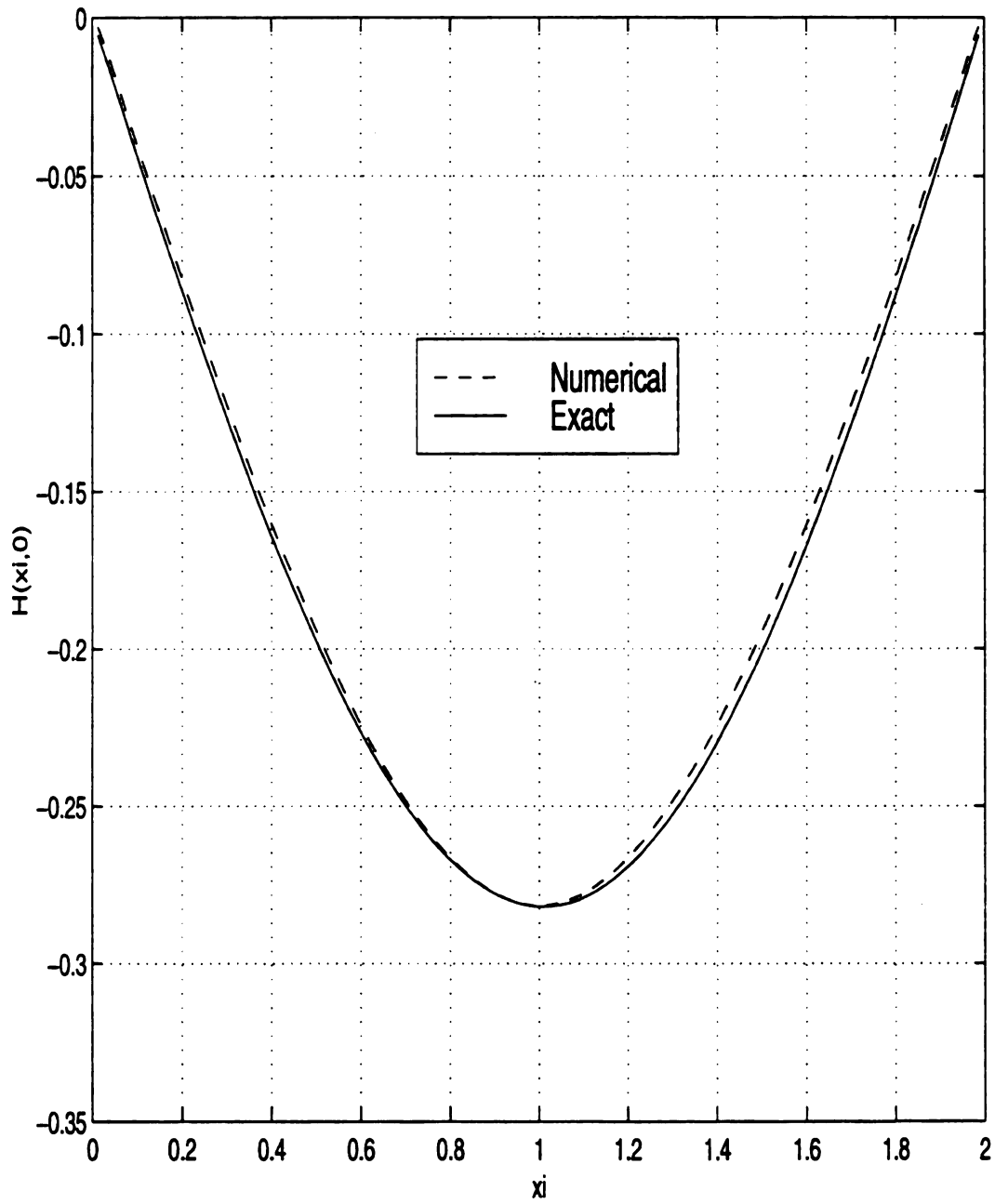


Figure 37 - Excess enthalpy distribution at the exit plane when  $\phi = 1$

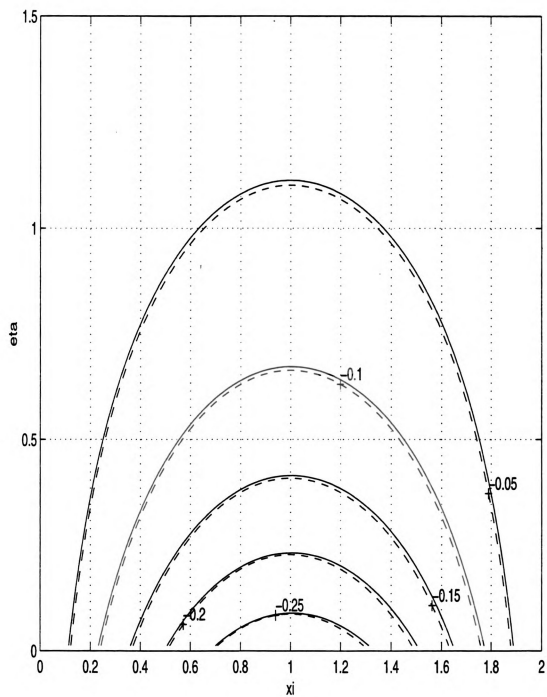


Figure 38 - Excess enthalpy contours when  $\phi = 1$

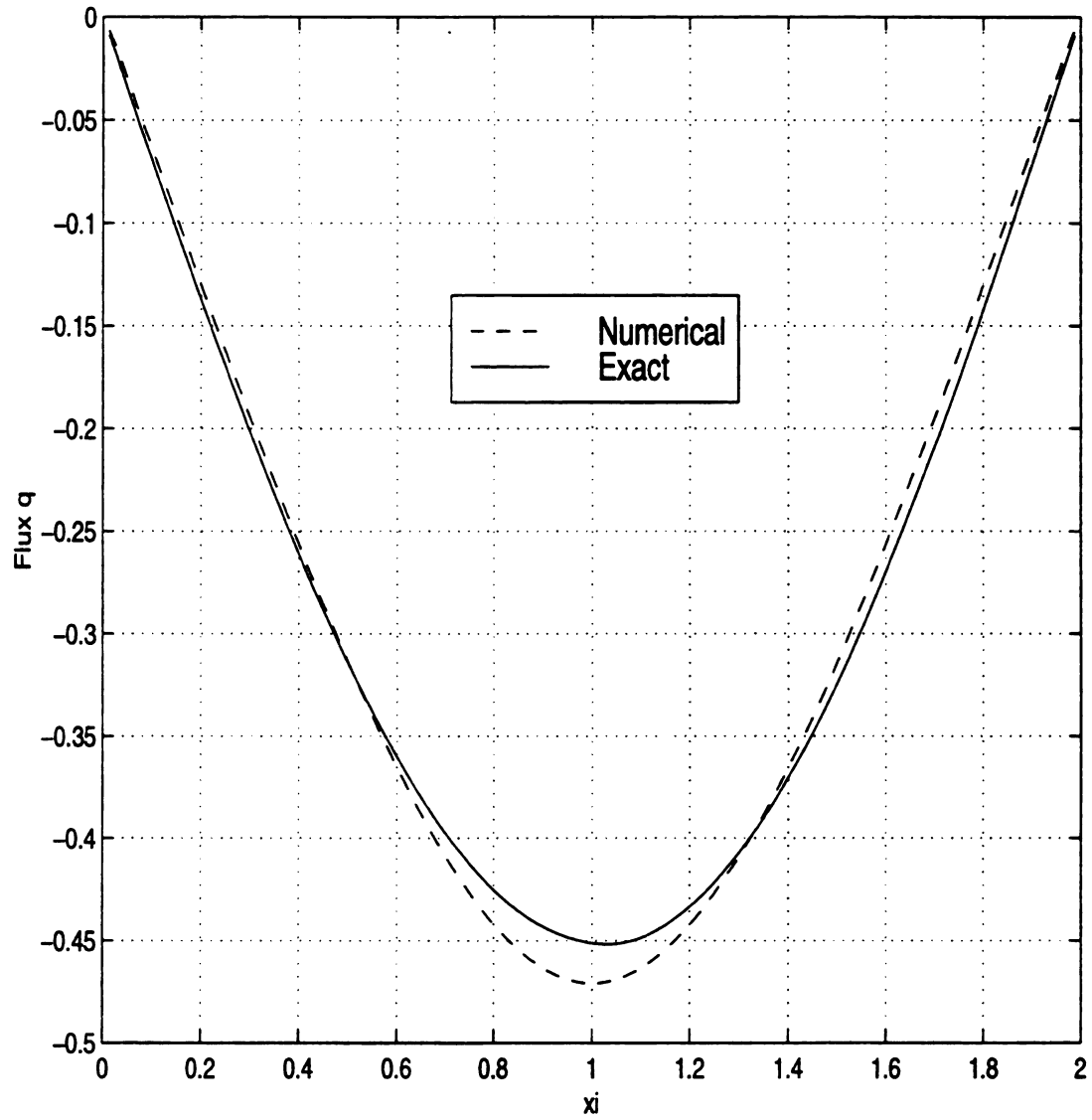


Figure 39 - Exact and numerical values of heat flux to when  $\phi = 1$

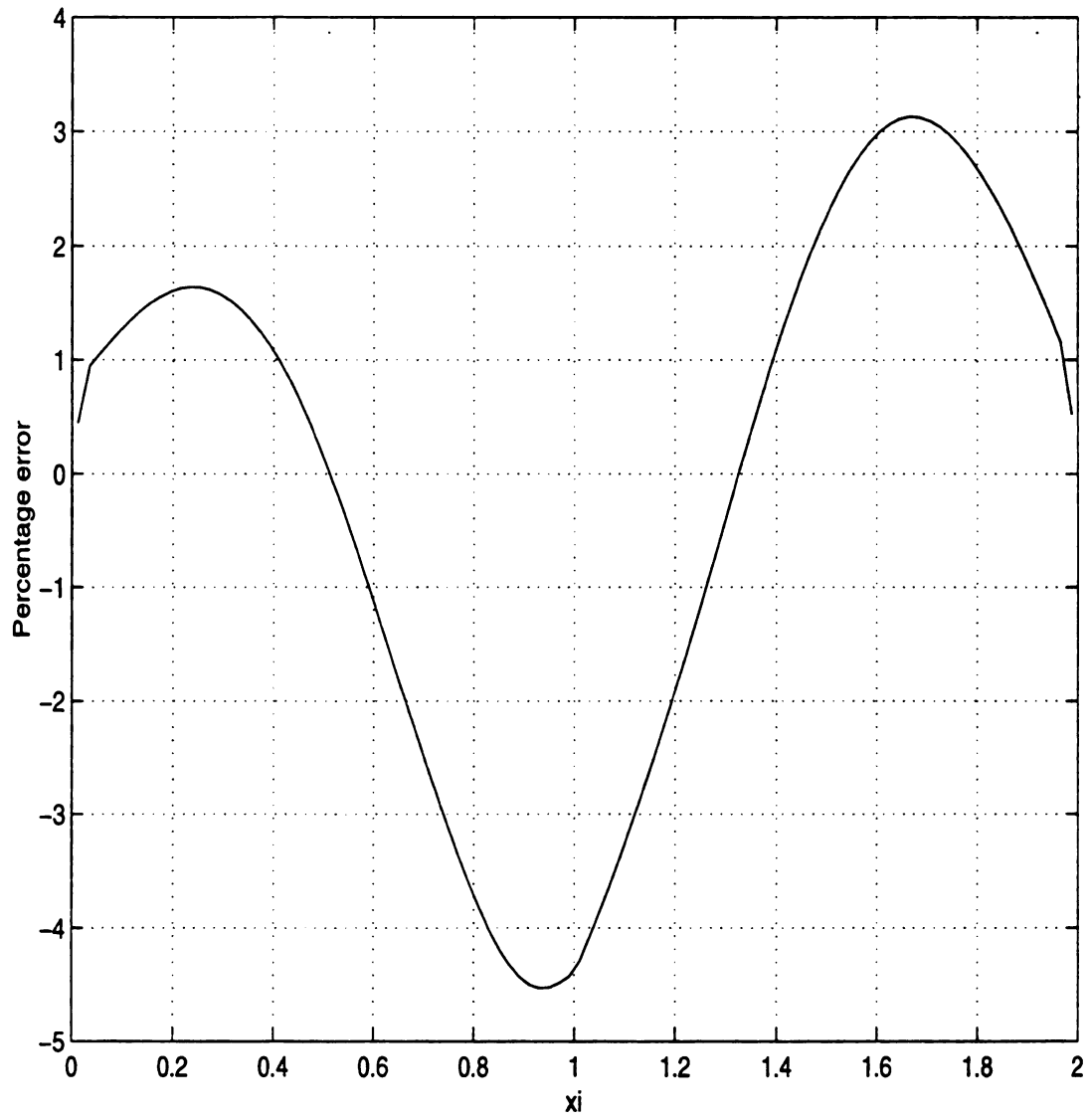


Figure 40 - Error in the approximation to the heat flux vs  $x$

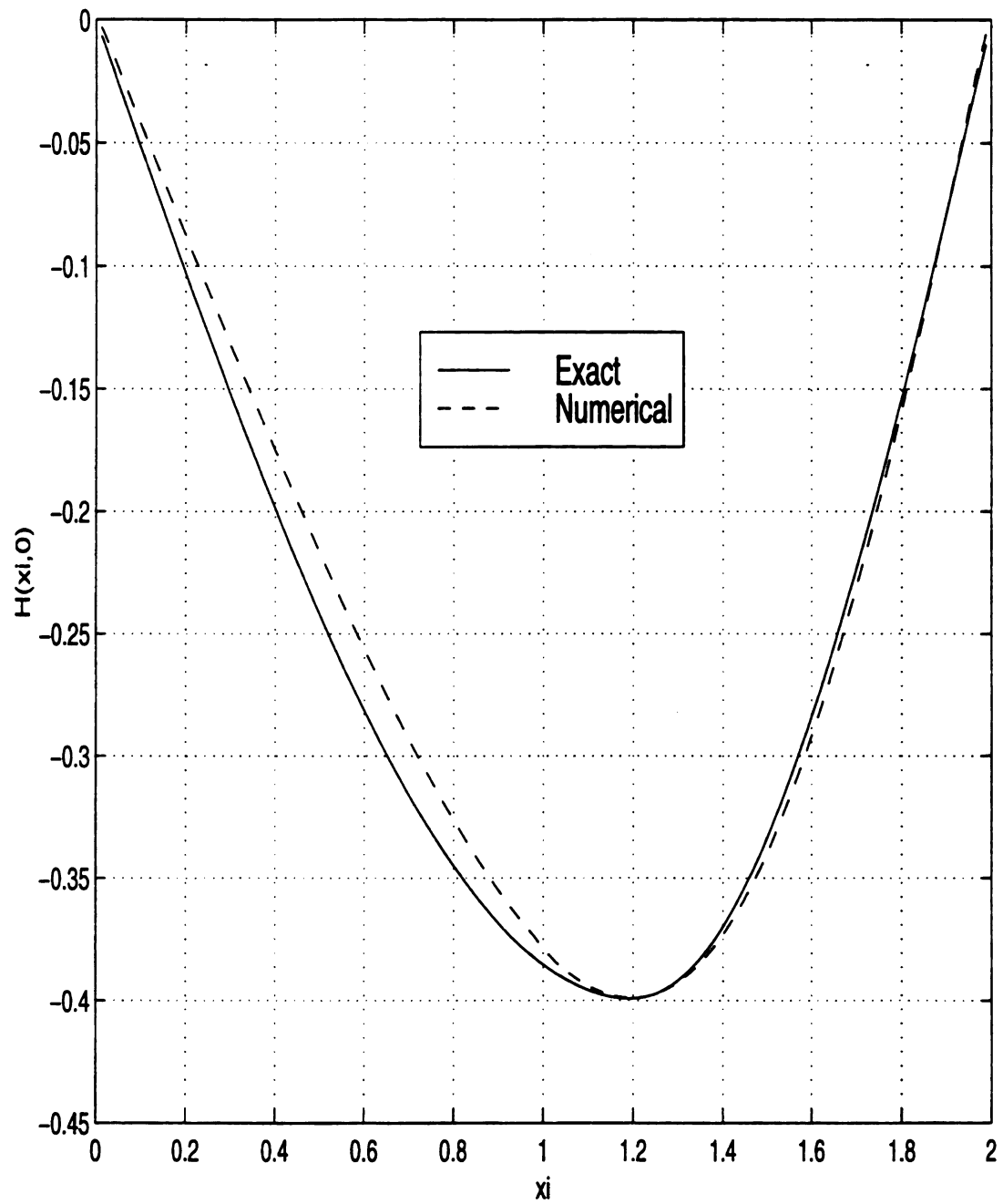


Figure 41 - Excess enthalpy distribution at the exit plane when  $\phi = 5$

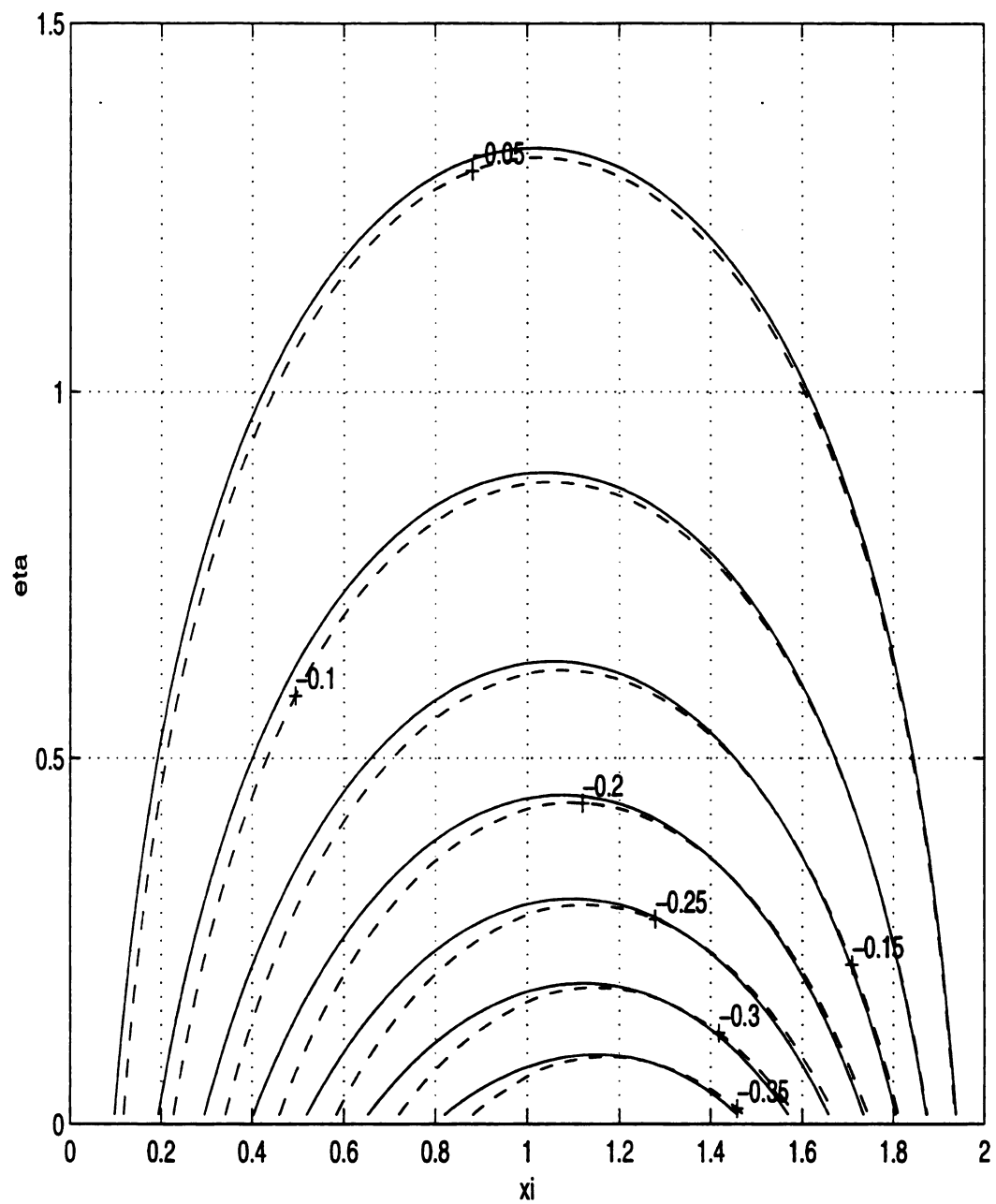


Figure 42 - Excess enthalpy contours when  $\phi = 5$

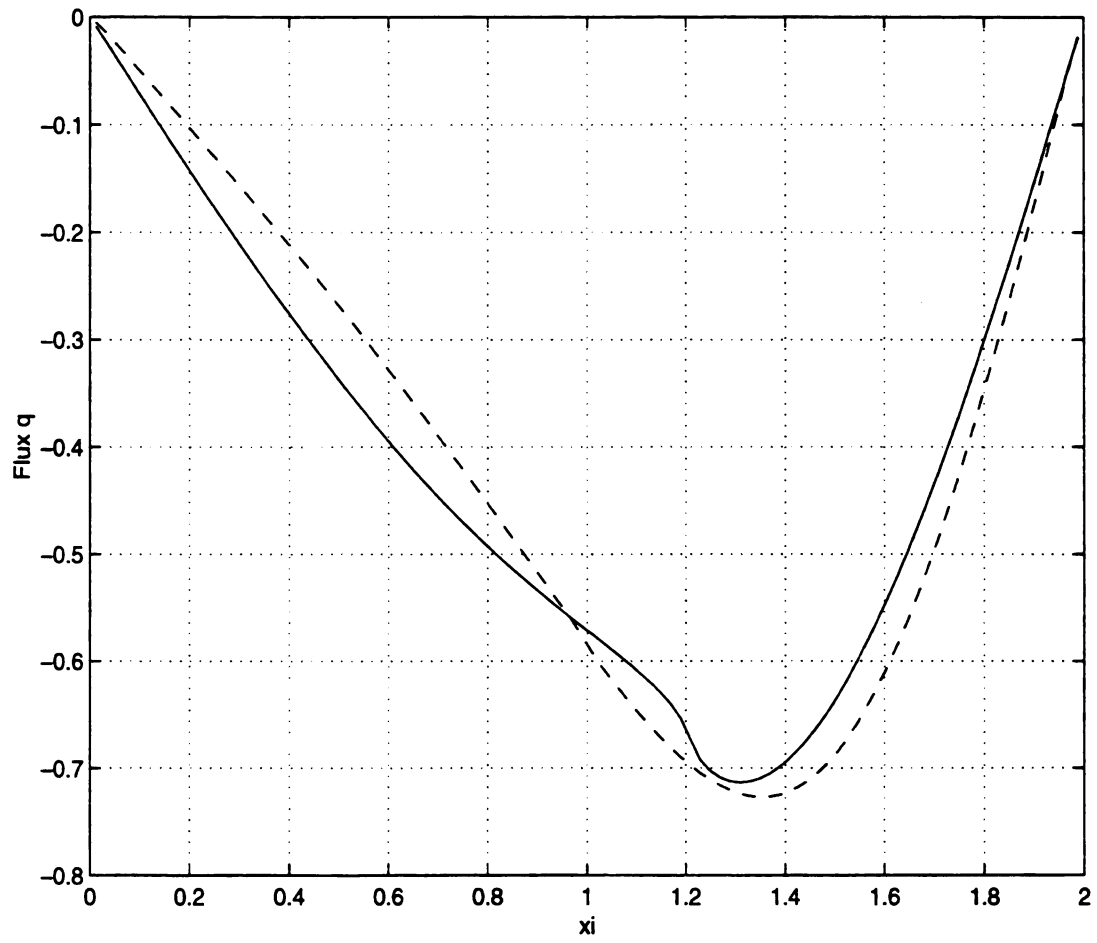


Figure 43 - Heat flux distribution when  $\phi = 5$

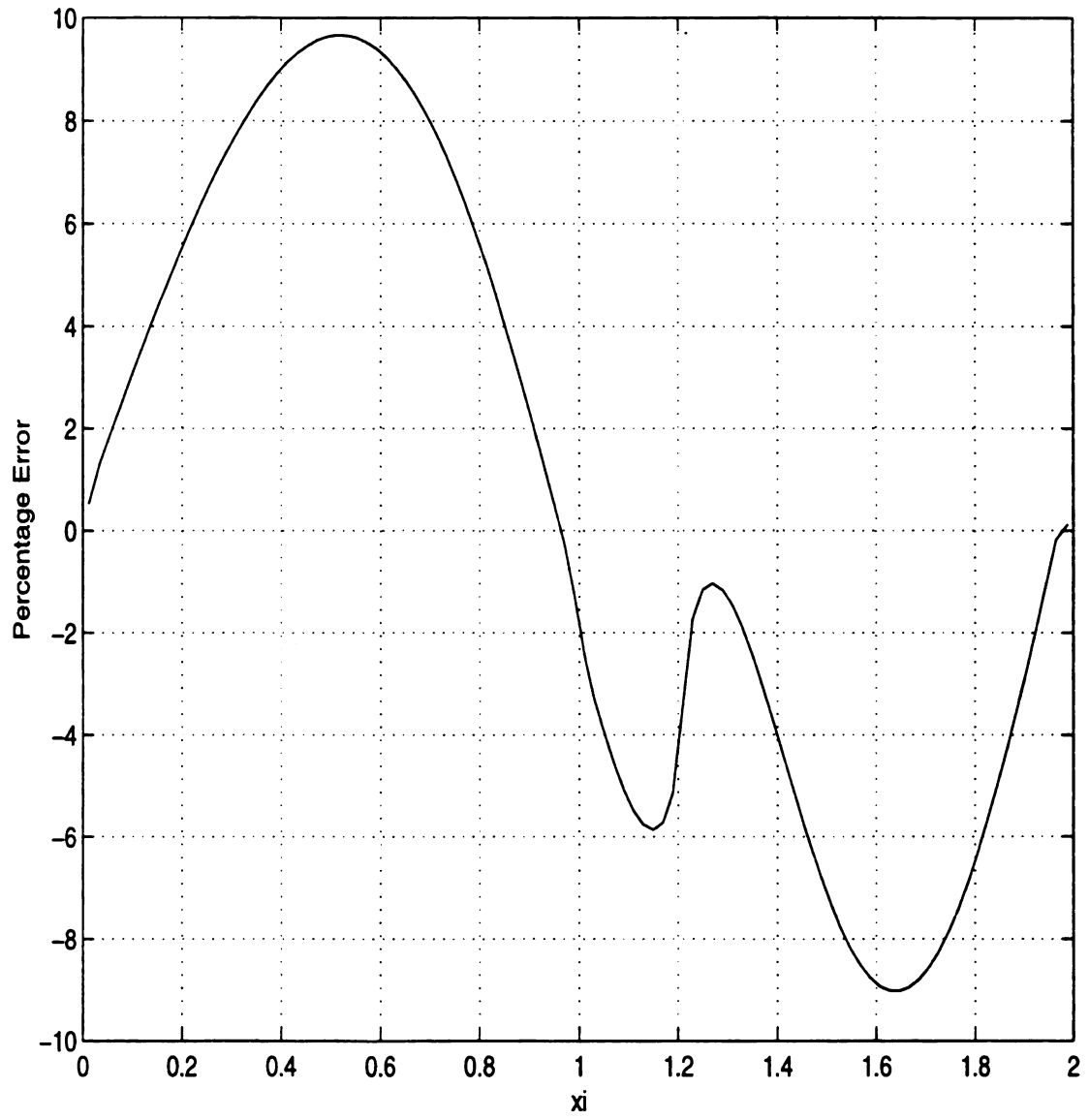


Figure 44 - Error in heat flux approximation when  $\phi = 5$

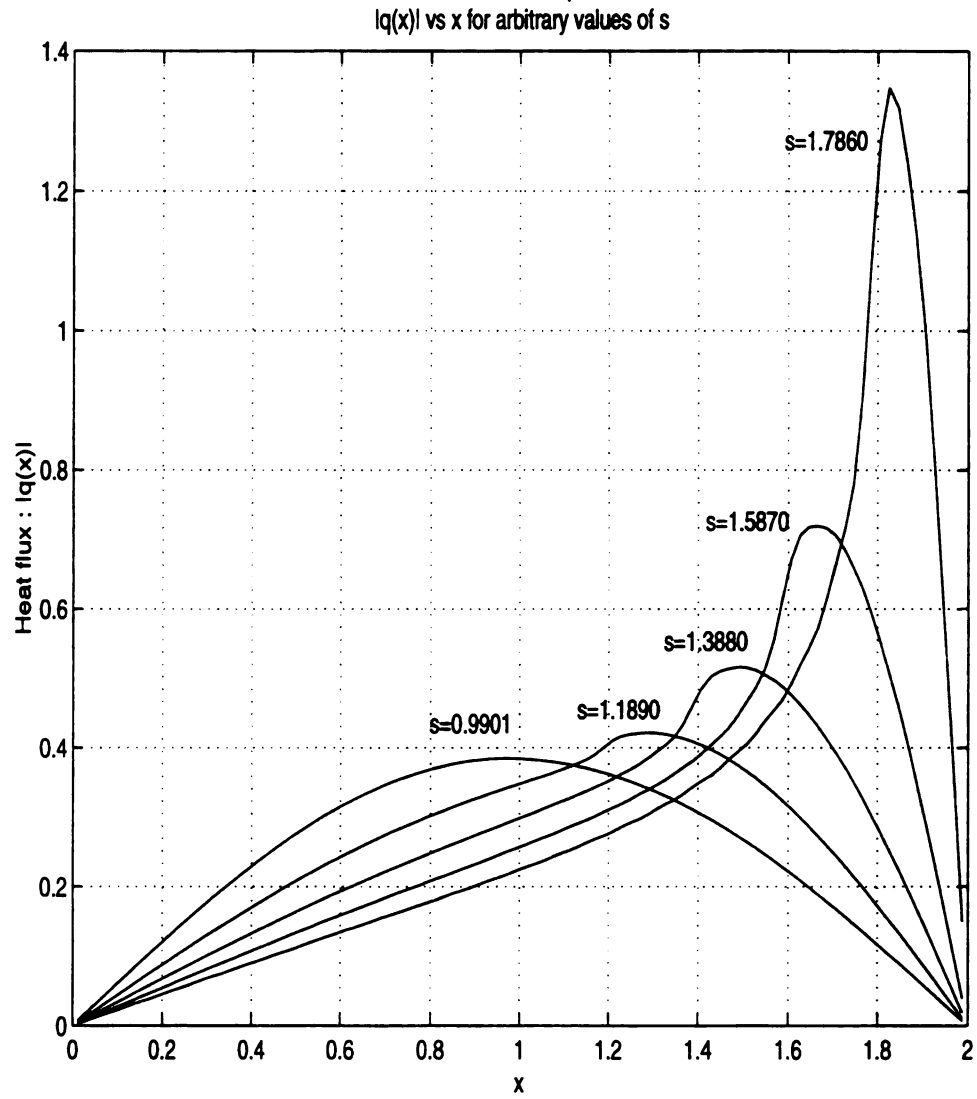
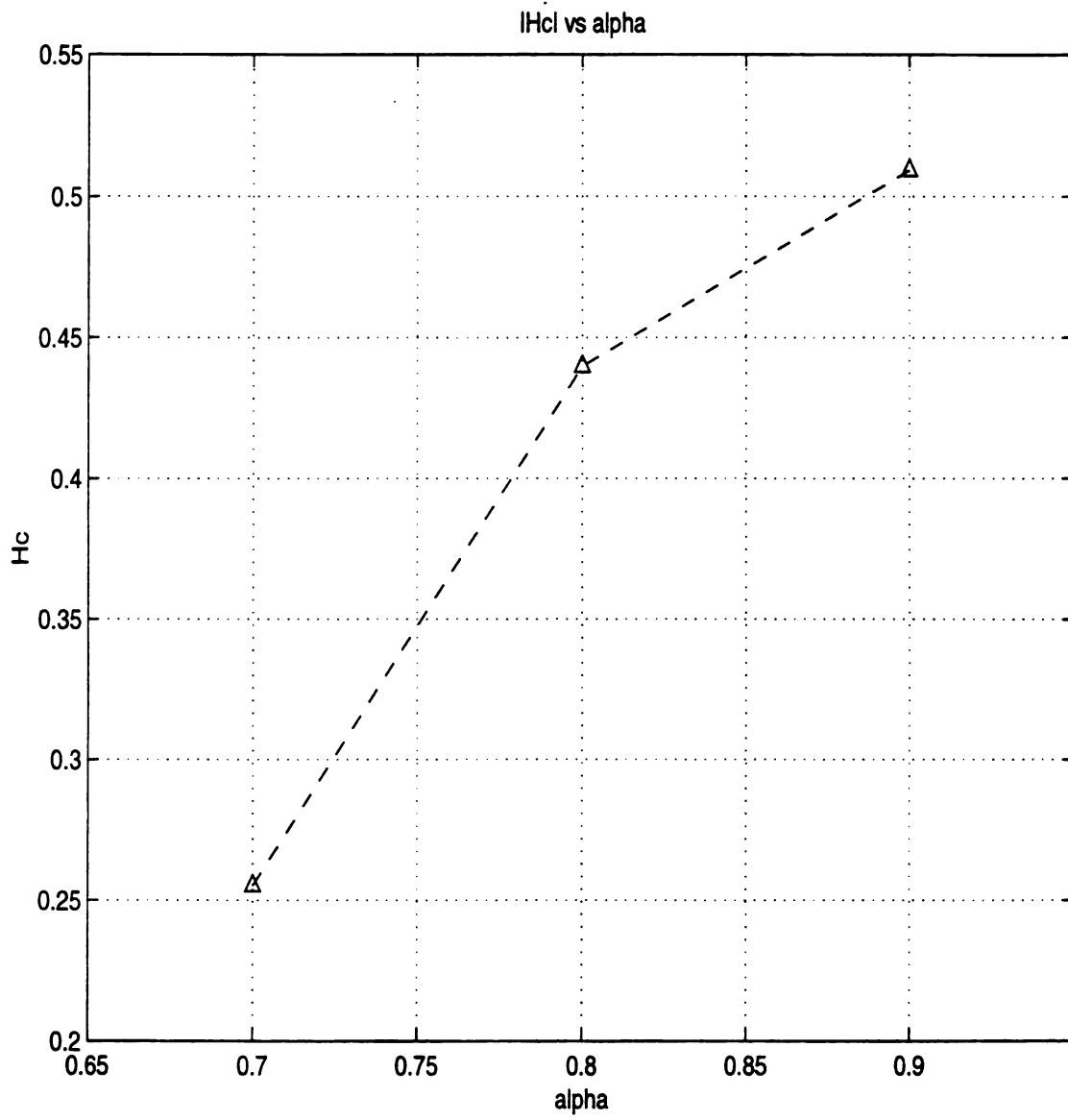
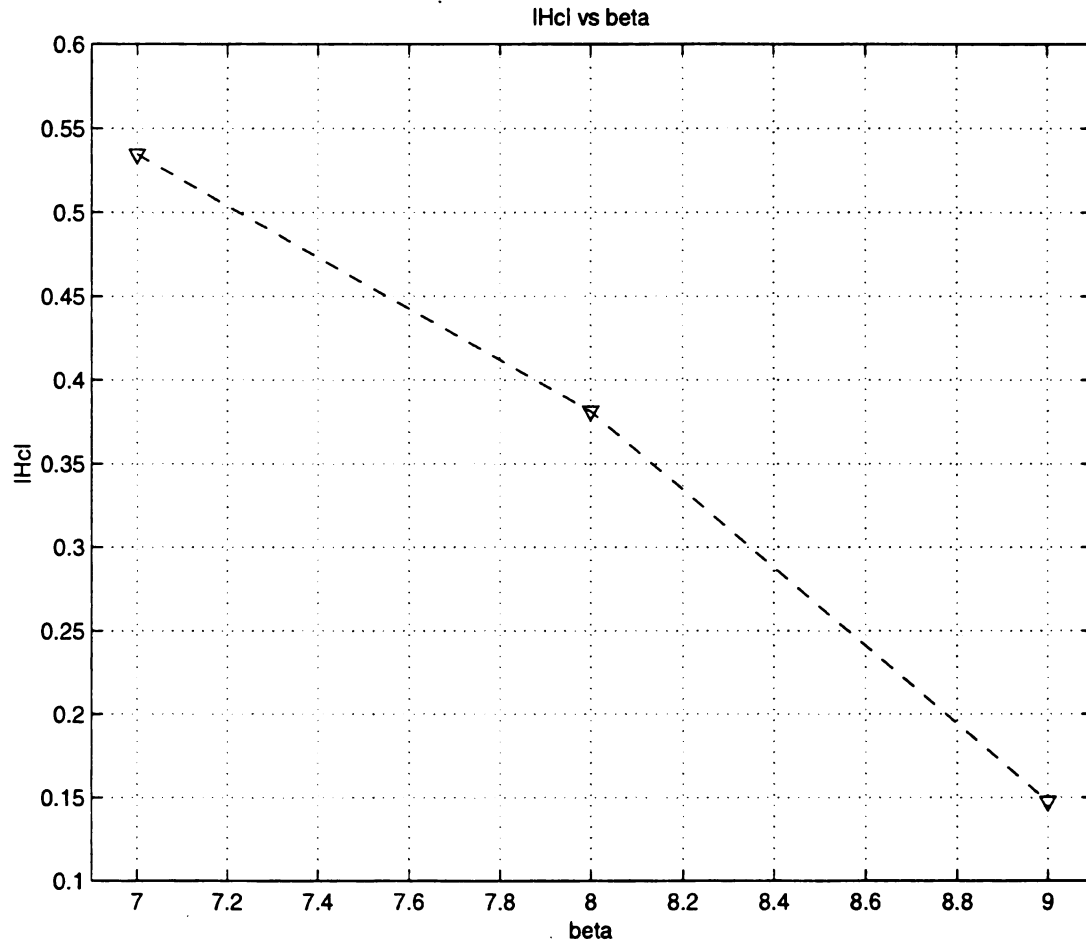
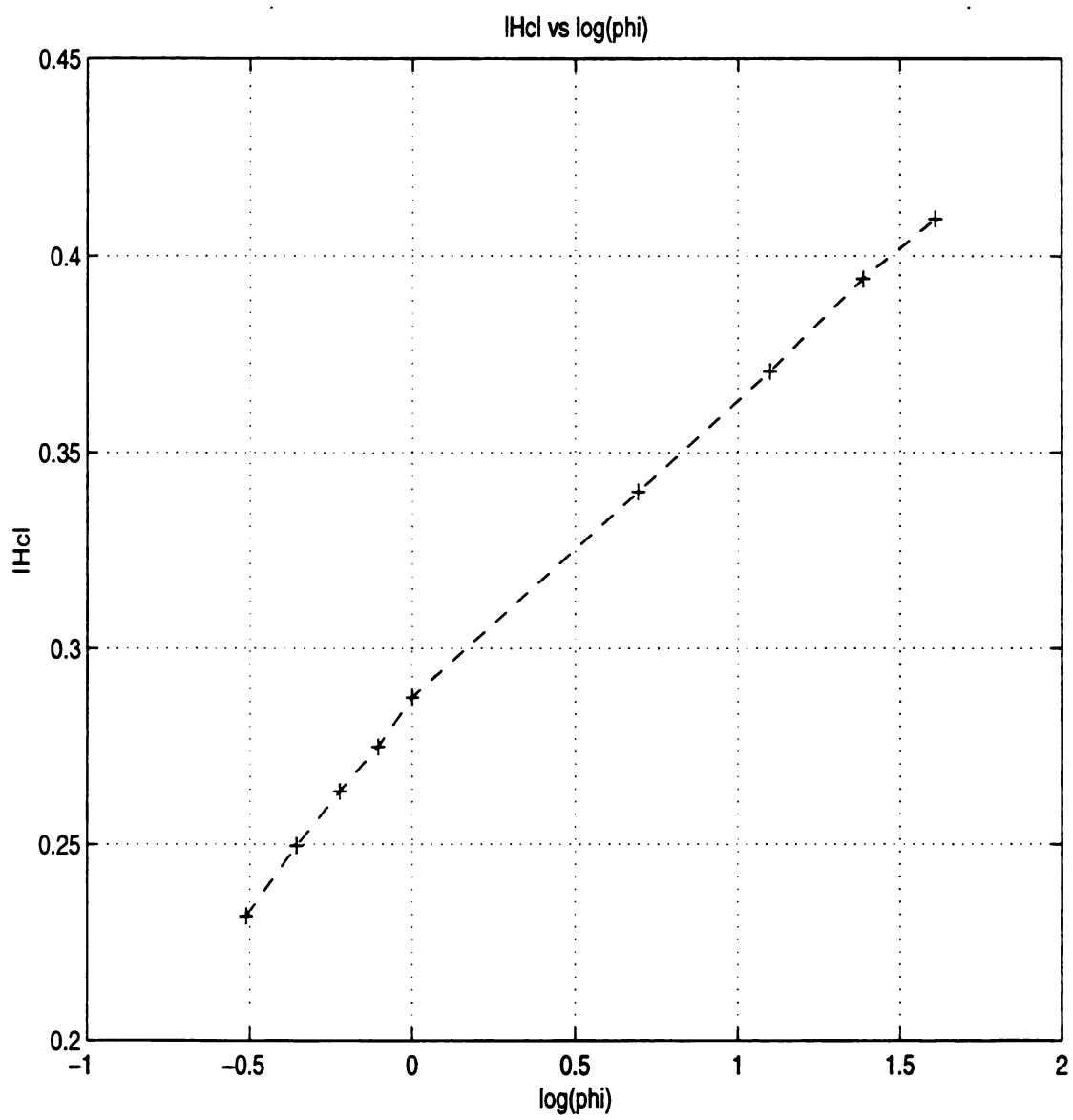
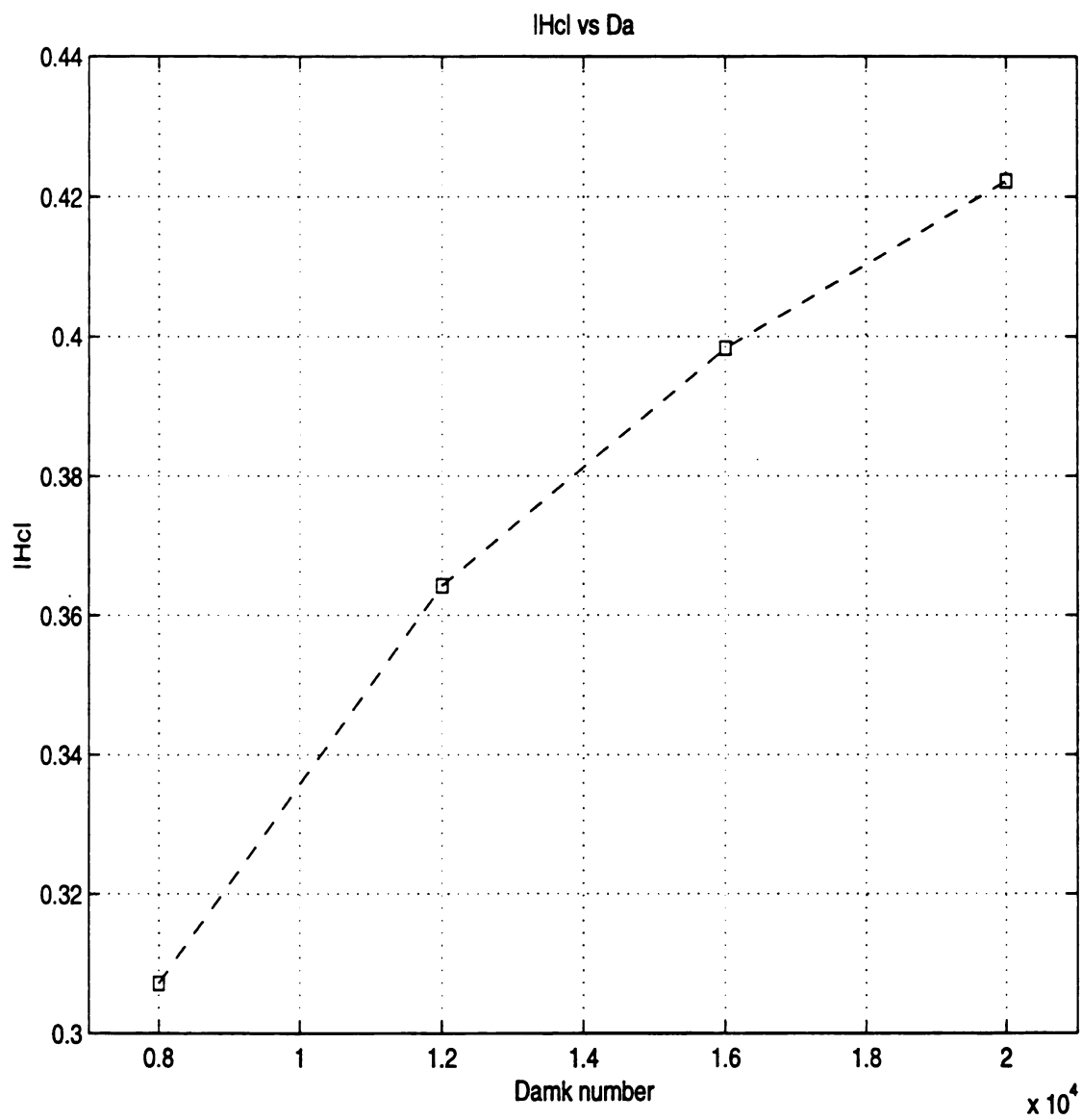


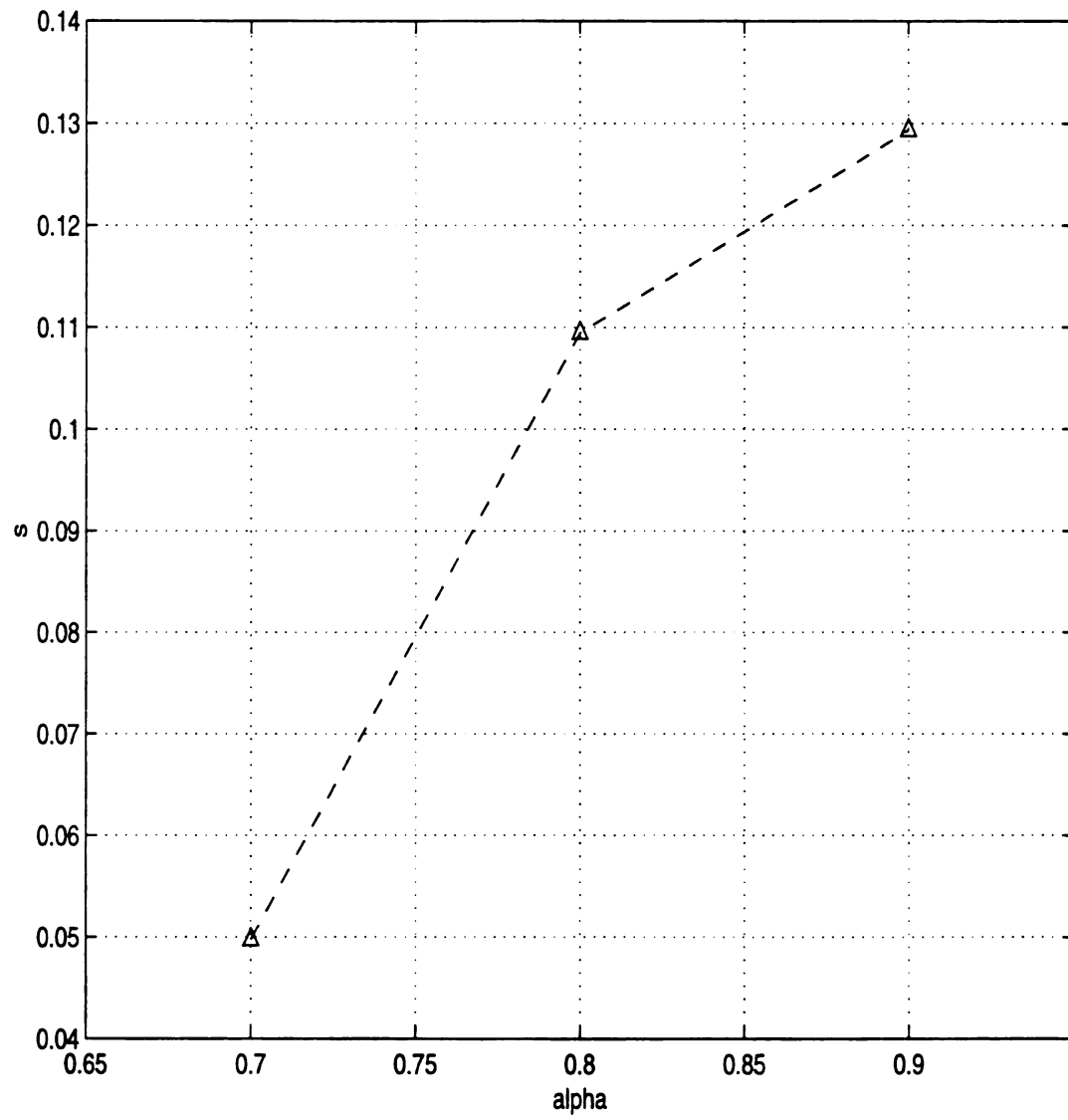
Figure 45 - Heat flux for fictitious values of 's'

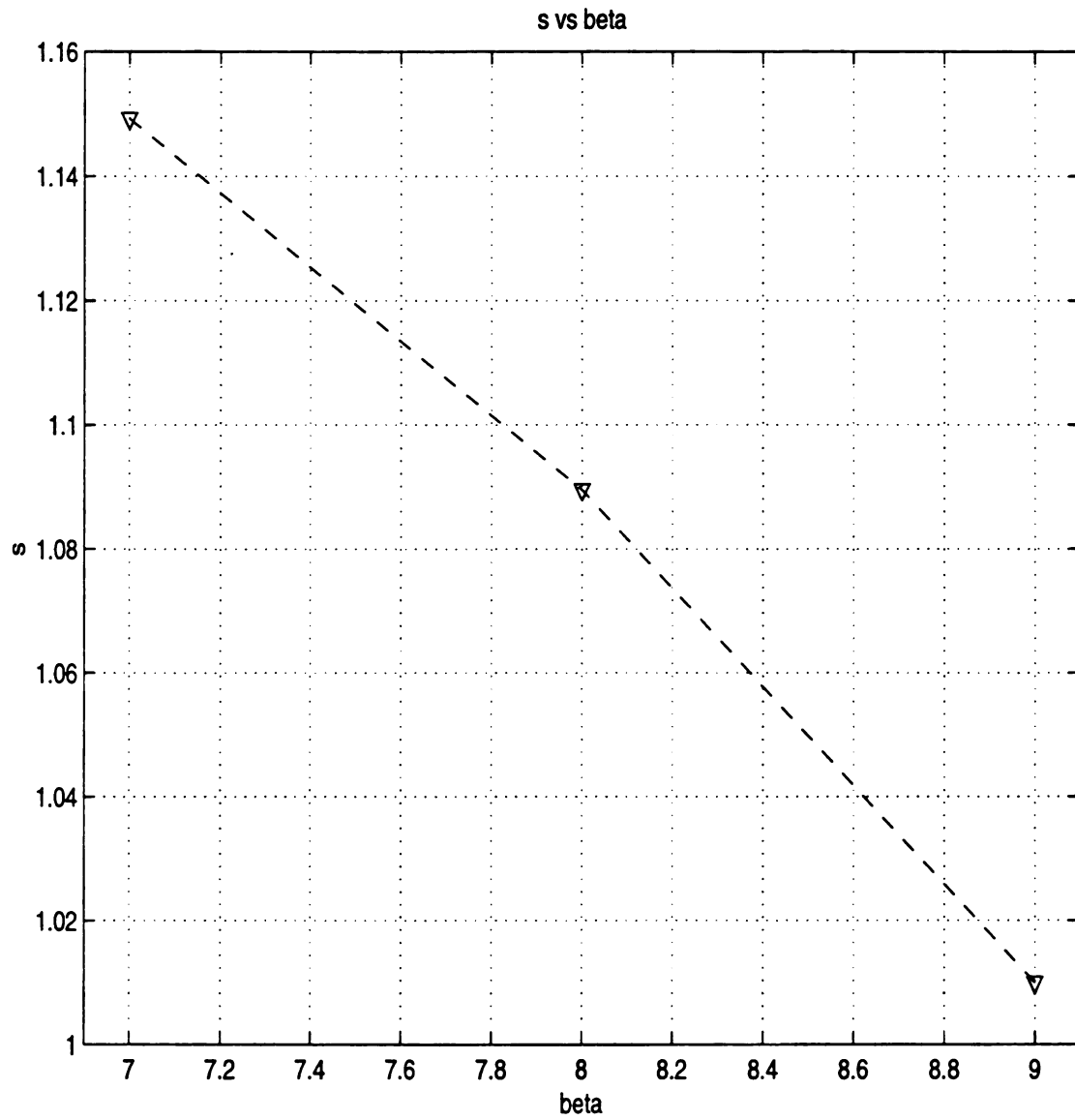
Figure 46 - |H<sub>c</sub>| vs  $\alpha$

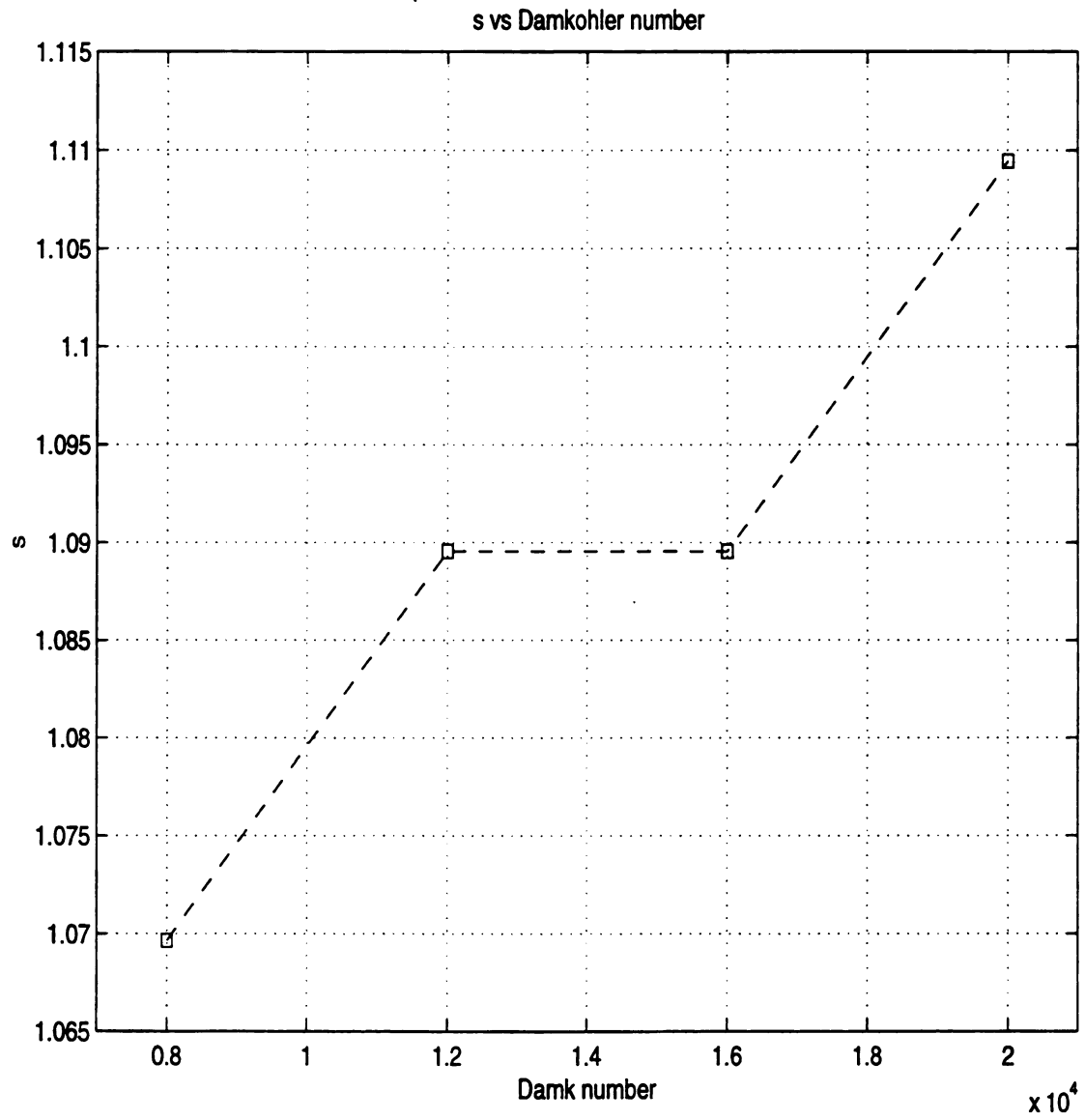
Figure 47 -  $|H_c|$  vs  $\beta$

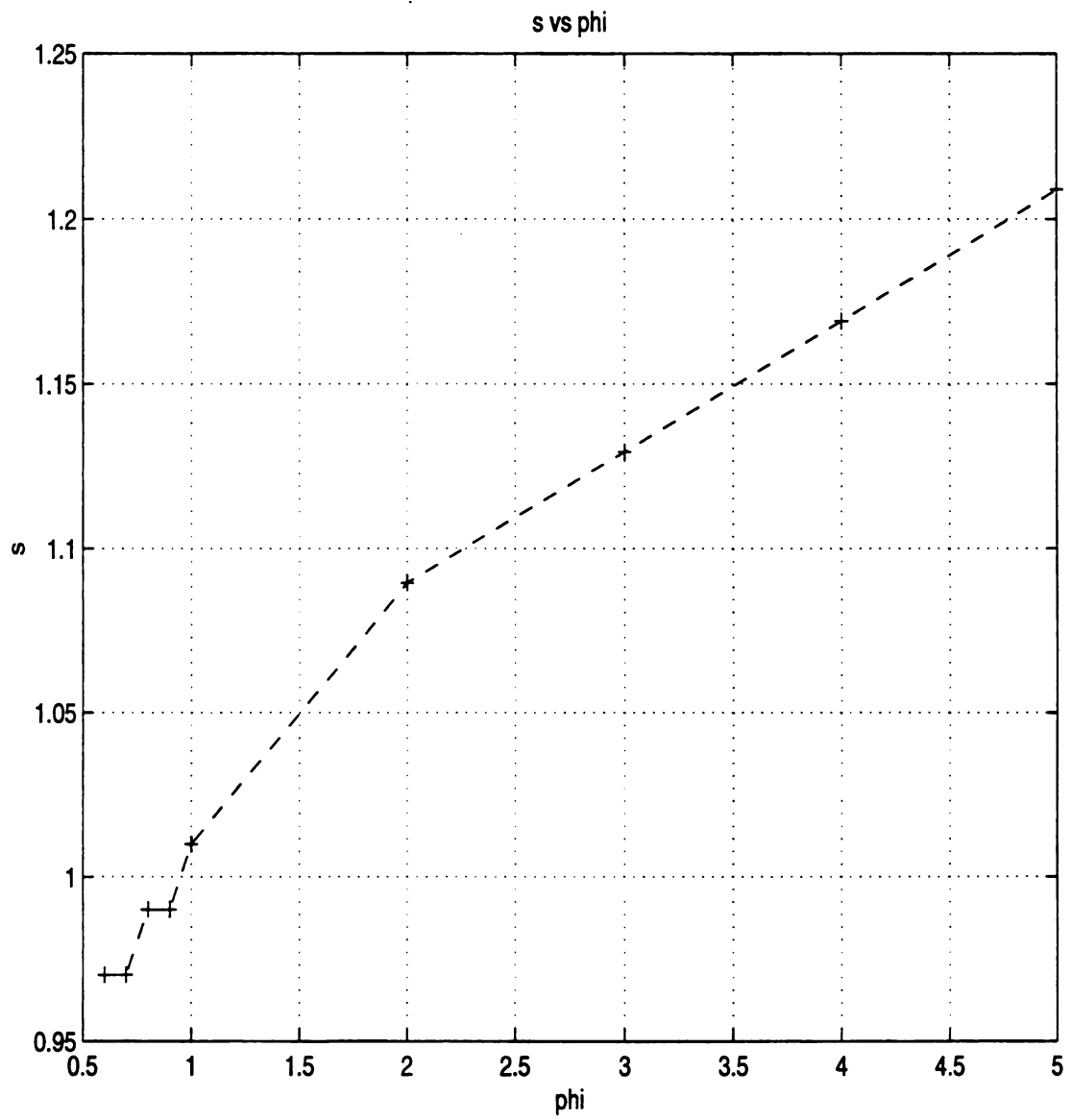
Figure 48 -  $|H_c|$  vs  $\ln(\phi)$

Figure 49 -  $|H_c|$  vs  $D_a$

Figure 50 -  $s$  vs  $\alpha$

Figure 51 -  $s$  vs  $\beta$

Figure 52 -  $s$  vs  $D_a$

Figure 53 - s vs  $\phi$

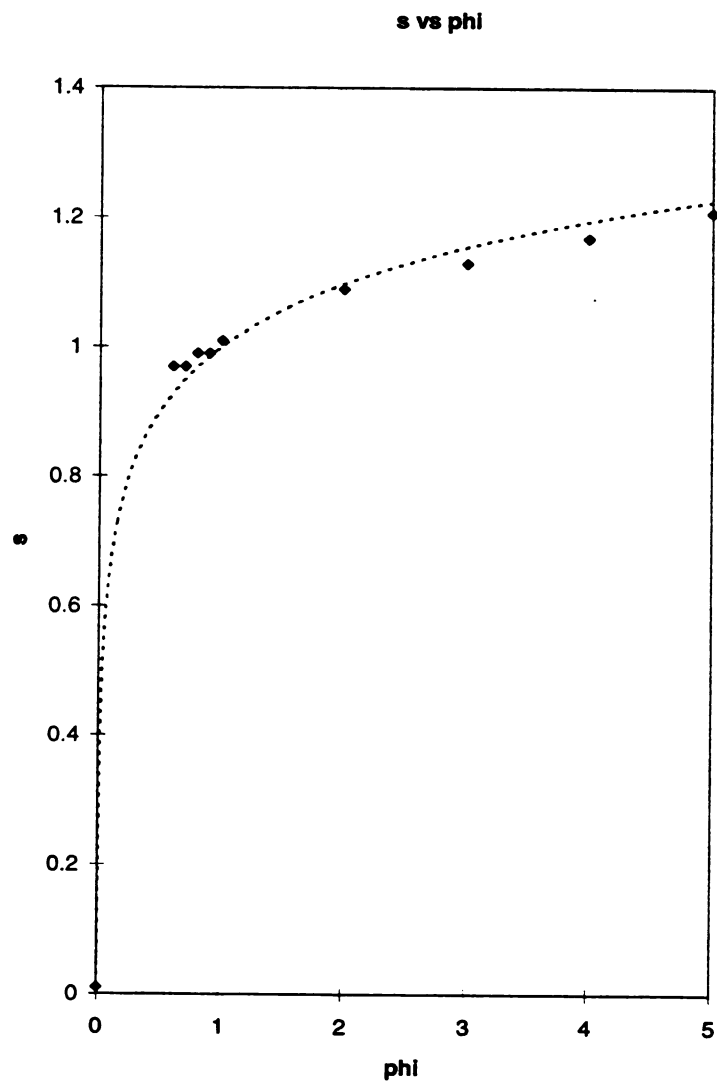


Figure 54 - s vs  $\phi$  with trendline

## CHAPTER V

### Conclusions

The features of diffusion flame behavior near cold chemically inert surfaces, with emphasis on the structure of triple flames, were examined using a model problem that permits two dimensional effects near the flame tip. In Chapter 1, the generic features were studied. The stoichiometric PF tip postulate was analyzed in Chapter 2, while the heat flux distribution in the cold wall was examined in Chapter 3.

The generic features of triple flames were studied using a model problem formulated in Chapter 1.

- The analysis shows the existence of three distinct regions: the mixing region, the triple flame region and the diffusion flame region. The mass fraction profiles show unique characteristics in each of these three regions.
- The influence of the various parameters in the model on the solution contours was examined. In particular the parameter  $\alpha$  influences the maximum of the reactivity contour while  $\beta$  and  $D_a$  also influence the location of the flame. The flow parameter  $Pe$  influences the mass fraction profiles and results in a characteristic 'onion' or a 'heart' shape.  $Pe$  also influences the location of the quench point through the Damkohler number. The divider thickness influences the quench radius and also the maximum of the reactivity field.
- Some differential relations that are valid when the excess enthalpy field is identically zero throughout the field were presented. These served as a check on the numerical

code and are also useful as generic results.

- The negativity of the excess enthalpy field near the cold wall was examined both from the physical and theoretical stand point. An exact solution to the excess enthalpy field is also presented.
- The validity of the postulate relating the mass fraction contours to the shape of the triple flame is examined. From our analysis, we conclude that mass fraction contours may not form a good approximation for the weak PF arc for high  $\phi$  values.

Many researchers have postulated the existence of stoichiometric PF tips with a velocity equal to that of a propagating PF. The validity of this postulate was examined. Our results show that the self-normal propagation velocity appears to be a useful concept only for lifted flames. The actual behavior and response for attached flame structures can be complicated.

In Chapter 4 the heat flux signatures to the cold wall were examined. From our knowledge of the excess enthalpy distribution on the cold wall, an exact solution was presented for both symmetric and unsymmetric flames. This solution in general depends on two parameters which are functions of the four basic parameters in the problem. An approximate expression for this dependence was stated.

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