# Some notes on the structure and extinction of an asymptotic flamelet (Peters 1983)

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## 1 Introduction

This document aims to add expository footnotes to Norbert Peters's seminal paper on non-premixed flame extinction. The problem solved is identical to that of Peters, but the procedure borrows heavily from C. K. Law's excellent combustion text. Notational variances aside, the analysis carried out here is fairly identical to C. K. Law's text in Chapter 9.

## 2 Notation

In Peters, there are no ambiguities of notational origin because most of the material is presented in terms of dimensional quantities. However, the analysis is greatly simplified by defining non-dimensional quantities that will be used in the asymptotic analysis.

The non-dimensionalization is in conformity with C. K. Law (in section 5).

The chemical reaction is proposed as

$$\nu'_F F + \nu'_O O \rightarrow \nu''_P P \tag{1}$$

which is a bimolecular reaction of order 2, in Peters's analysis. The reaction is assumed to follow Arrhenius kinetics taking the form (as in Peters)

$$w = \frac{B}{M_F M_O} \rho^2 Y_F Y_O e^{-E/T} \tag{2}$$

where $w$ is the fuel mass reaction rate; $M_F$ and $M_O$ are the fuel and oxidizer molecular weights; $Y_F$ and $Y_O$ are the fuel and oxidizer mass fractions; $E$ is the activation temperature; $T$ is the flame temperature.

In addition, the following symbols are used: $c_p$: specific heat (assumed constant), $\rho$:density, $D$: diffusion coefficient (assumed to be the same for all species and same for thermal and mass transport-unity Lewis numbers) $Z$: mixture fraction, $\chi$: scalar dissipation rate, $Da$: Dahmköhler number; $(\Delta h)$: the heat of formation of fuel (a negative quantity); $r_s$, the ratio of oxidizer to fuel consumed during the reaction. The fuel and air side boundary conditions are denoted by an additional subscript $F$ or $O$ ($T_F$, $T_O$, $Y_{F,F}$, $Y_{F,O} = 0$, $Y_{O,O}$, $Y_{O,F} = 0$).

A tilde above a quantity signifies that it has been non-dimensionalized (e.g., $\tilde{T}$, $\tilde{Y}_F$, $\tilde{Y}_O$).

# 3 Assumptions

The principal assumptions used are

- Unity Lewis numbers.
- Constant density and specific heat.
- Constant diffusivities.

# 4 Derivation of the flamelet equation

The flamelet equation in Peters will be the basis for the asymptotic analysis. The transport equations are cast into a mixture fraction formulation that is highly advantageous because of its one-dimensionality (in mixture fraction space).

We start with the mixture fraction equation

$$\frac{\rho\partial Z}{\partial t} + \rho u_j \frac{\partial Z}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial Z}{\partial x_j}\right) \tag{3}$$

where the mixture fraction is defined

$$Z = \frac{Y_F - (Y_O - Y_{O,O})/r_s}{Y_{F,F} + Y_{O,O}/r_s} \tag{4}$$

Do a Crocco transformation to orient the coordinate directions in terms of $Z$, $Z_2$, $Z_3$ instead of $x_1$, $x_2$, $x_3$.

Let $\tau = t$, $Z_2 = x_2$, $Z_3 = x_3$.

Apply the transformation rules

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t}\frac{\partial}{\partial Z} \tag{5}$$

$$\frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1}\frac{\partial}{\partial Z} \tag{6}$$

$$\frac{\partial}{\partial x_k} = \frac{\partial}{\partial Z_k}\frac{\partial}{\partial Z}, \qquad (k = 2, 3) \tag{7}$$

The energy equation may be written as

$$\frac{\rho \partial T}{\partial t} + \rho u_j \frac{\partial T}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial T}{\partial x_j}\right) \tag{8}$$

**While transforming, the convection term is seen to be negligible compared to the reaction term (in the vicinity of the reaction zone). This may be seen by stretching the $Z$ coordinate around $Z = Z_{st}$.** This is the basis for the flamelet equations, and one may bear in mind that it is valid only at the reaction zone. For the outer regions, one needs to solve the transport equation for $Z$ written down in the aforementioned. One may therefore not solve the outer equations in the $Z$ coordinate with neglect of the convection term, in which case, it will be seen that it is not of any use to solve the outer equations with $Z$ as the coordinate instead of $x$.

The transformed energy equation is written as follows (equation (11)) in Peters.

$$\rho\left(\frac{\partial T}{\partial \tau} + v_2\frac{\partial T}{\partial Z_2} + v_3\frac{\partial T}{\partial Z_3}\right) \tag{9}$$

$$-\rho D\left\{\left(\frac{\partial Z}{\partial x_k}\right)^2 \quad \frac{\partial^2 T}{\partial Z^2} + 2\frac{\partial Z}{\partial x_2}\frac{\partial^2 T}{\partial Z \partial Z_2} + 2\frac{\partial Z}{\partial x_3}\frac{\partial^2 T}{\partial Z \partial Z_3} + \frac{\partial^2 T}{\partial Z_2^2} + \frac{\partial^2 T}{\partial Z_3^2}\right\} = \frac{-\Delta h}{c_p} w$$

The equation is now transformed into its one dimensional form by introducing the stretched coordinate

$$\xi = \frac{Z - Z_{st}}{\epsilon} \tag{10}$$

into equation (9) and expanding around $Z = Z_{st}$. $\epsilon$ is a small parameter to be defined during the analysis.

Thus

$$\frac{\partial}{\partial Z} = \frac{1}{\epsilon}\frac{\partial}{\partial \xi} \tag{11}$$

The zeroth order expansion then gives

$$-(\rho D)_{st}\left(\frac{\partial Z}{\partial x_k}\right)^2\frac{\partial^2 T}{\partial^2 \xi}=\epsilon^2\frac{(-\Delta h)}{c_p}w_{st} \tag{12}$$

Rewrite equation (12) as the standard flamelet equation containing the scalar dissipation rate $\chi_{st}$

$$-\frac{\chi_{st}}{2}\frac{\partial^2 T}{\partial Z^2}=\frac{(-\Delta h)}{c_p}\left(\frac{w}{\rho}\right)_{st} \tag{13}$$

where

$$\chi_{st}=2D\left(\frac{\partial Z}{\partial x_k}\right)^2_{st} \tag{14}$$

One may similarly obtain flamelet equations for reacting scalars $Y_F$, $Y_O$

$$-\frac{\chi_{st}}{2}\frac{\partial^2 Y_F}{\partial Z^2}=-\left(\frac{w}{\rho}\right)_{st} \tag{15}$$

$$-\frac{\chi_{st}}{2}\frac{\partial^2 Y_O}{\partial Z^2}=-r_s\left(\frac{w}{\rho}\right)_{st} \tag{16}$$

# 5 Non-dimensionalization

We may now non-dimensionalize the scalars by defining variables as suggested by equations (13), (15) and (16).

Define

$$\tilde{T}=\frac{c_p T}{(-\Delta h Y_{F,F})} \tag{17}$$

$$\tilde{Y_F}=\frac{Y_F}{Y_{F,F}} \tag{18}$$

$$\tilde{Y_O}=\frac{Y_O}{r_s Y_{F,F}} \tag{19}$$

We may then obtain the coupling relation

$$\frac{d^2(\tilde{T}+\tilde{Y_i})}{dZ^2}=0 \tag{20}$$

The non-dimensionalized energy equation is

$$\frac{d^2\tilde{T}}{dZ^2}=-Da_C\tilde{Y_F}\tilde{Y_O}exp(-\frac{\tilde{T_a}}{\tilde{T}}) \tag{21}$$

where

$$Da_C = \frac{2r_s B \rho_{st} Y_{F,F}}{\chi_{st} M_O M_F} \tag{22}$$

Equation (21) is the form given in C. K. Law, and from here on the procedure is analogous to that taken in the combustion text.

# 6 Asymptotic structure of flamelet

The equation to be solved is

$$\frac{d^2\tilde{T}}{dZ^2} = -Da_C \tilde{Y}_O \tilde{Y}_F e^{-\tilde{T}_a/\tilde{T}} \tag{23}$$

subject to BCs

$$\tilde{Y}_F = 0; \qquad \text{at } Z = 0 \tag{24}$$
$$\tilde{Y}_F = 1; \qquad \text{at } Z = 1 \tag{25}$$
$$\tilde{Y}_O = 1; \qquad \text{at } Z = 0 \tag{26}$$
$$\tilde{Y}_O = 0; \qquad \text{at } Z = 1 \tag{27}$$
$$\tilde{T} = \tilde{T}_O; \qquad \text{at } Z = 0 \tag{28}$$
$$\tilde{T} = \tilde{T}_F; \qquad \text{at } Z = 1 \tag{29}$$

## 6.1 Inner expansions and the Zeldovich number

Do an inner expansion of $\tilde{T}$, $\tilde{Y}_F$ and $\tilde{Y}_O$ around the stoichiometric value as

$$\tilde{T} = \tilde{T}_{st} - \epsilon\theta + O(\epsilon^2) \tag{30}$$

$$\begin{aligned} \tilde{Y}_F = &\quad \tilde{Y}_{F,st} + \epsilon\psi + O(\epsilon^2) \\ = &\quad \epsilon\psi + O(\epsilon^2) \end{aligned} \tag{31}$$

Likewise for oxidizer

$$\begin{aligned} \tilde{Y}_O = &\quad \tilde{Y}_{O,st} + \epsilon\Xi + O(\epsilon^2) \\ = &\quad \epsilon\Xi + O(\epsilon^2) \end{aligned} \tag{32}$$

In the above, the zeroth order terms are those obtained at equilibrium, or inifinitely fast Chemistry. The fuel and oxidizer mass fractions have an $O(\epsilon)$ leakage from the equilibrium solution ($\epsilon$ is the small parameter that will be defined during the analysis). It may also be seen that in order to understand

the inner structure of the reaction zone, one needs to characterize the $O(\epsilon)$ terms, since the left hand side of equation (23) has vanishing $O(1)$ terms. Insert the perturbation expansions for $T$, $Y_F$ and $Y_O$ (equations (30), (31), (32)) into the energy equation (23). Using the stretched coordinate $\xi = (Z - Z_{st})/\epsilon$ in equation (23) and expanding around $Z = Z_{st}$ we get

$$\frac{d^2\theta}{d\xi^2} = \epsilon^3 Da_C \Xi \psi e^{-\tilde{T}_a/\tilde{T}} \tag{33}$$

Now we consider the exponential term $e^{-\tilde{T}_a/\tilde{T}}$ and define the small parameter $\epsilon$ and Zeldovich number $Ze$ as follows. Expand the temperature to be used in the exponential as

$$\tilde{T} = \tilde{T}_{st} - \epsilon\theta \tag{34}$$

Or

$$\frac{\tilde{T}}{T_{st}} = 1 - \epsilon\frac{\theta}{\tilde{T}_{st}} \tag{35}$$

so that

$$\frac{\tilde{T}_a}{\tilde{T}_{st}} = \frac{\tilde{T}_a}{\tilde{T}_{st}} \frac{1}{1 - \epsilon\frac{\theta}{T_{st}} + O(\epsilon^2)} \tag{36}$$

$$= \frac{\tilde{T}_a}{\tilde{T}_{st}} \left(1 + \epsilon\frac{\theta}{\tilde{T}_{st}} + O(\epsilon^2)\right) \tag{37}$$

Now we may write the equation (33) as

$$\frac{d^2\theta}{d\xi^2} = \epsilon^3 Da_C \Xi \psi e^{-\tilde{T}_a/\tilde{T}} \tag{38}$$

$$= (\epsilon^3 Da_c e^{-\frac{\tilde{T}_a}{\tilde{T}_{st}}}) \Xi \psi e^{-(\epsilon\tilde{T}_a/\tilde{T}_{st}^2)\theta} \tag{39}$$

As the quantity on the right hand side of equation (39) is of $O(1)$, we must have both

$$\epsilon\frac{\tilde{T}_a}{\tilde{T}_{st}^2} \sim O(1) \tag{40}$$

and

$$\epsilon^3 Da_c e^{-\tilde{T}_a/\tilde{T}_{st}} \sim O(1) \tag{41}$$

The expansion parameter $\epsilon$ is obtained by arbitrarily setting the right hand side of equation (40) to 1. This gives us the Zeldovich number

$$Ze = \frac{\tilde{T}_a}{\tilde{T}_{st}^2} = \frac{1}{\epsilon} \tag{42}$$

and

$$\epsilon = \frac{1}{Ze} = \frac{\tilde{T}_{st}^2}{\tilde{T}_a} \tag{43}$$

The equation (41) allows the definition of a reduced Dahmkohler number $\Delta$ arising as a consequence of the large Dahmköhler number

$$Da = Da_C e^{-\tilde{T}_a/\tilde{T}_{st}} \tag{44}$$

The reduced Damköhler number $\Delta$ is an $O(1)$ quantity defined as

$$\Delta = \epsilon^3 Da \tag{45}$$

In Peters, the author calls equation (40) the large activation energy expansion, and equation (41) the large Dahmköhler number expansion, which have now been interrelated by equation (45), the distinguished limit. With these refinements, our energy equation now takes the form

$$\frac{d^2\theta}{d\xi^2} = \Delta(\psi \Xi e^{-\theta}) \tag{46}$$

# 7 Simplification from Schwab-Zeldovich coupling

Use the coupling relation to obtain expressions for $\psi$ and $\Xi$ in the energy equation.

$$\frac{d^2(\tilde{T} + \tilde{Y}_i)}{dZ^2} = 0 \tag{47}$$

The solution to this equation is

$$\tilde{T} + \tilde{Y}_i = aZ + b \tag{48}$$

After recognizing that at $Z = 0$, $\tilde{Y}_F = 0, \tilde{Y}_O = \tilde{Y}_{O,O}, \tilde{T} = \tilde{T}_O$; at $Z = 1$, $\tilde{Y}_F = \tilde{Y}_{F,F}, \tilde{Y}_O = 0, \tilde{T} = \tilde{T}_F$, we get,

$$\tilde{Y}_F = (T_F + \tilde{Y}_{F,F} - \tilde{T}_O)Z + \tilde{T}_O - \tilde{T} \tag{49}$$

and

$$\tilde{Y}_O = (\tilde{T}_F - \tilde{T}_O - \tilde{Y}_{O,O})Z + \tilde{T}_O + \tilde{Y}_{O,O} - \tilde{T} \tag{50}$$

Here, the quantity $\alpha = \tilde{T}_F - \tilde{T}_O$ is the heat transfer parameter, important in determining fuel and air side leakages. Now we expand $\tilde{T}$ about $Z = Z_{st}$ and put in equations (49) and (50).

$$\tilde{T} = \tilde{T}_{st} - \epsilon\theta \tag{51}$$

$T_{st}$ may be obtained from the zeroth order expansion of (49) and (50).

$$\tilde{T_{st}} = (\alpha - \tilde{Y}_{O,O})Z_{st} + \tilde{Y}_{O,O} + \tilde{T_O} = (\alpha + \tilde{Y}_{F,F})Z_{st} + \tilde{T_O} \tag{52}$$

Get the mass fractions $\tilde{Y_F}$ and $\tilde{Y_O}$ as

$$\begin{aligned} \tilde{Y_F} = &\quad (\alpha + \tilde{Y}_{F,F})(Z - Z_{st}) + \epsilon\theta && (53)\\ = &\quad (\alpha + \tilde{Y}_{F,F})\epsilon\xi + \epsilon\theta && (54)\\ = &\quad \epsilon[(\alpha + \tilde{Y}_{F,F})\xi + \theta] && (55)\\ = &\quad \epsilon\psi && (56) \end{aligned}$$

$$\begin{aligned} \tilde{Y_O} = &\quad (\alpha - \tilde{Y}_{O,O})(Z - Z_{st}) + \epsilon\theta && (57)\\ = &\quad (\alpha - \tilde{Y}_{O,O})\xi\epsilon + \epsilon\theta && (58)\\ = &\quad \epsilon\{(\alpha - \tilde{Y}_{O,O})\xi + \theta\} && (59)\\ = &\quad \epsilon\Xi && (60) \end{aligned}$$

Thus,

$$\psi = (\alpha + \tilde{Y}_{F,F})\xi + \theta \tag{61}$$

and

$$\Xi = (\alpha - \tilde{Y}_{O,O})\xi + \theta \tag{62}$$

Our energy equation may now be cast into the form

$$\frac{d^2\theta}{d\xi^2} = \Delta[(\alpha + \tilde{Y}_{F,F})\xi + \theta]\{(\alpha - \tilde{Y}_{O,O})\xi + \theta\}e^{-\theta} \tag{63}$$

Note that this is identical to equation 9.3.18 (Chapter 9) of C. K. Law, with the difference that $\alpha = -\beta$ used in the book (in C. K. Law it seems to be written so that air is preheated, instead of fuel as done here).

The boundary conditions for this ordinary differential equation may be obtained by matching with the outer solutions.

# 8 Outer solutions and matching to obtain BCs

For the outer solutions, one needs to revert to nomal coordinates since the convection term can no longer be neglected. However, for purposes of matching, it suffices to say that as the stretched inner coordinate $\xi \to \pm\infty$, the leakage takes a *small* constant value. One may either set this to zero, or take

the derivative of this leakage, which will turn out to be zero. Either of these approaches are equivalent. On the fuel side one has the oxidizer leakage

$$\lim_{\xi\to\infty} \Xi = c_O \tag{64}$$

$$\tag{65}$$

Taking derivatives gives

$$\lim_{\xi\to\infty} \frac{d\Xi}{d\xi} = 0 \tag{66}$$

$$\text{Or} \qquad \lim_{\xi\to\infty} \frac{d\theta}{d\xi} = \tilde{Y}_{O,O} - \alpha \tag{67}$$

Likewise, for the air side one has the fuel leakage

$$\lim_{\xi\to-\infty} \psi = c_F \tag{68}$$

$$\tag{69}$$

Taking derivatives gives

$$\lim_{\xi\to-\infty} \frac{d\psi}{d\xi} = 0 \tag{70}$$

$$\text{Or} \qquad \lim_{\xi\to-\infty} \frac{d\theta}{d\xi} = -\tilde{Y}_{F,F} - \alpha \tag{71}$$

Alternate to the foregoing, one may also set the leakage values to zero in the outer solutions. This gives

$$\lim_{\xi\to-\infty} \theta = -(\alpha + \tilde{Y}_{F,F})\xi \tag{72}$$

$$\lim_{\xi\to\infty} \theta = -(\alpha - \tilde{Y}_{O,O})\xi \tag{73}$$

# 9 Recasting of inner equations into Liñan's form

Our problem is now completely defined and may be solved either analytically as in Liñan. The usual approach is to recast the inner equation into a more convenient form by making the transformation

$$\theta = \tilde{\theta} + \gamma\eta, \qquad \xi = \frac{2}{1 + \tilde{Y_{O,O}}}\eta \tag{74}$$

with

$$\delta = \frac{4\Delta}{1+\tilde{Y}_{O,O}^2}, \qquad \gamma = 1 - \frac{2(1+\alpha)}{1+\tilde{Y_{O,O}}} \tag{75}$$

The equations then become

$$\frac{d^2\tilde{\theta}}{d\eta^2} = \delta(\tilde{\theta}-\eta)(\tilde{\theta}+\eta)e^{-(\tilde{\theta}+\gamma\eta)} \tag{76}$$

with boundary conditions

$$\left(\frac{d\tilde{\theta}}{d\eta}\right)_{-\infty} = -1 \text{ and} \qquad \left(\frac{d\tilde{\theta}}{d\eta}\right)_{\infty} = 1 \tag{77}$$

# 10 Non unity fuel and air exponentes in reaction term

The analysis for varying fuel and air coefficients ($\nu_F$ and $\nu_O$ for fuel and air) is quite similar to the unity coefficients case. Here, one expands the quantities in powers of $\epsilon$, where $\epsilon$ has been identified in the foregoing as $\tilde{T}_{st}^2/\tilde{T}_a$. As usual, one is interested mostly in the first order behavior.

$$\tilde{T} = \tilde{T}_{st} - \epsilon\theta \tag{78}$$

$$\tilde{Y}_F = \epsilon\psi \tag{79}$$

$$\tilde{Y}_O = \epsilon\Xi \tag{80}$$

Upon insertion into the inner energy equation, one gets

$$\frac{d^2\theta}{d\xi^2} = \epsilon^{1+\nu_F+\nu_O} \exp\left(-\frac{\tilde{T}_a}{\tilde{T}_{st}}\right) Da_C \Xi^{\nu_O}\psi^{\nu_F}\exp(-\theta) \tag{81}$$

It then transpires that

$$\epsilon^{1+\nu_F+\nu_O} \sim Da_C^{-1}[\exp\left(-\frac{\tilde{T}_a}{\tilde{T}_{st}}\right)]^{-1} \sim Da_C^{-1} \tag{82}$$

Transposition into Liñan's form gives

$$\frac{d^2\tilde{\theta}}{d\eta^2} = \delta(\tilde{\theta}-\eta)^{\nu_F}(\tilde{\theta}+\eta)^{\nu_O}e^{-(\tilde{\theta}+\gamma\eta)} \tag{83}$$

subject to the boundary conditions

$$\left(\frac{d\tilde{\theta}}{d\eta}\right)_{-\infty} = -1 \text{ and} \qquad \left(\frac{d\tilde{\theta}}{d\eta}\right)_{\infty} = 1 \tag{84}$$

# 11 Extinction conditions for flame with non-unity fuel-air exponents

The equation (83) was solved using Matlab with $\nu_F = 0.1$, $\nu_O = 1.65$. $\delta$ was progressively reduced, leading to a state when Matlab cannot give a solition. The extinction scalar dissipation rate was obtained (approximately) as $\chi_{st} = 30/s$. The corresponding value with $a = 1$ and $b = 1$ is $\chi_{st} = 0.15/s$, differing approximately by a factor of 50.

The figure attached shows the variations of the $O(1)$ flame temperature when $\delta$ is reduced. For high values of $\delta$, the leakage zone is small. Progressive reduction of $\delta$ leads to an increase in the extent of the leakage region. $\delta = 0.22$ was the last value obtained, which gives $\chi_{st} = 28s^{-1}$. Note that in the following, the outer solutions are not shown. They will take the form of error functions (in space), and not directly amenable to solution by using the mixture fraction approach. In Peters, the solution is only implied as a special form using a similarity transformation, and this is not to be expected in the general case. One will have to solve for the outer solutions in normal space.

# 12 Conclusions and further work

The flame structure of a strained laminar flamelet (no radiation) (in $Z$ space) is obtained from asymptotic analysis. The resulting BVP is solved using Matlab, to obtain the extinction scalar dissipation rate. It is seen that non-unity fuel and oxidizer coefficients results in drastically different values of the extinction scalar dissipation rate, as compared with when the coefficients are unity. The value obtained compares favorably with Direct Numerical Simulations using S3D. It is emphasized here that the solutions obtained from Matlab may be refined to get a more accurate value, but even so, the results are fairly encouraging.

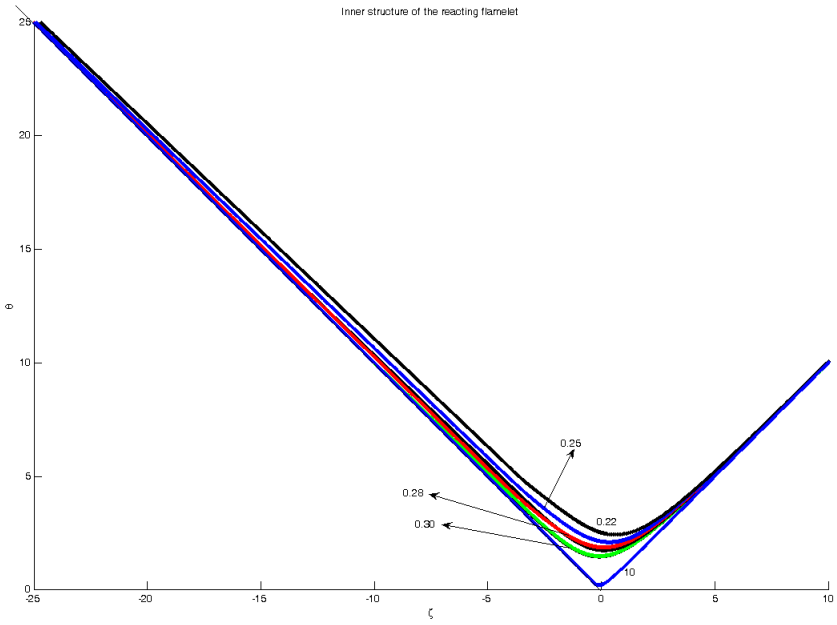


Figure 1: Variation of first order correction term for inner solution with reduced Damköher number $\delta$. The last solution obtained from Matlab was with $\delta = 0.22$ corresponding to $\chi_{st} = 29s^{-1}$.