ABSTRACT

Title of Document: AN ASYMPTOTIC ANALYSIS OF SPONTANEOUS IGNITION OF HYDROGEN JETS

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Analytical work is presented for the spontaneous ignition of a hydrogen jet emanating from a slot into air. A similarity solution of the flowfield was obtained. This was combined with the species and energy conservation equations, which were solved using activation energy asymptotics. Limits of spontaneous ignition were identified as functions of slot width, flow rate, and temperatures of the hydrogen jet and ambient air. Two scenarios are examined: a cool jet flowing into a hot ambient and a hot jet flowing into a cool ambient. For both scenarios, ignition is favored with an increase of either the ambient temperature or the hydrogen supply temperature. Moreover, for the hot ambient scenario, a decrease in local fuel Lewis number also promotes ignition. The Lewis number of the oxidizer only has a weak effect on ignition. Because spontaneous ignition is very sensitive to temperature, ignition is predicted to occur near the edge of the jet if the hydrogen is cooler than the air and on the centerline if the hydrogen is hotter than the air.

AN ASYMPTOTIC ANALYSIS OF SPONTANEOUS IGNITION OF HYDROGEN JETS

By

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dedication

To my dearest wife Jolene and precious son Zaccaeus. And to God, for His grace and providence, and for watching over me every step of the way.

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Table of Contents

List of Tables

List of Figures

Nomenclature

a_T	constant representing the temperature increase through reaction
B	pre-exponential factor
c_j	molar concentration of species j
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
Da	Damköhler number
$\tilde{D}a$	reduced Damköhler number; flow time divided by chemical time
Da_E	Damköhler number at extinction
Da_I	Damköhler number at ignition
D_j	mass diffusion coefficient of species j
E	extinction state (when used in Fig.1)
E	activation temperature
F	fuel
f	nondimensional stream function
h	half width of the slot
I	ignition state
Le_j	local Lewis number of species j; thermal diffusivity of mixture divided by mass diffusivity of species j into mixture
ℓ_F	perturbation of the fuel Lewis number from unity

M linear momentum per unit depth of the slot

O oxidizer

p pressure

p_a atmospheric pressure

P combustion products

Pr local Prandtl number; mixture viscosity divided by mixture thermal diffusivity

q_F heat of combustion per unit mass of the fuel

R ideal gas constant ($R°/W^*$)

$R°$ universal gas constant

Sc_j local Schmidt number of species j; mixture viscosity divided by mass diffusivity of species j into mixture

T temperature

u flow velocity in the x (streamwise) direction

v flow velocity in the y (transverse) direction

w thickness of the wall

W^* average molecular weight

W_j molecular weight of species j

x streamwise spatial coordinate

x_0 distance between the virtual origin of the jet to the exit of the slot

y transverse spatial coordinate ($y = 0$ on the plane of symmetry)

Y_j mass fraction of species j

Greek Symbols

α parameter defined as $\alpha = (\tilde{T}_\infty - \tilde{T}_0)/\tilde{Y}_{F,0}$

β parameter defined as $\beta = (\tilde{T}_0 - \tilde{T}_\infty)/\tilde{Y}_{O,\infty}$

ε small parameter, defined as $\varepsilon = \tilde{T}_\infty^{\,2}/\tilde{E}$, used for asymptotic expansion

ϕ_F perturbation of fuel concentration in the inner, reaction region (because of the weak reaction)

Φ_F perturbation of fuel concentration in the outer, chemically inert region (because of the weak reaction)

ϕ_O perturbation of oxidizer concentration in the inner, reaction region

Φ_O perturbation of oxidizer concentration in the outer, chemically inert region (because of the weak reaction)

γ specific heat ratio (c_p/c_v)

η similarity variable

λ thermal conductivity

μ dynamic viscosity

ν_j stoichiometric coefficient of species j

θ perturbation of temperature in the inner, reaction region (because of the weak reaction)

Θ perturbation of temperature in the outer, chemically inert region (because of the weak reaction)

ρ gas density

σ parameter defined as $\sigma = \tilde{Y}_{F,0} / \tilde{x}^{1/3}$

ω reaction rate function

ξ spatial coordinate defined as $\xi = \operatorname{sech}^2 \eta$

ψ streamfunction

ζ stretched spatial coordinate in the inner, reaction region (inner variable)

$\bar{\zeta}$ rescaled inner spatial coordinate defined as $\bar{\zeta} = \sigma\zeta$

Subscripts

0 value of variables at the exit of the slot

f frozen solution

F fuel

i value of variables in the fuel supply

O oxidizer

P combustion products

T temperature

∞ value of variables at the ambient

Superscripts

nj reaction order of species *j*

~ nondimensional quantity

$\wedge$ rescaled nondimensional quantity

Chapter 1: Introduction

1.1 Motivation for Project

Concerns about the emissions of greenhouse gases have led to extensive consideration of hydrogen as a major fuel carrier. Hydrogen presents several unusual fire hazards, including high leak propensity, ease of ignition, and invisible flames. Heated air jets flowing into hydrogen ignite spontaneously at an air temperature of 943 K [1]. This is cooler than for most other fuels [2,3], including gasoline and methane, and is not much higher than the autoignition temperature of stoichiometric hydrogen/air mixtures, 858 K [4]. Occasional unintended hydrogen leaks will be unavoidable, and some may involve heated hydrogen and/or air. Thus an improved understanding of limits of spontaneous ignition of hydrogen jets is sought here, with the aid of activation-energy asymptotics.

1.2 Literature Review

Asymptotic flame theories can provide valuable insights into combustion reactions [5-7]. Quantitative and predictive derivations can be made using the concept of distinguished limits in activation energy asymptotics. Based largely on the concept of Zel'dovich number, asymptotic analysis enables derivation and establishing of temperature effects on reaction rates despite the narrowness of the reaction zone relative to the preheat zone of the laminar flame structure.

Im et al. [8,9] analyzed thermal ignition in supersonic hydrogen/air mixing layers and obtained ignition characteristics over a wide range of conditions. The findings were however based on reduced mechanisms and supersonic flows, which are more applicable for scramjets. An investigation of different combustion regimes by Damköhler-number and activation-energy asymptotics in a stagnant mixing layer, based on an eight-step reduced mechanisms was performed by Lee and Chung [10]. Helenbrook and Law investigated the ignition of hydrogen/air mixing layer with reduced reaction mechanisms which they developed [11,12]. However, no single-step reaction mechanism was developed. Compared to a single-step, overall, irreversible reaction with second order Arrhenius kinetics and a high activation energy (which was used in the research), the reduced mechanism has different assumptions in length scales in determining the reaction rates, which will yield different results with emphasis on temperature dependence for thermal runaway. This is because the emphasis for reduced mechanisms is on the role of chemical kinetic mechanisms, involving chain-branching and termination reactions, in effecting a non-linear feedback in the concentrations of certain radicals and consequently, thermal runaway.

Zheng and Law [13] identified ignition limits of premixed hydrogen-air flames where ignition was by heated counterflow. Ignition limits of non-premixed hydrogen-air flames from jets will be different because of the non-premixed combustion mode and the absence of strain due to counterflow heating. Toro et al. [14] examined in detail the structure of laminar hydrogen jet flames both experimentally and numerically. For completeness, analytical results should be obtained to enable comparison with experimental and numerical results, under the same conditions and scenarios. Chaos et al. [15] examined Lewis-number effects in unsteady laminar hydrogen jet flames, which will have different effects compared to a steady laminar hydrogen jet flame. Liu and Pei [16] examined autoignition and explosion limits of hydrogen-oxygen mixtures in homogenous systems, which involved reduced mechanisms. Dryer et al. [17] examined spontaneous ignition of pressurized releases of hydrogen and natural gas into air, which investigated multi-dimensional transient flows involving shock formation, reflection and interactions which resulted in the transition to turbulent jet diffusive combustion. This is a different aspect of risk associated with rapid failures of compressed storages, as compared to the scenario being considered here, involving small leaks/cracks that are undetected, and that ignite spontaneously when the limits are reached.

1.3 Combustion S-curve

In understanding and analyzing the limits of spontaneous ignition of hydrogen jets, it is important to appreciate the fundamentals of flame ignition and extinction, which can be characterized and explained by the famous combustion S-curve [5,7,18]. The S-curve, as shown in Fig. 1.1, comprises 3 branches, the lower, middle and upper branches. The y-axis represents the reaction temperature, and the x-axis represents the Damköhler-number (Da). Starting with the left end of the lower branch, at $Da = 0$, we have the chemically frozen flow limit. By increasing Da along this branch, every possible weakly reacting state that the system can have was covered. Da_I represents the ignition Da, at which weak reactions transition to vigorous burning with a sudden jump to the upper branch. Anywhere beyond this Da will result in spontaneous combustion. We define this point as the ignition state. Conversely, as we decrease the Da for an intense burning flame on the upper branch to the point Da_E, there will be another jump of the temperature down to the lower branch. This point is defined as the extinction Da.

Physically, the existence of turning points implies that there exist states for which the chemical reaction rate cannot balance the heat transport rate in steady state. Thus for the lower branch, beyond Da_I, the chemical heat is generated so fast in the reaction zone that it cannot be transported away in steady manner. The middle branch is never observed because it has a negative slope which implies that reaction temperature decreases as *Da* increases, which is physically unrealistic.

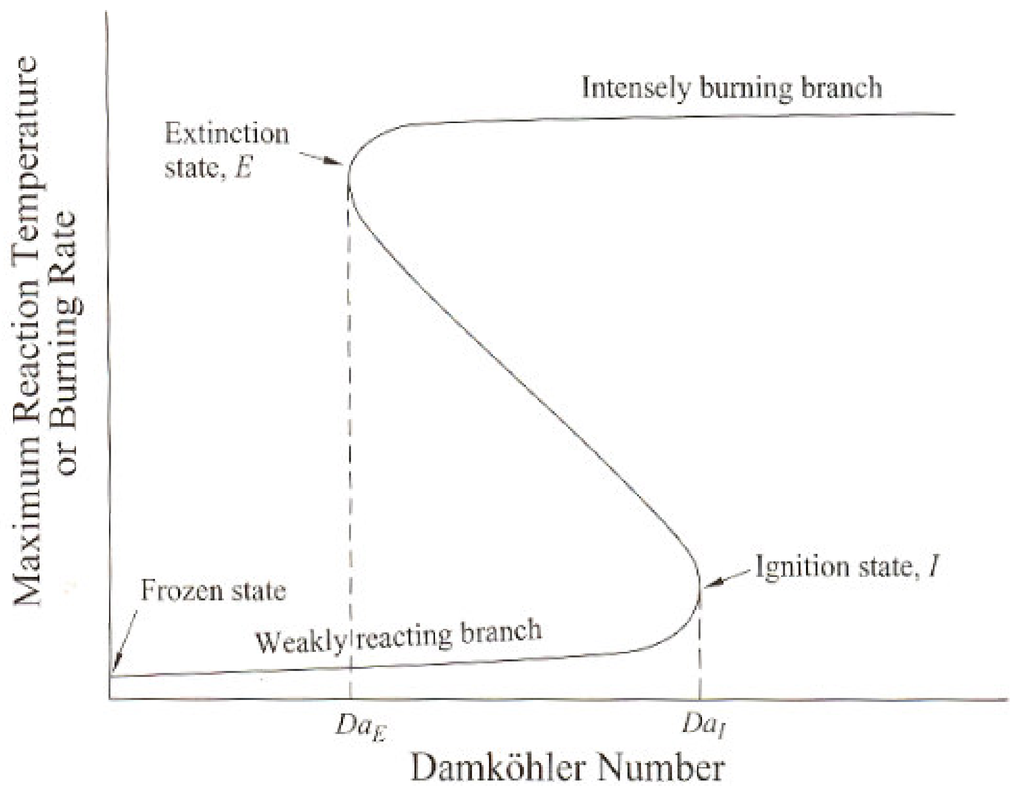

Fig. 1.1: Combustion S-Curve reproduced from [18].

<u>*1.4 Activation Energy Asymptotics*</u>

There are a number of possible approaches to modeling the influences of finite-rate chemistry on diffusion flames. Known rates of elementary reaction steps may be employed in the full set of conservation equations, with solutions sought by numerical integration and computational fluid dynamics (CFD). While CFD is like an experiment, with only one condition considered at a time, other modeling such as activation-energy asymptotics (AEA) can quickly identify trends and give additional physical insights. Complexities of diffusion flame problems motivates searches for simplifications of the chemical kinetics [19]. With simplified chemical kinetics, perturbation methods [20] are attractive for improving understanding and also for seeking quantitative comparison with experiment results. Two types of perturbation approaches have been developed, Damköhler-number asymptotics and AEA. In the former, the ratio of a flow time to reaction time, one of the dimensionless groups introduced by Damköhler [21] is treated as a large parameter. And in the latter, the ratio of the activation energy to the thermal energy, emphasized as important by Frank-Kamenetskii [22], is taken to be large. Damköhler-number asymptotics can provide estimates of reaction zone broadening in near-equilibrium situations [23,24], and also affords possibilities of investigating other regimes [25].

Analyses of phenomena such as sharp ignition and extinction events cannot be performed on the basis of Damköhler-number asymptotics, but they can be treated by activation-energy asymptotics. Moreover, activation-energy asymptotics may lead to results valid for all Damköhler numbers, and therefore results of Damköhler-number asymptotics may be extracted from those of activation-energy asymptotics. Activation-energy asymptotics is the more general of the two types of perturbation approaches. As compared to CFD, AEA was selected for our study as it provides the complete physics of the problem instead of just providing exact solutions for individual points, and provides a good representation of trends and limit behavior, which is sought here.

In the research, the AEA approach which was adopted to derive the exact solutions to the Navier-Stokes Equations can be summarized as:

1) Solutions of the flowfield for the scenario of hydrogen jet emanating from a rectangular slot were derived. A similarity solution of the non-reacting flowfield is obtained, and then used in the energy and species conservation equations. Coordinate transformation is necessary to investigate the effects of perturbations because the reaction zone of concern is a very small thin one.
2) Frozen solutions were then obtained. These represent the solutions in very low *Da* regime whereby there are no reactions.
3) Outer solutions were derived. These solutions deviate from the frozen solution by a small amount due to perturbation, and are present in outer regions where there is no reaction due to the low temperature. Before ignition, there are only weak reactions.
4) Inner solutions were derived for the reaction zone where weak chemical reactions occur.
5) Matching of inner and outer solutions is then performed to determine the conditions whereby ignition can occur. Ignition can occur when the heat generated from the chemical reaction is sufficient to overcome heat losses. The results are presented in terms of *Da*, T_o, T_∞, Le_F, and Le_o.

1.5 Project Objectives

The present analysis considers the spontaneous ignition of a jet of hydrogen or other gaseous fuel leaking through a slot into air. The slot is taken to be straight and long, yielding a two-dimensional flow field. The ignition analysis identifies limits of spontaneous ignition.

The objectives of this work are to:

1) develop a model of spontaneous ignition for two cases: a cool fuel jet flowing into heated air and a heated fuel jet flowing into cool air,
2) identify limits of spontaneous ignition as functions of slot width, flow rate, fuel Lewis number, and temperatures of the fuel jet and the ambient air, and
3) identify the location of ignition.

Chapter 2: Formulation

2.1 Introduction

The problem of interest is a steady, isobaric laminar jet of fuel (e.g. hydrogen) at temperature T_0 issuing from a rectangular slot into an oxidizing environment (e.g. atmospheric air) at a temperature of T_∞, as shown schematically in Figs. 2.1 and 2.2 for the two scenarios. Spontaneous ignition occurs when either T_0 or T_∞ is sufficiently high that the weak reaction between the fuel and the oxidizer transitions to a vigorous burning flame. This study analyzes the ignition state as a function of various physical properties including Lewis number, T_0, T_∞, the flow velocity at the slot exit, u_0, and the width of the slot. The slot is considered sufficiently long that end effects are negligible. The reaction chemistry is simulated by a single-step, overall, irreversible reaction with second order Arrhenius kinetics and a high activation energy.

The formulation that follows is an exact solution of the conservation of mass, momentum, energy and species. The key assumptions are boundary layer behavior $(\frac{\partial}{\partial y} \gg \frac{\partial}{\partial x})$ and single-step chemistry. A similarity solution of the non-reacting flowfield is obtained. This is then used in the conservation of energy and species equations.

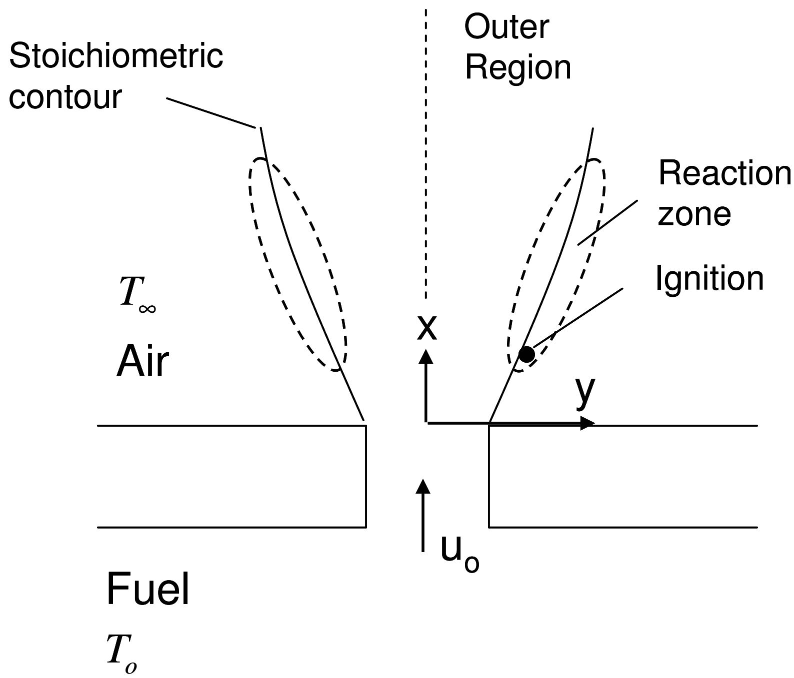

Fig. 2.1: Schematic of slot and hydrogen leak for hot ambient case

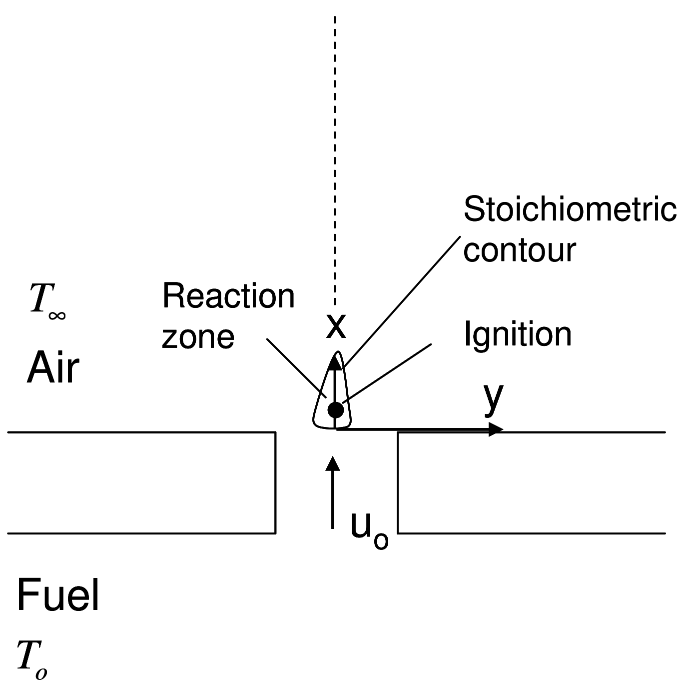

Fig. 2.2: Schematic of slot and hydrogen leak for hot jet case

2.2 Assumptions

The assumptions are as follow:

(1) steady, 2D flow, negligible body force

(2) reaction follows Arrhenius kinetics

(3) high activation energy reaction

(4) isobaric flow

(5) symmetric with respect to the plane of symmetry

(6) c_p, $\rho\,\lambda$, $\rho\,\mu$, and $\rho^2\,D_i$ do not vary with position

These assumptions are reasonable in light of the mathematical simplicity they introduce. Similar assumptions are commonly invoked in this type of analysis. [11,12]

2.3 Slot Flowfield

The reaction is

$$\nu_F\,F + \nu_O\,O \rightarrow \nu_P\,P \tag{2.1}$$

The flowfield is described by conservation of mass,

$$\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}=0 \tag{2.2}$$

conservation of momentum, x-direction

$$\rho u\frac{\partial u}{\partial x}+\rho v\frac{\partial u}{\partial y}-\frac{\partial}{\partial x}\left\{\mu\left[2\frac{\partial u}{\partial x}-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)\right]\right\}-\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]=-\frac{\partial p}{\partial x} \tag{2.3}$$

and conservation of momentum, y-direction

$$\rho u\frac{\partial v}{\partial x}+\rho v\frac{\partial v}{\partial y}-\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)\right]-\frac{\partial}{\partial y}\left\{\mu\left[2\frac{\partial v}{\partial y}-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)\right]\right\}=-\frac{\partial p}{\partial y} \tag{2.4}$$

Within the slot, the only velocity component is u along the x direction : $v = 0$

$$\frac{\partial(\rho u)}{\partial x} = 0 \quad \text{Therefore, } \rho u \text{ is independent of } x_o \tag{2.5}$$

Conservation of momentum becomes

$$\rho u \frac{\partial u}{\partial x} - \frac{4}{3}\frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) = -\frac{\partial p}{\partial x} \tag{2.6}$$

$$\frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial y}\right) - \frac{2}{3}\frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial x}\right) = \frac{\partial p}{\partial y} \tag{2.7}$$

$y = 0$: $\partial u / \partial x = 0$

Case I Uniform flow

A uniform flow is possible when the effect of viscosity is negligible ($\mu \approx 0$).

At any x, u is uniform for all y

$\frac{\partial p}{\partial y} = 0$ leading to $p = p(x)$

$\rho u \frac{du}{dx} = -\frac{dp}{dx}$ leading to $\rho u^2 = c - p$ (Bernoulli Equation)

In the tank : $u = 0$, $p = p_i$, therefore $c = p_i$

At the exit : $u = u_0$, $p = p_0$, $\rho = \rho_0$ therefore, $\rho_0 u_0^2 = p_i - p_0$ or

$$u_0 = \sqrt{(p_i - p_0)/\rho_0} \tag{2.8}$$

$$M = \int_{-h}^{h} \rho_0 u_0^2 \, dy = \int_{-h}^{h} (p_i - p_0) dy = (p_i - p_0) \int_{-h}^{h} dy = 2h(p_i - p_0) \tag{2.9}$$

For this case, there is no friction. The flow is supported by the expansion caused by the pressure reduction so ρ cannot be considered constant. If the pressure difference is large, the flow is choked (Ma = 1 at the exit).

If there is no heat addition or generation during the expansion, the gas temperature density and velocity at the exit (T_0, ρ_0 and u_0) are (isentropic compressible flow)

$$T_0/T_i = 2/(\gamma+1) \quad , \quad \gamma = c_p/c_v \tag{2.10}$$

$$p_0/p_i = [2/(\gamma+1)]^{\gamma/(\gamma-1)} \tag{2.11}$$

$$\rho_0/\rho_i = [2/(\gamma+1)]^{1/(\gamma-1)} \tag{2.12}$$

An expansion wave exists if $p_a < p_0$.

Case II Fully developed flow in a channel : $u = u(y)$

The flow velocity is relatively low so the flow can be considered incompressible and isothermal

$\frac{\partial p}{\partial y} = 0$ leading to $p = p(x)$ ($\mu = \mu_i = \mu_0$ = constant when ρ = constant)

$$\frac{d}{dy}\left(\mu_0 \frac{du}{dy}\right) = \frac{dp}{dx} \tag{2.13}$$

since lefthand side is a function of *y* only and righthand side is a function of *x* only,

$\frac{dp}{dx}$ = constant.

$$dp/dx = -(p_i - p_0)/w \quad w \text{ is the thickness of the wall,} \quad p_0 = p_a \tag{2.14}$$

$$\frac{du}{dy} = \frac{1}{\mu_0}\frac{dp}{dx}y + c_1 = -\frac{p_i - p_0}{\mu_0 w}y + c_1 \quad \text{and} \quad u = -\frac{p_i - p_0}{2\mu_0 w}y^2 + c_1 y + c_2 \tag{2.15}$$

At $y = 0$ (centerline) : $\frac{du}{dy} = 0$

$$\text{therefore} \quad c_1 = 0 \quad \text{leading to} \quad u = -\frac{p_i - p_0}{2\mu_0 w}y^2 + c_2 \tag{2.16}$$

At $y = h$ (channel wall) : $u = 0$

$$\text{therefore} \quad c_2 = \frac{p_i - p_0}{2\mu_0 w}h^2 \quad \text{leading to} \quad u = \frac{p_i - p_0}{2\mu_0 w}(h^2 - y^2) \tag{2.17}$$

$$M=\int_{-h}^{h}\rho_0 u^2\,dy=\int_{-h}^{h}\rho_0\left[\frac{p_i-p_0}{2\mu_0 w}(h^2-y^2)\right]^2 dy=\rho_0\left(\frac{p_i-p_0}{2\mu_0 w}\right)^2\int_{-h}^{h}(h^4-2h^2y^2+y^4)\,dy \qquad (2.18)$$

$$=\rho_0\left(\frac{p_i-p_0}{2\mu_0 w}\right)^2\left(h^4y-\frac{2}{3}h^2y^3+\frac{1}{5}y^5\right)_{-h}^{h}=\rho_0\left(\frac{p_i-p_0}{2\mu_0 w}\right)^2[h^4(2h)-\frac{2}{3}h^2(2h^3)+\frac{1}{5}(2h^5)]=\frac{4}{15}\rho_0 h^5\left(\frac{p_i-p_0}{\mu_0 w}\right)^2$$

At $y=0$: $u=u_0$ $\quad\therefore\quad$ $u_0=\dfrac{p_i-p_0}{2\mu_0 w}h^2$

2.4 Conservation Equations and Boundary Conditions in the Jet

(a) Conservation equations

$p=\rho RT$ or $\rho=p/(RT)$; R = ideal gas constant , p = constant (isobaric flow)

$$\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}=0 \qquad (2.19)$$

$\dfrac{\partial p}{\partial y}=0$ leading to $p=p(x)$

$\rho u\dfrac{\partial u}{\partial x}+\rho v\dfrac{\partial u}{\partial y}-\dfrac{\partial}{\partial y}\left(\mu\dfrac{\partial u}{\partial y}\right)=-\dfrac{\partial p}{\partial x}=-\dfrac{dp}{dx}=0$ (At any x, as $y\to\pm\infty$, $u\to 0$ therefore $\dfrac{dp}{dx}=0$)

Conservation of energy is,

$$\rho u c_p\frac{\partial T}{\partial x}+\rho v c_p\frac{\partial T}{\partial y}-\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)=\nu_F W_F q_F\omega \qquad (2.20)$$

Conservation of fuel is,

$$\rho u\frac{\partial Y_F}{\partial x}+\rho v\frac{\partial Y_F}{\partial y}-\frac{\partial}{\partial y}\left(\rho D_F\frac{\partial Y_F}{\partial y}\right)=-\nu_F W_F\omega \qquad (2.21)$$

Conservation of oxidizer is,

$$\rho u \frac{\partial Y_O}{\partial x} + \rho v \frac{\partial Y_O}{\partial y} - \frac{\partial}{\partial y}\left(\rho D_O \frac{\partial Y_O}{\partial y} \right) = -\nu_O W_O \, \omega \tag{2.22}$$

Conservation of oxidizer is,

$$\omega = B c_F^{n_F} c_O^{n_O} T^{n_T} \exp(-E/T) = B(\rho Y_F / W_F)^{n_F} (\rho Y_O / W_O)^{n_O} T^{n_T} \exp(-E/T)$$

$$= (B / W_F^{n_F} W_O^{n_O}) \rho^{n_F + n_O} Y_F^{n_F} Y_O^{n_O} T^{n_T} \exp(-E/T) \tag{2.23}$$

(b) Boundary and interface conditions

Let $x = 0$ be the virtual origin of the jet and $x = x_0$ be the exit of the jet.

$x = x_0^-$, $-h < y < h$: $T = T_0$, $Y_F = Y_{F,0}$, $Y_O = 0$, $u = u_0$, $v = 0$

$y = 0$, $x = x_0^+$: $T = T_0$, $Y_F = Y_{F,0}$, $Y_O = 0$, $u = u_0$, $y = 0$, $x > x_0$:

$\partial T / \partial y = \partial Y_F / \partial y = \partial Y_O / \partial y = \partial u / \partial y = 0$, $v = 0$

$y \to \infty$: $T \to T_\infty$, $Y_F \to 0$, $Y_O \to Y_{O,\infty}$, $u \to 0$

2.5 Coordinate Transformation and the Solution of Momentum Equation

A stream function ψ is defined such that the continuity equation is satisfied :

$$\frac{\rho u}{\rho_\infty u_0} = \frac{\partial \psi}{\partial y} \quad , \quad \frac{\rho v}{\rho_\infty u_0} = -\frac{\partial \psi}{\partial x} \tag{2.24}$$

A new coordinate system is defined using similarity variables [26,27].

$$\eta = \frac{\alpha_1}{x^{2/3}} \int_0^y \frac{\rho}{\rho_\infty} dy' \quad , \quad \psi = \alpha_2 x^{1/3} f(\eta) \quad , \quad \tilde{x} = x / x_0 \tag{2.25}$$

(α_1 and α_2 are constants that are defined later to simplify the expression)

It is assumed that a similarity solution exists so that f is a function of η only.

Coordinate transformation from (x, y) to (x, η) yields

$$\frac{\partial}{\partial x}=\frac{\partial}{\partial x}\frac{\partial x}{\partial x}+\frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial x}=\frac{\partial}{\partial x}+\left[-\frac{2}{3}\frac{\alpha_1}{x^{5/3}}\int_0^y\frac{\rho}{\rho_\infty}d\,y'+\frac{\alpha_1}{x^{2/3}}\frac{\partial}{\partial x}\left(\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\right]\frac{\partial}{\partial \eta}$$

$$=\frac{\partial}{\partial x}-\frac{2\eta}{3x}\frac{\partial}{\partial \eta}+\frac{\alpha_1}{x^{2/3}}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\frac{\partial}{\partial \eta} \tag{2.26}$$

$$\frac{\partial}{\partial y}=\frac{\partial}{\partial x}\frac{\partial x}{\partial y}+\frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial y}=\frac{\partial}{\partial \eta}\left[\frac{\alpha_1}{x^{2/3}}\frac{\partial}{\partial y}\left(\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\right]=\frac{\alpha_1}{x^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta} \tag{2.27}$$

$$\frac{\rho u}{\rho_\infty u_0}=\frac{\partial \psi}{\partial y}=\frac{\alpha_1}{x^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta}\left[\alpha_2 x^{1/3} f(\eta)\right]=\frac{\alpha_1\alpha_2}{x^{1/3}}\frac{\rho}{\rho_\infty}\frac{df}{d\eta} \tag{2.28}$$

We define $\alpha_1\alpha_2=x_0{}^{1/3}$ or $\alpha_2=x_0{}^{1/3}/\alpha_1$ such that $\frac{u}{u_0}=\frac{x_0{}^{1/3}}{x^{1/3}}\frac{df}{d\eta}$ or $u=\frac{u_0}{\tilde{x}^{1/3}}\frac{df}{d\eta}$

$$\frac{\rho v}{\rho_\infty u_0}=-\frac{\partial \psi}{\partial x}=-\frac{\partial}{\partial x}\left[\frac{x_0{}^{1/3}}{\alpha_1}x^{1/3}f(\eta)\right]+\frac{2}{3x}\eta\frac{\partial}{\partial \eta}\left[\frac{x_0{}^{1/3}}{\alpha_1}x^{1/3}f(\eta)\right]$$
$$-\alpha_1 x^{-2/3}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\frac{\partial}{\partial \eta}\left[\frac{x_0{}^{1/3}}{\alpha_1}x^{1/3}f(\eta)\right]$$

$$=-\frac{x_0{}^{1/3}}{3\alpha_1 x^{2/3}}\left(f-2\eta\frac{df}{d\eta}\right)-\frac{x_0{}^{1/3}}{x^{1/3}}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\frac{df}{d\eta} \tag{2.29}$$

$$\frac{\partial u}{\partial x}=\frac{\partial}{\partial x}\left(\frac{x_0{}^{1/3}u_0}{x^{1/3}}\frac{df}{d\eta}\right)-\frac{2\eta}{3x}\frac{\partial}{\partial \eta}\left(\frac{x_0{}^{1/3}u_0}{x^{1/3}}\frac{df}{d\eta}\right)+\frac{\alpha_1}{x^{2/3}}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\frac{\partial}{\partial \eta}\left(\frac{x_0{}^{1/3}u_0}{x^{1/3}}\frac{df}{d\eta}\right)$$

$$=-\frac{x_0{}^{1/3}u_0}{3x^{4/3}}\left(\frac{df}{d\eta}+2\eta\frac{d^2f}{d\eta^2}\right)+\frac{\alpha_1 x_0{}^{1/3}u_0}{x}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\frac{d^2f}{d\eta^2} \tag{2.30}$$

$$\frac{\partial u}{\partial y}=\frac{\alpha_1}{x^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta}\left(\frac{x_0{}^{1/3}u_0}{x^{1/3}}\frac{df}{d\eta}\right)=\frac{\alpha_1 x_0{}^{1/3}u_0}{x}\frac{\rho}{\rho_\infty}\frac{d^2f}{d\eta^2} \tag{2.31}$$

$$\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)=\frac{\alpha_1}{x^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta}\left[\frac{\alpha_1 x_0{}^{1/3}u_0}{x}\frac{\rho\mu}{\rho_\infty}\frac{d^2f}{d\eta^2}\right]=\frac{\alpha_1{}^2 x_0{}^{1/3}u_0}{x^{5/3}}\frac{\rho^2\mu}{\rho_\infty{}^2}\frac{d^3f}{d\eta^3}$$
$$=\frac{\alpha_1{}^2 x_0{}^{1/3}u_0}{x^{5/3}}\frac{\rho\rho_\infty\mu_\infty}{\rho_\infty{}^2}\frac{d^3f}{d\eta^3}=\frac{\alpha_1{}^2 x_0{}^{1/3}u_0}{x^{5/3}}\frac{\rho\mu_\infty}{\rho_\infty}\frac{d^3f}{d\eta^3} \tag{2.32}$$

(It is assumed that $\rho\mu = \rho_\infty \mu_\infty$ =constant)

Momentum equation is given by,

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} - \frac{\partial}{\partial y}\left(\mu \frac{\partial u}{\partial y}\right) = 0 \tag{2.33}$$

$$\frac{\rho x_0^{1/3} u_0}{x^{1/3}} \frac{df}{d\eta}\left[-\frac{x_0^{1/3} u_0}{3x^{4/3}}\left(\frac{df}{d\eta} + 2\eta \frac{d^2 f}{d\eta^2}\right) + \frac{\alpha_1 x_0^{1/3} u_0}{x}\left(\frac{\partial}{\partial x}\int_0^y \frac{\rho}{\rho_\infty} dy'\right)\frac{d^2 f}{d\eta^2}\right]$$

$$+\left[-\frac{\rho_\infty u_0 x_0^{1/3}}{3\alpha_1 x^{2/3}}\left(f - 2\eta \frac{df}{d\eta}\right) - \frac{\rho_\infty u_0 x_0^{1/3}}{x^{1/3}}\left(\frac{\partial}{\partial x}\int_0^y \frac{\rho}{\rho_\infty} dy'\right)\frac{df}{d\eta}\right]\frac{\alpha_1 x_0^{1/3} u_0}{x}\frac{\rho}{\rho_\infty}\frac{d^2 f}{d\eta^2}$$

$$-\frac{\alpha_1^2 x_0^{1/3} u_0}{x^{5/3}}\frac{\rho \mu_\infty}{\rho_\infty}\frac{d^3 f}{d\eta^3} - \frac{\rho u_0^2 x_0^{2/3}}{3x^{5/3}}\left[\left(\frac{df}{d\eta}\right)^2 + f\frac{d^2 f}{d\eta^2} + \alpha_1^2 \frac{3\mu_\infty}{\rho_\infty u_0 x_0^{1/3}}\frac{d^3 f}{d\eta^3}\right] = 0 \tag{2.34}$$

We define $\alpha_1^2 \frac{3\mu_\infty}{\rho_\infty u_0 x_0^{1/3}} = \frac{1}{2}$ such that it leads to $\alpha_1 = \sqrt{\frac{\rho_\infty u_0 x_0^{1/3}}{6\mu_\infty}}$ and

$$\frac{1}{2}\frac{d^3 f}{d\eta^3} + f\frac{d^2 f}{d\eta^2} + \left(\frac{df}{d\eta}\right)^2 = 0 \tag{2.35}$$

$$\eta = \frac{\alpha_1}{x^{2/3}}\int_0^y \frac{\rho}{\rho_\infty} dy' = \sqrt{\frac{\rho_\infty u_0 x_0^{1/3}}{6\mu_\infty}}\frac{1}{x^{2/3}}\int_0^y \frac{\rho}{\rho_\infty} dy' = \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}}\frac{1}{\tilde{x}^{2/3}}\int_0^y \frac{\rho}{\rho_\infty} dy' \tag{2.36}$$

$$\psi = \alpha_2 x^{1/3} f(\eta) = \frac{x_0^{1/3}}{\alpha_1} x^{1/3} f(\eta) = x_0^{1/3}\sqrt{\frac{6\mu_\infty}{\rho_\infty u_0 x_0^{1/3}}}\, x^{1/3} f(\eta) = \sqrt{\frac{6\mu_\infty x_0}{\rho_\infty u_0}}\,\tilde{x}^{1/3} f(\eta) \tag{2.37}$$

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x} - \frac{2\eta}{3x}\frac{\partial}{\partial \eta} + \frac{\alpha_1}{x^{2/3}}\left(\frac{\partial}{\partial x}\int_0^y \frac{\rho}{\rho_\infty} dy'\right)\frac{\partial}{\partial \eta} = \frac{\partial}{\partial (x_0 \tilde{x})} - \frac{2\eta}{3x_0 \tilde{x}}\frac{\partial}{\partial \eta}$$
$$+\sqrt{\frac{\rho_\infty u_0 x_0^{1/3}}{6\mu_\infty}}\frac{1}{x_0^{2/3}\tilde{x}^{2/3}}\left(\frac{\partial}{\partial x}\int_0^y \frac{\rho}{\rho_\infty} dy'\right)\frac{\partial}{\partial \eta}$$

$$= \frac{1}{x_0}\frac{\partial}{\partial \tilde{x}} - \frac{1}{x_0}\frac{2\eta}{3\tilde{x}}\frac{\partial}{\partial \eta} + \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}}\frac{1}{\tilde{x}^{2/3}}\left(\frac{\partial}{\partial x}\int_0^y \frac{\rho}{\rho_\infty} dy'\right)\frac{\partial}{\partial \eta} \tag{2.38}$$

$$\frac{\partial}{\partial y} = \frac{\alpha_1}{x^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta} = \sqrt{\frac{\rho_\infty u_0 x_0^{1/3}}{6\mu_\infty}}\frac{1}{x_0^{2/3}\tilde{x}^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta} = \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}}\frac{1}{\tilde{x}^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial}{\partial \eta} \tag{2.39}$$

Boundary conditions

$y=0$, $x=x_0^+$: $u=u_0$ $\Rightarrow$ $\eta=0$: $df/d\eta=1$ (f is independent of x)

$y=0$, $x>x_0$: $\partial u/\partial y=v=0$ $\Rightarrow$ $\eta=0$, $x>x_0$: $f=d^2f/d\eta^2=0$

$y\to\infty$: $u\to 0$ $\Rightarrow$ $\eta\to\infty$: $df/d\eta\to 0$

Solution in the jet ($x>x_0$ or $\tilde{x}>1$)

$$0=\frac{1}{2}\frac{d^3f}{d\eta^3}+f\frac{d^2f}{d\eta^2}+\left(\frac{df}{d\eta}\right)^2=\frac{1}{2}\frac{d^3f}{d\eta^3}+\frac{d}{d\eta}\left(f\frac{df}{d\eta}\right)=\frac{d}{d\eta}\left(\frac{1}{2}\frac{d^2f}{d\eta^2}+f\frac{df}{d\eta}\right) \quad \text{therefore} \tag{2.40}$$

$$\frac{1}{2}\frac{d^2f}{d\eta^2}+f\frac{df}{d\eta}=c$$

$\eta=0$: $f=d^2f/d\eta^2=0$ therefore $c=0$ leading to $\frac{1}{2}\frac{d^2f}{d\eta^2}+f\frac{df}{d\eta}=0$

$$0=\frac{1}{2}\frac{d^2f}{d\eta^2}+f\frac{df}{d\eta}=\frac{1}{2}\frac{d^2f}{d\eta^2}+\frac{1}{2}\frac{df^2}{d\eta}=\frac{1}{2}\frac{d}{d\eta}\left(\frac{df}{d\eta}+f^2\right) \quad \text{therefore} \quad \frac{df}{d\eta}+f^2=c \tag{2.41}$$

Let $z=a\,\eta$, $f=a\,F(z)$, $c=a^2$ then $\frac{df}{d\eta}=\frac{d(aF)}{dz}\frac{dz}{d\eta}=a\frac{dF}{dz}a=a^2\frac{dF}{dz}$

$a^2\frac{dF}{dz}+\frac{(aF)^2}{2}=a^2$ or $\frac{dF}{dz}+F^2=1$ $\Rightarrow$ $\frac{dF}{dz}=1-F^2$ or $\frac{dF}{1-F^2}=dz$

$\tanh^{-1}F=z+c$ or $F=\tanh(z+c)$ or $\frac{f}{a}=\tanh(a\eta+c)$ or $f=a\tanh(a\eta+c)$

$\eta=0$: $f=0$, $df/d\eta=1$

$\tanh c=0$ or $c=0$ $\Rightarrow$ $f=a\tanh(a\,\eta)$ and $df/d\eta=a^2\,\mathrm{sech}^2(a\,\eta)$

$a^2\,\mathrm{sech}^2(0)=1$ therefore $a^2=1$ or $a=1$

Thus : $f=\tanh\eta$, $df/d\eta=\mathrm{sech}^2\,\eta$,

$$u=(u_0/\tilde{x}^{1/3})(df/d\eta)=u_0(\mathrm{sech}^2\eta)/\tilde{x}^{1/3} \tag{2.42}$$

$$\rho v = \rho_\infty u_0 \left[-\frac{x_0^{1/3}}{3\alpha_1 x^{2/3}} \left(f - 2\eta \frac{df}{d\eta} \right) - \frac{x_0^{1/3}}{x^{1/3}} \left(\frac{\partial}{\partial x} \int_0^y \frac{\rho}{\rho_\infty} dy' \right) \frac{df}{d\eta} \right] \tag{2.43}$$

$$= -\rho_\infty u_0 \left[\sqrt{\frac{6\mu_\infty}{\rho_\infty u_0 x_0^{1/3}}} \frac{x_0^{1/3}}{3x_0^{2/3} \tilde{x}^{2/3}} \left(f - 2\eta \frac{df}{d\eta} \right) + \frac{1}{\tilde{x}^{1/3}} \left(\frac{\partial}{\partial x} \int_0^y \frac{\rho}{\rho_\infty} dy' \right) \frac{df}{d\eta} \right] \tag{2.44}$$

$$= -\rho_\infty u_0 \left\{ \sqrt{\frac{6\mu_\infty}{\rho_\infty u_0 x_0}} \frac{(\tanh \eta) - 2\eta (\operatorname{sech}^2 \eta)}{3\tilde{x}^{2/3}} + \frac{\operatorname{sech}^2 \eta}{\tilde{x}^{1/3}} \left(\frac{\partial}{\partial x} \int_0^y \frac{\rho}{\rho_\infty} dy' \right) \right\} \tag{2.45}$$

Determination of x_0 by momentum conservation

$$\int_{-\infty}^{\infty} \rho u^2 \, dy = \int_{-h}^{h} \rho_0 u_0^2 \, dy = M$$

$$M = \int_{-\infty}^{\infty} \rho u^2 \, dy = \int_{-\infty}^{\infty} \rho \left(\frac{u_0}{\tilde{x}^{1/3}} \operatorname{sech}^2 \eta \right)^2 \left(\sqrt{\frac{6\mu_\infty x_0}{\rho_\infty u_0}} \tilde{x}^{2/3} \frac{\rho_\infty}{\rho} d\eta \right)$$

$$= u_0 \sqrt{6 x_0 u_0 \rho_\infty \mu_\infty} \int_{-\infty}^{\infty} (\operatorname{sech}^4 \eta) \, d\eta \tag{2.46}$$

$$= u_0 \sqrt{6 x_0 u_0 \rho_\infty \mu_\infty} \left[\left. \frac{(\operatorname{sech}^2 \eta)(\tanh \eta)}{3} \right|_{-\infty}^{\infty} + \frac{2}{3} \int_{-\infty}^{\infty} (\operatorname{sech}^2 \eta) d\eta \right]$$

$$= u_0 \sqrt{6 x_0 u_0 \rho_\infty \mu_\infty} \left[0 + \frac{2}{3} \tanh \eta \Big|_{-\infty}^{\infty} \right] = \frac{4}{3} u_0 \sqrt{6 x_0 u_0 \rho_\infty \mu_\infty} \tag{2.47}$$

Therefore $\quad \frac{32}{3} u_0^3 x_0 \rho_\infty \mu_\infty = M^2 \quad$ or $\quad x_0 = \frac{3M^2}{32 u_0^3 \rho_\infty \mu_\infty} \qquad (2.48)$

In summary, the flowfield solution is :

$\eta = \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \int_0^y \frac{\rho}{\rho_\infty} dy'$ (2.36), $\psi = \sqrt{\frac{6\mu_\infty x_0}{\rho_\infty u_0}} \tilde{x}^{1/3} f(\eta)$ (2.37), $x_0 = \frac{3M^2}{32 u_0^3 \rho_\infty \mu_\infty}$ (2.48)

$f = \tanh \eta \quad , \quad df/d\eta = \operatorname{sech}^2 \eta \quad , \quad u = u_0 (\operatorname{sech}^2 \eta) / \tilde{x}^{1/3} \qquad (2.42)$

$$\frac{\partial}{\partial x} = \frac{1}{x_0} \frac{\partial}{\partial \tilde{x}} - \frac{1}{x_0} \frac{2\eta}{3\tilde{x}} \frac{\partial}{\partial \eta} + \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \left(\frac{\partial}{\partial x} \int_0^y \frac{\rho}{\rho_\infty} dy' \right) \frac{\partial}{\partial \eta} \tag{2.38}$$

$$\frac{\partial}{\partial y} = \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \frac{\rho}{\rho_\infty} \frac{\partial}{\partial \eta} \tag{2.39}$$

$$\rho v = -\rho_\infty u_0 \left\{ \sqrt{\frac{6\mu_\infty}{\rho_\infty u_0 x_0}} \frac{(\tanh \eta) - 2\eta (\operatorname{sech}^2 \eta)}{3\tilde{x}^{2/3}} + \frac{\operatorname{sech}^2 \eta}{\tilde{x}^{1/3}} \left(\frac{\partial}{\partial x} \int_0^y \frac{\rho}{\rho_\infty} dy' \right) \right\} \tag{2.45}$$

2.6 Nondimensionalizing the Energy and Species Equations

The following nondimensional quantities are defined as :

$$\tilde{T} = \frac{c_p T}{q_F} \quad , \quad \tilde{Y}_F = Y_F \quad , \quad \tilde{Y}_O = \frac{\nu_F W_F}{\nu_O W_O} Y_O \quad , \quad \tilde{E} = \frac{c_p E}{q_F} \tag{2.49}$$

Damköhler number: $$Da = \frac{6 x_0 \nu_O^{n_O} B}{\nu_F^{n_O - 1} W_F^{n_O + n_F - 1} u_0} \left(\frac{q_F}{c_p}\right)^{n_T - n_F - n_O + 1} \left(\frac{p}{R}\right)^{n_F + n_O - 1} \tag{2.50}$$

Prandtl number : $$Pr = \frac{\mu}{\lambda / c_p} = \frac{\rho\mu}{\rho\lambda / c_p} = \text{constant} \tag{2.51}$$

Schmidt number of species j : $$Sc_j = \frac{\mu}{\rho D_j} = \frac{\rho\mu}{\rho^2 D_j} = \text{constant} \tag{2.52}$$

Lewis number of species j : $$Le_j = \frac{\lambda / c_p}{\rho D_j} = \frac{Sc_j}{Pr} = \text{constant} \tag{2.53}$$

Nondimensionlizing the energy equation:

(1) $$\rho = p/(RT) = (p/R)(c_p/q_F)/\tilde{T} \tag{2.54}$$

(2) $$\rho u c_p \frac{\partial T}{\partial x} + \rho v c_p \frac{\partial T}{\partial y} - \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) = \frac{\nu_F W_F B}{W_F^{n_F} W_O^{n_O}} q_F \rho^{n_F + n_O} Y_F^{n_F} Y_O^{n_O} T^{n_T} \exp(-E/T)$$

$$\frac{q_F}{c_p}\left[\rho u c_p \frac{\partial \tilde{T}}{\partial x} + \rho v c_p \frac{\partial \tilde{T}}{\partial y} - \frac{1}{\Pr}\frac{\partial}{\partial y}\left(\mu c_p \frac{\partial \tilde{T}}{\partial y}\right)\right]$$
$$= \frac{\nu_F W_F B}{W_F^{n_F} W_O^{n_O}} q_F \rho^{n_F + n_O} Y_F^{n_F} \left(\frac{\nu_O W_O}{\nu_F W_F}\tilde{Y}_O\right)^{n_O} \left(\frac{q_F}{c_p}\tilde{T}\right)^{n_T} \exp(-\tilde{E}/\tilde{T}) \tag{2.55}$$

$$\rho u \frac{\partial \tilde{T}}{\partial x} + \rho v \frac{\partial \tilde{T}}{\partial y} - \frac{1}{\Pr}\frac{\partial}{\partial y}\left(\mu \frac{\partial \tilde{T}}{\partial y}\right)$$
$$= \frac{\nu_O^{n_O} B}{\nu_F^{n_O - 1} W_F^{n_O + n_F - 1}} (q_F / c_p)^{n_T} \rho^{n_F + n_O} \tilde{Y}_F^{n_F} \tilde{Y}_O^{n_O} \tilde{T}^{n_T} \exp(-\tilde{E}/\tilde{T}) \tag{2.56}$$

$$\frac{\partial \tilde{T}}{\partial x} = \frac{1}{x_0}\frac{\partial \tilde{T}}{\partial \tilde{x}} - \frac{1}{x_0}\frac{2\eta}{3\tilde{x}}\frac{\partial \tilde{T}}{\partial \eta} + \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \left(\frac{\partial}{\partial x}\int_0^y \frac{\rho}{\rho_\infty} dy'\right) \frac{\partial \tilde{T}}{\partial \eta} \quad ; \quad \frac{\partial \tilde{T}}{\partial y} = \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \frac{\rho}{\rho_\infty} \frac{\partial \tilde{T}}{\partial \eta}$$

$$\frac{\partial}{\partial y}\left(\mu \frac{\partial \tilde{T}}{\partial y}\right) = \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \frac{\rho}{\rho_\infty} \frac{\partial}{\partial \eta}\left(\mu \sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}} \frac{1}{\tilde{x}^{2/3}} \frac{\rho}{\rho_\infty} \frac{\partial \tilde{T}}{\partial \eta}\right) = \frac{\rho u_0}{6 x_0} \frac{1}{\tilde{x}^{4/3}} \frac{\partial^2 \tilde{T}}{\partial \eta^2} \tag{2.57}$$

($\rho\mu = \rho_\infty \mu_\infty$ = constant)

$$\rho u\frac{\partial\tilde{T}}{\partial x}+\rho v\frac{\partial\tilde{T}}{\partial y}-\frac{1}{Pr}\frac{\partial}{\partial y}\left(\mu\frac{\partial\tilde{T}}{\partial y}\right)=$$

$$\rho u_0\frac{\operatorname{sech}^2\eta}{\tilde{x}^{1/3}}\left[\frac{1}{x_0}\frac{\partial\tilde{T}}{\partial\tilde{x}}-\frac{1}{x_0}\frac{2\eta}{3\tilde{x}}\frac{\partial\tilde{T}}{\partial\eta}+\sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}}\frac{1}{\tilde{x}^{2/3}}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\frac{\partial\tilde{T}}{\partial\eta}\right]$$
$$-\frac{1}{\Pr}\frac{\rho u_0}{6x_0}\frac{1}{\tilde{x}^{4/3}}\frac{\partial^2\tilde{T}}{\partial\eta^2}-\rho_\infty u_0\left\{\sqrt{\frac{6\mu_\infty}{\rho_\infty u_0 x_0}}\frac{(\tanh\eta)-2\eta(\operatorname{sech}^2\eta)}{3\tilde{x}^{2/3}}+\frac{\operatorname{sech}^2\eta}{\tilde{x}^{1/3}}\left(\frac{\partial}{\partial x}\int_0^y\frac{\rho}{\rho_\infty}d\,y'\right)\right\}$$
$$\left(\sqrt{\frac{\rho_\infty u_0}{6\mu_\infty x_0}}\frac{1}{\tilde{x}^{2/3}}\frac{\rho}{\rho_\infty}\frac{\partial\tilde{T}}{\partial\eta}\right)$$

$$=\frac{\rho u_0}{x_0}\frac{(\operatorname{sech}^2\eta)}{\tilde{x}^{1/3}}\frac{\partial\tilde{T}}{\partial\tilde{x}}-\frac{\rho u_0}{x_0}\frac{(\tanh\eta)}{3\tilde{x}^{4/3}}\frac{\partial\tilde{T}}{\partial\eta}-\frac{1}{\Pr}\frac{\rho u_0}{6x_0}\frac{1}{\tilde{x}^{4/3}}\frac{\partial^2\tilde{T}}{\partial\eta^2}$$
$$=-\frac{\rho u_0}{6x_0\tilde{x}^{4/3}}\left[\frac{1}{\Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2}+2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right] \tag{2.58}$$

$$\frac{1}{Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2}+2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}$$

$$=-\frac{6x_0\tilde{x}^{4/3}}{\rho u_0}\frac{\nu_O{}^{n_O}B}{\nu_F{}^{n_O-1}W_F{}^{n_O+n_F-1}}\left(\frac{q_F}{c_p}\right)^{n_T}\rho^{n_F+n_O}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T}\exp(-\tilde{E}/\tilde{T})$$

$$=-Da\tilde{x}^{4/3}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}) \tag{2.59}$$

(3) $\rho u\frac{\partial Y_F}{\partial x}+\rho v\frac{\partial Y_F}{\partial y}-\frac{\partial}{\partial y}\left(\rho D_F\frac{\partial Y_F}{\partial y}\right)=-\frac{\nu_F W_F B}{W_F{}^{n_F}W_O{}^{n_O}}\rho^{n_F+n_O}Y_F{}^{n_F}Y_O{}^{n_O}T^{n_T}\exp(-E/T)$

$$\rho u\frac{\partial\tilde{Y}_F}{\partial x}+\rho v\frac{\partial\tilde{Y}_F}{\partial y}-\frac{\partial}{\partial y}\left(\frac{\rho D_F}{\mu}\mu\frac{\partial\tilde{Y}_F}{\partial y}\right)$$

$$=-\frac{\nu_F W_F B}{W_F{}^{n_F}W_O{}^{n_O}}\rho^{n_F+n_O}Y_F{}^{n_F}\left(\frac{\nu_O W_O}{\nu_F W_F}\tilde{Y}_O\right)^{n_O}\left(\frac{q_F}{c_p}\tilde{T}\right)^{n_T}\exp(-\tilde{E}/\tilde{T})\ \rho u\frac{\partial\tilde{Y}_F}{\partial x}+\rho v\frac{\partial\tilde{Y}_F}{\partial y}-\frac{1}{Sc_F}\frac{\partial}{\partial y}\left(\mu\frac{\partial\tilde{Y}_F}{\partial y}\right)$$
$$=-\frac{\nu_O{}^{n_O}B}{\nu_F{}^{n_O-1}W_F{}^{n_O+n_F-1}}(q_F/c_p)^{n_T}\rho^{n_F+n_O}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T}\exp(-\tilde{E}/\tilde{T}) \tag{2.60}$$

By the same analysis as that of (2), we have (change Pr to Sc_F and the sign of the righthand side)

$$\frac{1}{Sc_F}\frac{\partial^2\tilde{Y}_F}{\partial\eta^2}+2(\tanh\eta)\frac{\partial\tilde{Y}_F}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}=Da\tilde{x}^{4/3}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}) \tag{2.61}$$

(4) $\rho u \dfrac{\partial Y_O}{\partial x} + \rho v \dfrac{\partial Y_O}{\partial y} - \dfrac{\partial}{\partial y}\left(\rho D_O \dfrac{\partial Y_O}{\partial y}\right) = -\dfrac{\nu_O W_O B}{W_F{}^{n_F} W_O{}^{n_O}} \rho^{n_F+n_O} Y_F{}^{n_F} Y_O{}^{n_O} T^{n_T} \exp(-E/T)$

$$\frac{\nu_O W_O}{\nu_F W_F}\left[\rho u \frac{\partial \tilde{Y}_O}{\partial x} + \rho v \frac{\partial \tilde{Y}_O}{\partial y} - \frac{\partial}{\partial y}\left(\frac{\rho D_O}{\mu}\mu \frac{\partial \tilde{Y}_O}{\partial y}\right)\right]$$
$$= -\frac{\nu_O W_O B}{W_F{}^{n_F} W_O{}^{n_O}} q_F \rho^{n_F+n_O} Y_F{}^{n_F}\left(\frac{\nu_O W_O}{\nu_F W_F}\tilde{Y}_O\right)^{n_O}\left(\frac{q_F}{c_p}\tilde{T}\right)^{n_T} \exp(-\tilde{E}/\tilde{T})$$

$$\rho u \frac{\partial \tilde{Y}_O}{\partial x} + \rho v \frac{\partial \tilde{Y}_O}{\partial y} - \frac{1}{Sc_O}\frac{\partial}{\partial y}\left(\mu \frac{\partial \tilde{Y}_O}{\partial y}\right)$$
$$= -\frac{\nu_O{}^{n_O} B}{\nu_F{}^{n_O-1} W_F{}^{n_O+n_F-1}} (q_F/c_p)^{n_T} \rho^{n_F+n_O} \tilde{Y}_F{}^{n_F} \tilde{Y}_O{}^{n_O} \tilde{T}^{n_T} \exp(-\tilde{E}/\tilde{T}) \qquad (2.62)$$

Similar to (3), we have

$$\frac{1}{Sc_O}\frac{\partial^2 \tilde{Y}_O}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{Y}_O}{\partial \eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial \tilde{Y}_O}{\partial \tilde{x}} = Da\tilde{x}^{4/3}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}) \qquad (2.63)$$

(5) $y = 0$, $x = x_0{}^+$: $\quad T = T_0$, $\quad Y_F = Y_{F,0}$, $\quad Y_O = 0$

leading to $\quad \eta = 0$, $\tilde{x} = 1^+$: $\quad \tilde{T} = \tilde{T}_0 = \dfrac{c_p T_0}{q_F}$, $\quad \tilde{Y}_F = \tilde{Y}_{F,0} = Y_{F,0}$, $\quad \tilde{Y}_O = 0$

$y = 0$, $x > x_0$: $\quad \partial T/\partial y = \partial Y_F/\partial y = \partial Y_O/\partial y = 0$

leading to $\quad \eta = 0$, $\tilde{x} > 1$: $\quad \partial \tilde{T}/\partial \eta = \partial \tilde{Y}_F/\partial \eta = \partial \tilde{Y}_O/\partial \eta = 0$

$y \to \infty$: $\quad T \to T_\infty$, $\quad Y_F \to 0$, $\quad Y_O \to Y_{O,\infty}$, $\quad u \to 0$

leading to $\quad \eta \to \infty$: $\quad \tilde{T} \to \tilde{T}_\infty = \dfrac{c_p T_\infty}{q_F}$, $\quad \tilde{Y}_F \to 0$, $\quad \tilde{Y}_O \to \tilde{Y}_{O,\infty} = \dfrac{\nu_F W_F}{\nu_O W_O} Y_{O,\infty}$

(6) In summary

$$\frac{1}{Pr}\frac{\partial^2 \tilde{T}}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{T}}{\partial \eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial \tilde{T}}{\partial \tilde{x}} = -Da\tilde{x}^{4/3}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}) \qquad (2.59)$$

$$\frac{1}{Sc_F}\frac{\partial^2 \tilde{Y}_F}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{Y}_F}{\partial \eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial \tilde{Y}_F}{\partial \tilde{x}} = Da\tilde{x}^{4/3}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}) \qquad (2.61)$$

$$\frac{1}{Sc_O}\frac{\partial^2 \tilde{Y}_O}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{Y}_O}{\partial \eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial \tilde{Y}_O}{\partial \tilde{x}} = Da\tilde{x}^{4/3}\tilde{Y}_F{}^{n_F}\tilde{Y}_O{}^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}) \qquad (2.63)$$

$\eta = 0$, $\tilde{x} = 1$: $\tilde{T} = \tilde{T}_0$, $\tilde{Y}_F = \tilde{Y}_{F,0}$, $\tilde{Y}_O = 0$

$\eta = 0$, $\tilde{x} > 1$: $\partial\tilde{T}/\partial\eta = \partial\tilde{Y}_F/\partial\eta = \partial\tilde{Y}_O/\partial\eta = 0$

$\eta \to \infty$: $\tilde{T} \to \tilde{T}_\infty$, $\tilde{Y}_F \to 0$, $\tilde{Y}_O \to \tilde{Y}_{O,\infty}$

2.7 Frozen Solution

In the frozen limit (designated by a subscript "*f*"), there is no reaction

$$(1)\quad \frac{1}{Pr}\frac{\partial^2 \tilde{T}_f}{\partial \eta^2} + 2(\tanh\ \eta)\frac{\partial \tilde{T}_f}{\partial \eta} - 6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial \tilde{T}_f}{\partial \tilde{x}} = 0 \tag{2.64}$$

Since the energy and momentum equations are similar, it is expected that

$$\tilde{T}_f = c_1 + \hat{T}(\eta)/\tilde{x}^{1/3}$$

$$\frac{\partial \tilde{T}_f}{\partial \tilde{x}} = -\frac{1}{3}\frac{\hat{T}}{\tilde{x}^{4/3}} \quad , \quad \frac{\partial \tilde{T}_f}{\partial \eta} = \frac{1}{\tilde{x}^{1/3}}\frac{d\hat{T}}{d\eta} \quad , \quad \frac{\partial^2 \tilde{T}_f}{\partial \eta^2} = \frac{1}{\tilde{x}^{1/3}}\frac{d^2\hat{T}}{d\eta^2}$$

$$\frac{1}{\mathrm{Pr}}\frac{\partial^2 \tilde{T}_f}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{T}_f}{\partial \eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial \tilde{T}_f}{\partial \tilde{x}}$$
$$= \frac{1}{\mathrm{Pr}}\left(\frac{1}{\tilde{x}^{1/3}}\frac{d^2\hat{T}}{d\eta^2}\right) + 2(\tanh\eta)\left(\frac{1}{\tilde{x}^{1/3}}\frac{d\hat{T}}{d\eta}\right) - 6(\mathrm{sech}^2\eta)\tilde{x}\left(-\frac{1}{3}\frac{\hat{T}}{\tilde{x}^{4/3}}\right)$$

$$= \frac{1}{\tilde{x}^{1/3}}\left[\frac{1}{Pr}\frac{d^2\hat{T}}{d\eta^2} + 2(\tanh\ \eta)\frac{d\hat{T}}{d\eta} + 2(\mathrm{sech}^2\ \eta)\hat{T}\right] = \frac{1}{Pr\tilde{x}^{1/3}}\left\{\frac{d^2\hat{T}}{d\eta^2} + 2Pr\frac{d[(\tanh\ \eta)\hat{T}]}{d\eta}\right\} = 0 \tag{2.65}$$

Therefore $\frac{1}{Pr}\frac{d^2\hat{T}}{d\eta^2} + 2\frac{d[(\tanh\ \eta)\hat{T}]}{d\eta} = 0$ or $\frac{d\hat{T}}{d\eta} + 2Pr(\tanh\ \eta)\hat{T} = c_2$

$\eta = 0$: $\partial\tilde{T}_f/\partial\eta = d\hat{T}/\partial\eta = 0$ $\therefore$ $c_2 = 0$ (tanh 0 = 0) and

$$\frac{d\hat{T}}{d\eta} = -2Pr(\tanh\ \eta)\hat{T}$$

$$\frac{d\hat{T}}{\hat{T}} = -2Pr(\tanh\ \eta)d\eta = -2Pr\frac{(\sinh\ \eta)}{(\cosh\ \eta)}d\eta = -2Pr\frac{d(\cosh\ \eta)}{(\cosh\ \eta)} \tag{2.66}$$

Therefore $\ell n(\hat{T}) = -2Pr\,\ell n(\cosh\eta) + c'$ or $\hat{T} = c_2(\cosh\eta)^{-2Pr} = c_2(\operatorname{sech}^{2Pr}\eta)$

leading to $\tilde{T}_f = c_1 + c_2(\operatorname{sech}^{2Pr}\eta)/\,\tilde{x}^{1/3}$

$\eta \to \infty$: $\tilde{T}_f \to \tilde{T}_\infty$ therefore $c_1 = \tilde{T}_\infty$ and $\tilde{T}_f = \tilde{T}_\infty + c_2(\operatorname{sech}^{2Pr}\eta)/\,\tilde{x}^{1/3}$

$(\operatorname{sech}(\infty) \to 0)$

$\eta = 0$, $\tilde{x} = 1$: $\tilde{T} = \tilde{T}_0$ therefore $\tilde{T}_0 = \tilde{T}_\infty + c_2$ or $c_2 = \tilde{T}_0 - \tilde{T}_\infty$ $(\operatorname{sech}(0) = 1)$

Thus : $\tilde{T}_f = \tilde{T}_\infty + (\tilde{T}_0 - \tilde{T}_\infty)(\operatorname{sech}^{2Pr}\eta)/\,\tilde{x}^{1/3}$ (2.67)

(2) $\frac{1}{Sc_F}\frac{\partial^2 \tilde{Y}_{F,f}}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{Y}_{F,f}}{\partial \eta} - 6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial \tilde{Y}_{F,f}}{\partial \tilde{x}} = 0$

Similar to (1), the solution of $\tilde{Y}_{F,f}$ is $\tilde{Y}_{F,f} = c_1 + c_2(\operatorname{sech}^{2Sc_F}\eta)/\,\tilde{x}^{1/3}$

$\eta \to \infty$: $\tilde{Y}_{F,f} \to 0$ therefore $c_1 = 0$ and $\tilde{Y}_{F,f} = c_2(\operatorname{sech}^{2Sc_F}\eta)/\,\tilde{x}^{1/3}$

$\eta = 0$, $\tilde{x} = 1$: $\tilde{Y}_{F,f} = \tilde{Y}_{F,0}$ therefore $c_2 = \tilde{Y}_{F,0}$

Thus : $\tilde{Y}_{F,f} = \tilde{Y}_{F,0}(\operatorname{sech}^{2Sc_F}\eta)/\,\tilde{x}^{1/3}$ (2.68)

(3) $\frac{1}{Sc_O}\frac{\partial^2 \tilde{Y}_{O,f}}{\partial \eta^2} + 2(\tanh\eta)\frac{\partial \tilde{Y}_{O,f}}{\partial \eta} - 6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial \tilde{Y}_{O,f}}{\partial \tilde{x}} = 0$

Similar to (2), the solution of $\tilde{Y}_{O,f}$ is $\tilde{Y}_{O,f} = c_1 + c_2(\operatorname{sech}^{2Sc_O}\eta)/\,\tilde{x}^{1/3}$

$\eta \to \infty$: $\tilde{Y}_{O,f} \to \tilde{Y}_{O,\infty}$ therefore $c_1 = \tilde{Y}_{O,\infty}$ and $\tilde{Y}_{O,f} = \tilde{Y}_{O,\infty} + c_2(\operatorname{sech}^{2Sc_O}\eta)/\,\tilde{x}^{1/3}$

$\eta = 0$, $\tilde{x} = 1$: $\tilde{Y}_{O,f} = 0$ therefore $0 = \tilde{Y}_{O,\infty} + c_2$ or $c_2 = -\tilde{Y}_{O,\infty}$

Thus : $\tilde{Y}_{O,f} = \tilde{Y}_{O,\infty}[1 - (\operatorname{sech}^{2Sc_O}\eta)/\,\tilde{x}^{1/3}]$ (2.69)

(4) Summary

$\tilde{T}_f = \tilde{T}_\infty + (\tilde{T}_0 - \tilde{T}_\infty)(\operatorname{sech}^{2Pr}\eta)/\,\tilde{x}^{1/3}$ (2.67)

$$\tilde{Y}_{F,f} = \tilde{Y}_{F,0}(\operatorname{sech}^{2Sc_F}\eta)/\tilde{x}^{1/3} \tag{2.68}$$

$$\tilde{Y}_{O,f} = \tilde{Y}_{O,\infty}[1-(\operatorname{sech}^{2Sc_O}\eta)/\tilde{x}^{1/3}] \tag{2.69}$$

2.8 Summary of Formulation

$$\eta = \sqrt{\frac{\rho_\infty u_0}{3\mu_\infty x_0}}\,\frac{1}{\tilde{x}^{2/3}}\int_0^y \frac{\rho}{\rho_\infty}\,dy' \quad , \quad \psi = \sqrt{\frac{3\mu_\infty x_0}{\rho_\infty u_0}}\,\tilde{x}^{1/3} f(\eta) \quad , \quad x_0 = \frac{3M^2}{32 u_0^3 \rho_\infty \mu_\infty}$$

$$\tilde{T} = \frac{c_p T}{q_F} \quad , \quad \tilde{Y}_F = Y_F \quad , \quad \tilde{Y}_O = \frac{\nu_F W_F}{\nu_O W_O} Y_O \quad , \quad \tilde{E} = \frac{c_p E}{q_F} \quad ,$$

$$Da = \frac{6 x_0 \nu_O^{n_O} B}{\nu_F^{n_O-1} W_F^{n_O+n_F-1} u_0}\left(\frac{q_F}{c_p}\right)^{n_T-n_F-n_O+1}\left(\frac{p}{R}\right)^{n_F+n_O-1}$$

$$Pr = \frac{\mu}{\lambda/c_p} = \frac{\rho\mu}{\rho\lambda/c_p} \quad , \quad Sc_i = \frac{\mu}{\rho D_i} = \frac{\rho\mu}{\rho^2 D_i} \quad , \quad Le_i = \frac{\lambda/c_p}{\rho D_i} = \frac{Sc_i}{Pr}$$

$$f = \tanh\eta \quad , \quad df/d\eta = \operatorname{sech}^2\eta \quad , \quad u = u_0(\operatorname{sech}^2\eta)/\tilde{x}^{1/3}$$

$$\frac{1}{Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta} - 6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}} = -Da\,\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$\frac{1}{Sc_F}\frac{\partial^2\tilde{Y}_F}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{Y}_F}{\partial\eta} - 6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}} = Da\,\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$\frac{1}{Sc_O}\frac{\partial^2\tilde{Y}_O}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{Y}_O}{\partial\eta} - 6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{Y}_O}{\partial\tilde{x}} = Da\,\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$\eta = 0 \ , \ \tilde{x} = 1 \ : \quad \tilde{T} = \tilde{T}_0 \quad , \quad \tilde{Y}_F = \tilde{Y}_{F,0} \quad , \quad \tilde{Y}_O = 0$$

$$\eta = 0 \ , \ \tilde{x} > 1 \ : \quad \partial\tilde{T}/\partial\eta = \partial\tilde{Y}_F/\partial\eta = \partial\tilde{Y}_O/\partial\eta = 0$$

$$\eta\to\infty \ : \quad \tilde{T}\to\tilde{T}_\infty \quad , \quad \tilde{Y}_F\to 0 \quad , \quad \tilde{Y}_O\to\tilde{Y}_{O,\infty}$$

$$\tilde{T}_f = \tilde{T}_\infty + (\tilde{T}_0 - \tilde{T}_\infty)(\operatorname{sech}^{2Pr}\eta)/\tilde{x}^{1/3}$$

$$\tilde{Y}_{F,f} = \tilde{Y}_{F,0}(\operatorname{sech}^{2Sc_F}\eta)/\tilde{x}^{1/3}$$

$$\tilde{Y}_{O,f} = \tilde{Y}_{O,\infty}[1-(\operatorname{sech}^{2Sc_O}\eta)/\tilde{x}^{1/3}]$$

Chapter 3: Ignition Analysis

3.1 Description of Analysis

A total of three ignition analyses will be presented in this chapter. The first two analyses pertains to the cool jet flowing into hot ambient scenario, for two categories of fuels with local $Le_F < 1$ (hydrogen belongs to this category) and $Le_F \approx 1$ (for fuels like methane). The third analysis is for the hot jet flowing into cool ambient scenario.

The results and discussion will be based on ignition analysis I (for cool jet case) and analysis III (for hot jet case), as the main focus is on the spontaneous ignition of hydrogen, which occur when the temperature and reaction rate conditions in the inner region (which is the reaction zone) match the outer region (which lies outside the reaction zone). The second analysis is presented for comparison purposes between hydrogen and other common fuels like methane and propane.

3.2 Ignition Analysis I : $T\infty > T_0$, $Le_F < 1$

Because spontaneous ignition is primarily controlled by temperature, ignition occurs at $\eta \to \infty$ if successful. This is the outer edge of the jet.

(A) Outer Solutions

In the outer region, there is no reaction because of the low temperature.

Before ignition, there is only weak reaction. All the variables deviate from the frozen solutions by $O(\varepsilon)$.

$$\tilde{T} = \tilde{T}_f + \varepsilon\Theta + O(\varepsilon^2) \quad ; \quad \tilde{T}_f = \tilde{T}_\infty + (\tilde{T}_0 - \tilde{T}_\infty)(\mathrm{sech}^{2Pr}\eta)/\tilde{x}^{1/3} = \tilde{T}_\infty - (\tilde{T}_\infty - \tilde{T}_0)(\mathrm{sech}^{2Pr}\eta)/\tilde{x}^{1/3}$$

$$\tilde{Y}_F = \tilde{Y}_{F,f} + \varepsilon\Phi_F + O(\varepsilon^2) \quad ; \quad \tilde{Y}_{F,f} = \tilde{Y}_{F0}(\mathrm{sech}^{2Sc_F}\eta)/\tilde{x}^{1/3}$$

$\tilde{Y}_O=\tilde{Y}_{O,f}+\varepsilon\Phi_O+O(\varepsilon^2)$; $\tilde{Y}_{O,f}=\tilde{Y}_{O,\infty}[1-(\operatorname{sech}^{2Sc_O}\eta)/\tilde{x}^{1/3}]$

$\eta=0$, $\tilde{x}=1$: $\tilde{T}=\tilde{T}_0$, $\tilde{Y}_F=\tilde{Y}_{F,0}$, $\tilde{Y}_O=0$; $\eta=0$, $\tilde{x}>1$:

$\partial\tilde{T}/\partial\eta=\partial\tilde{Y}_F/\partial\eta=\partial\tilde{Y}_O/\partial\eta=0$

(1) $\dfrac{1}{Pr}\dfrac{\partial^2\tilde{T}}{\partial\eta^2}+2(\tanh\ \eta)\dfrac{\partial\tilde{T}}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\dfrac{\partial\tilde{T}}{\partial\tilde{x}}=0$

$$\frac{1}{Pr}\frac{\partial^2[\tilde{T}_f+\varepsilon\Theta+O(\varepsilon^2)]}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial[\tilde{T}_f+\varepsilon\Theta+O(\varepsilon^2)]}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial[\tilde{T}_f+\varepsilon\Theta+O(\varepsilon^2)]}{\partial\tilde{x}}=0$$

$$\left[\frac{1}{\Pr}\frac{\partial^2\tilde{T}_f}{\partial\eta^2}+2(\tanh\eta)\frac{\partial\tilde{T}_f}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}_f}{\partial\tilde{x}}\right]$$
$$+\varepsilon\left[\frac{1}{\Pr}\frac{\partial^2\Theta}{\partial\eta^2}+2(\tanh\eta)\frac{\partial\Theta}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\Theta}{\partial\tilde{x}}\right]+O(\varepsilon^2)=0$$

Since $\dfrac{1}{Pr}\dfrac{\partial^2\tilde{T}_f}{\partial\eta^2}+2(\tanh\ \eta)\dfrac{\partial\tilde{T}_f}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\dfrac{\partial\tilde{T}_f}{\partial\tilde{x}}=0$, we have

$$\frac{1}{Pr}\frac{\partial^2\Theta}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\Theta}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial\Theta}{\partial\tilde{x}}=0 \tag{3.1}$$

By the same approach as that for the frozen solution, we obtain

$\Theta=a_T+\bar{a}_T(\operatorname{sech}^{2Pr}\eta)/\tilde{x}^{1/3}$

$\eta=0$, $\tilde{x}=1$: $\tilde{T}=\tilde{T}_f+\varepsilon\Theta+O(\varepsilon^2)=\tilde{T}_0$ $\therefore$ $\Theta=0$ $\Rightarrow$ $0=a_T+\bar{a}_T$ and

$\Theta=a_T[1-(\operatorname{sech}^{2Pr}\eta)/\tilde{x}^{1/3}]$

The condition $\eta=0$, $\tilde{x}>1$: $\partial\tilde{T}/\partial\eta=0$ is automatically satisfied.

Thus : $\tilde{T}=\tilde{T}_f+\varepsilon\Theta+O(\varepsilon^2)=(\tilde{T}_\infty+\varepsilon a_T)-[(\tilde{T}_\infty-\tilde{T}_0)+\varepsilon a_T](\operatorname{sech}^{2Pr}\eta)/\tilde{x}^{1/3}+O(\varepsilon^2)$

(2) $\dfrac{1}{Sc_F}\dfrac{\partial^2\tilde{Y}_F}{\partial\eta^2}+2(\tanh\ \eta)\dfrac{\partial\tilde{Y}_F}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\dfrac{\partial\tilde{Y}_F}{\partial\tilde{x}}=0$

$$\frac{1}{Sc_F}\frac{\partial^2[\tilde{Y}_{F,f}+\varepsilon\Phi_F+O(\varepsilon^2)]}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial[\tilde{Y}_{F,f}+\varepsilon\Phi_F+O(\varepsilon^2)]}{\partial\eta}-6(\operatorname{sech}^2\eta)\tilde{x}\frac{\partial[\tilde{Y}_{F,f}+\varepsilon\Phi_F+O(\varepsilon^2)]}{\partial\tilde{x}}=0$$

$$\left[\frac{1}{Sc_F}\frac{\partial^2 \tilde{Y}_{F,f}}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_{F,f}}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_{F,f}}{\partial\tilde{x}}\right]+$$
$$+\varepsilon\left[\frac{1}{Sc_F}\frac{\partial^2 \Phi_F}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\Phi_F}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\Phi_F}{\partial\tilde{x}}\right]+O(\varepsilon^2)=0$$

Since $\frac{1}{Sc_F}\frac{\partial^2 \tilde{Y}_{F,f}}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_{F,f}}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_{F,f}}{\partial\tilde{x}}=0$, we have

$$\frac{1}{Sc_F}\frac{\partial^2 \Phi_F}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\Phi_F}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\Phi_F}{\partial\tilde{x}}=0 \qquad (3.2)$$

By the same approach as that for the frozen solution, we obtain

$$\Phi_F=a_F+\bar{a}_F(\mathrm{sech}^{2Sc_F}\ \eta)/\ \tilde{x}^{1/3}$$

$\eta=0$, $\tilde{x}=1$: $\tilde{Y}_F=\tilde{Y}_{F,f}+\varepsilon\Phi_F+O(\varepsilon^2)=\tilde{Y}_{F,0}$ $\therefore$ $\Phi_F=0$ $\Rightarrow$ $0=a_F+\bar{a}_F$ and

$$\Phi_F=a_F[1-(\mathrm{sech}^{2Sc_F}\ \eta)/\ \tilde{x}^{1/3}]$$

Thus : $\tilde{Y}_F=\tilde{Y}_{F,f}+\varepsilon\Phi_F+O(\varepsilon^2)=\varepsilon a_F+(\tilde{Y}_{F,0}-\varepsilon a_F)(\mathrm{sech}^{2Sc_F}\ \eta)/\ \tilde{x}^{1/3}+O(\varepsilon^2)$

(3) $\frac{1}{Sc_O}\frac{\partial^2 \tilde{Y}_O}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_O}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_O}{\partial\tilde{x}}=0$

$$\frac{1}{Sc_O}\frac{\partial^2[\tilde{Y}_{O,f}+\varepsilon\Phi_O+O(\varepsilon^2)]}{\partial\eta^2}+2(\tanh\eta)\frac{\partial[\tilde{Y}_{O,f}+\varepsilon\Phi_O+O(\varepsilon^2)]}{\partial\eta}-6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial[\tilde{Y}_{O,f}+\varepsilon\Phi_O+O(\varepsilon^2)]}{\partial\tilde{x}}=0$$

$$\left[\frac{1}{Sc_O}\frac{\partial^2 \tilde{Y}_{O,f}}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_{O,f}}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_{O,f}}{\partial\tilde{x}}\right]+$$
$$+\varepsilon\left[\frac{1}{Sc_O}\frac{\partial^2 \Phi_O}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\Phi_O}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\Phi_O}{\partial\tilde{x}}\right]+O(\varepsilon^2)=0$$

Since $\frac{1}{Sc_O}\frac{\partial^2 \tilde{Y}_{O,f}}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_{O,f}}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_{O,f}}{\partial\tilde{x}}=0$, we have

$$\frac{1}{Sc_O}\frac{\partial^2 \Phi_O}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\Phi_O}{\partial\eta}-6(\mathrm{sech}^2\ \eta)\tilde{x}\frac{\partial\Phi_O}{\partial\tilde{x}}=0 \qquad (3.3)$$

By the same approach as that for the frozen solution, we obtain

$$\Phi_O=a_O+\bar{a}_O(\mathrm{sech}^{2Sc_O}\ \eta)/\ \tilde{x}^{1/3}$$

$\eta = 0$, $\tilde{x}=1$: $\tilde{Y}_O = \tilde{Y}_{O,f} + \varepsilon\Phi_O + O(\varepsilon^2) = 0$ $\therefore$ $\Phi_O = 0$ $\Rightarrow$ $0 = a_O + \bar{a}_O$ and

$\Phi_O = a_O[1-(\mathrm{sech}^{2Sc_O}\,\eta)/\,\tilde{x}^{1/3}]$

Thus : $\tilde{Y}_O = \tilde{Y}_{O,f} + \varepsilon\Phi_O + O(\varepsilon^2) = (\tilde{Y}_{O,\infty} + \varepsilon a_O)[1-(\mathrm{sech}^{2Sc_O}\,\eta)/\,\tilde{x}^{1/3}] + O(\varepsilon^2)$

(4) Summary

$$\tilde{T} = (\tilde{T}_\infty + \varepsilon a_T) - [(\tilde{T}_\infty - \tilde{T}_0) + \varepsilon a_T](\mathrm{sech}^{2Pr}\,\eta)/\,\tilde{x}^{1/3} + O(\varepsilon^2) \tag{3.4}$$

$$\tilde{Y}_F = \varepsilon a_F + (\tilde{Y}_{F,0} - \varepsilon a_F)(\mathrm{sech}^{2Sc_F}\,\eta)/\,\tilde{x}^{1/3} + O(\varepsilon^2) \quad ; \tag{3.5}$$

$$\tilde{Y}_O = (\tilde{Y}_{O,\infty} + \varepsilon a_O)[1-(\mathrm{sech}^{2Sc_O}\,\eta)/\,\tilde{x}^{1/3}] + O(\varepsilon^2) \tag{3.6}$$

(B) Coordination Transformation

Define $\xi = \mathrm{sech}^2\eta$ then at $\eta = 0$, $\xi = 1$; as $\eta \to \infty$, $\xi \to 0$;

$\tanh^2\eta = 1 - \mathrm{sec}h^2\eta = 1-\xi$; $d(\tanh\eta)/d\eta = \mathrm{sech}^2\xi = \xi$

$$\frac{\partial}{\partial\eta} = \frac{\partial}{\partial\xi}\frac{d\xi}{d\eta} = \frac{d(\mathrm{sech}^2\eta)}{d\eta}\frac{\partial}{\partial\xi} = 2(\mathrm{sech}\,\eta)[-(\mathrm{sech}\,\eta)(\tanh\eta)]\frac{\partial}{\partial\xi} =$$

$$-2(\mathrm{sech}^2\eta)(\tanh\eta)\frac{\partial}{\partial\xi} = -2(\tanh\eta)\xi\frac{\partial}{\partial\xi}$$

$$\frac{\partial^2}{\partial\eta^2} = \frac{\partial}{\partial\eta}\left[-2(\tanh\eta)\xi\frac{\partial}{\partial\xi}\right] = -2\left[\frac{d(\tanh\eta)}{d\eta}\xi\frac{\partial}{\partial\xi} + (\tanh\eta)\frac{\partial}{\partial\eta}\left(\xi\frac{\partial}{\partial\xi}\right)\right]$$

$$= -2\left\{\xi^2\frac{\partial}{\partial\xi} + (\tanh\eta)\left[-2(\tanh\eta)\xi\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right)\right]\right\}$$

$$= -2\xi^2\frac{\partial}{\partial\xi} + 4(\tanh^2\eta)\left(\xi\frac{\partial}{\partial\xi} + \xi^2\frac{\partial^2}{\partial\xi^2}\right) = 4\xi(1-\xi)\left(\xi\frac{\partial^2}{\partial\xi^2} + \frac{\partial}{\partial\xi}\right) - 2\xi^2\frac{\partial}{\partial\xi} \tag{3.7}$$

(1) $\frac{1}{Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}} = -Da\,\tilde{x}^{4/3}\,\tilde{Y}_F^{n_F}\,\tilde{Y}_O^{n_O}\,\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$

$$\frac{1}{Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}$$

$$= \frac{1}{Pr}\left[4\xi(1-\xi)\left(\xi\frac{\partial^2\tilde{T}}{\partial\xi^2} + \frac{\partial\tilde{T}}{\partial\xi}\right) - 2\xi^2\frac{\partial\tilde{T}}{\partial\xi}\right] + 2(\tanh\eta)\left[-2(\mathrm{sech}^2\eta)(\tanh\eta)\frac{\partial\tilde{T}}{\partial\xi}\right] - 6\xi\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}$$

$$=\frac{1}{Pr}\left[4\xi(1-\xi)\left(\xi\frac{\partial^2\tilde{T}}{\partial\xi^2}+\frac{\partial\tilde{T}}{\partial\xi}\right)-2\xi^2\frac{\partial\tilde{T}}{\partial\xi}\right]-4\xi(1-\xi)\frac{\partial\tilde{T}}{\partial\xi}-6\xi\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}$$

$$=4\xi(1-\xi)\left[\frac{1}{Pr}\xi\frac{\partial^2\tilde{T}}{\partial\xi^2}+(\frac{1}{Pr}-1)\frac{\partial\tilde{T}}{\partial\xi}\right]-\frac{2}{Pr}\xi^2\frac{\partial\tilde{T}}{\partial\xi}-6\xi\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}$$

Thus :

$$4(1-\xi)\left[\frac{1}{Pr}\xi^2\frac{\partial^2\tilde{T}}{\partial\xi^2}+(\frac{1}{Pr}-1)\xi\frac{\partial\tilde{T}}{\partial\xi}\right]-\xi\left(\frac{2}{Pr}\xi\frac{\partial\tilde{T}}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)=-Da\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

(3.8)

(2) $$\frac{1}{Sc_F}\frac{\partial^2\tilde{Y}_F}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_F}{\partial\eta}-6(\text{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}=Da\,\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

The equation is similar to (1). By the same approach as that of (1), we have

$$4(1-\xi)\left[\frac{1}{Sc_F}\xi^2\frac{\partial^2\tilde{Y}_F}{\partial\xi^2}+(\frac{1}{Sc_F}-1)\xi\frac{\partial\tilde{Y}_F}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_F}\xi\frac{\partial\tilde{Y}_F}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}\right)=Da\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

(3.9)

(3) $$\frac{1}{Sc_O}\frac{\partial^2\tilde{Y}_O}{\partial\eta^2}+2(\tanh\ \eta)\frac{\partial\tilde{Y}_O}{\partial\eta}-6(\text{sech}^2\ \eta)\tilde{x}\frac{\partial\tilde{Y}_O}{\partial\tilde{x}}=Da\,\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

The equation is similar to (1). By the same approach as that of (1), we have

$$4(1-\xi)\left[\frac{1}{Sc_O}\xi^2\frac{\partial^2\tilde{Y}_O}{\partial\xi^2}+(\frac{1}{Sc_O}-1)\xi\frac{\partial\tilde{Y}_O}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_O}\xi\frac{\partial\tilde{Y}_O}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_O}{\partial\tilde{x}}\right)=Da\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

(3.10)

(4) $\eta\to\infty$: $\tilde{T}\to\tilde{T}_\infty$, $\tilde{Y}_F\to 0$, $\tilde{Y}_O\to\tilde{Y}_{O,\infty}$ $\Rightarrow$ $\xi=0$: $\tilde{T}=\tilde{T}_\infty$,

$\tilde{Y}_F=0$, $\tilde{Y}_O=\tilde{Y}_{O,\infty}$

(5) Frozen solutions

$$\tilde{T}_f=\tilde{T}_\infty-(\tilde{T}_\infty-\tilde{T}_0)(\text{sech}^{2Pr}\,\eta)/\,\tilde{x}^{1/3}\quad\Rightarrow\tilde{T}_f=\tilde{T}_\infty-(\tilde{T}_\infty-\tilde{T}_0)\xi^{Pr}/\,\tilde{x}^{1/3}\tag{3.11}$$

$$\tilde{Y}_{F,f}=\tilde{Y}_{F0}(\text{sech}^{2Sc_F}\,\eta)/\tilde{x}^{1/3}\quad\Rightarrow\quad\tilde{Y}_{F,f}=\tilde{Y}_{F0}\,\xi^{Sc_F}/\tilde{x}^{1/3}\tag{3.12}$$

$$\tilde{Y}_{O,f}=\tilde{Y}_{O,\infty}[1-(\mathrm{sech}^{2Sc_O}\,\eta)/\tilde{x}^{1/3}] \quad \Rightarrow \quad \tilde{Y}_{O,f}=\tilde{Y}_{O,\infty}(1-\xi^{Sc_O}/\tilde{x}^{1/3}) \tag{3.13}$$

(6) Outer solutions :

$$\tilde{T}=(\tilde{T}_\infty+\varepsilon a_T)-[(\tilde{T}_\infty-\tilde{T}_0)+\varepsilon a_T]\xi^{Pr}/\tilde{x}^{1/3}+O(\varepsilon^2) \tag{3.14}$$

$$\tilde{Y}_F=\varepsilon a_F+(\tilde{Y}_{F,0}-\varepsilon a_F)\xi^{Sc_F}/\tilde{x}^{1/3}+O(\varepsilon^2) \quad ; \tag{3.15}$$

$$\tilde{Y}_O=(\tilde{Y}_{O,\infty}+\varepsilon a_O)(1-\xi^{Sc_O}/\tilde{x}^{1/3})+O(\varepsilon^2) \tag{3.16}$$

(7) Summary

$$4(1-\xi)\left[\frac{1}{Pr}\xi^2\frac{\partial^2\tilde{T}}{\partial\xi^2}+(\frac{1}{Pr}-1)\xi\frac{\partial\tilde{T}}{\partial\xi}\right]-\xi\left(\frac{2}{Pr}\xi\frac{\partial\tilde{T}}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)=-Da\tilde{x}^{4/3}\,\tilde{Y}_F^{n_F}\,\tilde{Y}_O^{n_O}\,\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$4(1-\xi)\left[\frac{1}{Sc_F}\xi^2\frac{\partial^2\tilde{Y}_F}{\partial\xi^2}+(\frac{1}{Sc_F}-1)\xi\frac{\partial\tilde{Y}_F}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_F}\xi\frac{\partial\tilde{Y}_F}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}\right)=Da\tilde{x}^{4/3}\,\tilde{Y}_F^{n_F}\,\tilde{Y}_O^{n_O}\,\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$4(1-\xi)\left[\frac{1}{Sc_O}\xi^2\frac{\partial^2\tilde{Y}_O}{\partial\xi^2}+(\frac{1}{Sc_O}-1)\xi\frac{\partial\tilde{Y}_O}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_O}\xi\frac{\partial\tilde{Y}_O}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_O}{\partial\tilde{x}}\right)=Da\tilde{x}^{4/3}\,\tilde{Y}_F^{n_F}\,\tilde{Y}_O^{n_O}\,\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$\xi=0$: $\tilde{T}=\tilde{T}_\infty$, $\tilde{Y}_F=0$, $\tilde{Y}_O=\tilde{Y}_{O,\infty}$

Frozen solutions : $\tilde{T}_f=\tilde{T}_\infty-(\tilde{T}_\infty-\tilde{T}_0)\xi^{Pr}/\tilde{x}^{1/3}$; $\tilde{Y}_{F,f}=\tilde{Y}_{F,0}\xi^{Sc_F}/\tilde{x}^{1/3}$;

$\tilde{Y}_{O,f}=\tilde{Y}_{O,\infty}(1-\xi^{Sc_O}/\tilde{x}^{1/3})$

Outer solutions : $\tilde{T}=(\tilde{T}_\infty+\varepsilon a_T)-[(\tilde{T}_\infty-\tilde{T}_0)+\varepsilon a_T]\xi^{Pr}/\tilde{x}^{1/3}+O(\varepsilon^2)$

$\tilde{Y}_F=\varepsilon a_F+(\tilde{Y}_{F,0}-\varepsilon a_F)\xi^{Sc_F}/\tilde{x}^{1/3}+O(\varepsilon^2)$; $\tilde{Y}_O=(\tilde{Y}_{O,\infty}+\varepsilon a_O)(1-\xi^{Sc_O}/\tilde{x}^{1/3})+O(\varepsilon^2)$

(C) Inner Expansion

Define inner variable : $\xi^{Pr}=\varepsilon\tilde{x}^{1/3}\zeta/\tilde{Y}_{F,0}$ or $\zeta=\tilde{Y}_{F,0}\xi^{Pr}/(\varepsilon\tilde{x}^{1/3})$, $\varepsilon=\tilde{T}_\infty{}^2/\tilde{E}$,

$$\alpha=(\tilde{T}_\infty-\tilde{T}_0)/\tilde{Y}_{F,0} \quad ; \quad \xi=0 \;:\; \zeta=0 \tag{3.17}$$

$$\tilde{T}=\tilde{T}_f(\xi^{Pr}=\varepsilon\tilde{x}^{1/3}\zeta/\tilde{Y}_{F,0})+\varepsilon\theta+O(\varepsilon^2)=\tilde{T}_\infty-(\tilde{T}_\infty-\tilde{T}_0)(\varepsilon\tilde{x}^{1/3}\zeta/\tilde{Y}_{F,0})/\tilde{x}^{1/3}+\varepsilon\theta+O(\varepsilon^2)=\tilde{T}_\infty+\varepsilon(\theta-\alpha\zeta)+O(\varepsilon^2)$$

$$\tilde{Y}_F=\tilde{Y}_{F,f}(\xi^{Pr}=\varepsilon\tilde{x}^{1/3}\zeta/\tilde{Y}_{F,0})+\varepsilon\phi_F+O(\varepsilon^2)=\tilde{Y}_{F,0}(\varepsilon\tilde{x}^{1/3}\zeta/\tilde{Y}_{F,0})^{Sc_F/Pr}/\tilde{x}^{1/3}+\varepsilon\phi_F+O(\varepsilon^2)=\varepsilon^{Le_F}(\tilde{Y}_{F,0}/\tilde{x}^{1/3})^{1-Le_F}\zeta^{Le_F}+\varepsilon\phi_F+O(\varepsilon^2)$$

For $Le_F<1$ (for hydrogen, $Le_F\approx 0.5$) , $\varepsilon^{Le_F}>>\varepsilon$ and

$$\tilde{Y}_F = \varepsilon^{Le_F} (\tilde{Y}_{F0} / \tilde{x}^{1/3})^{1-Le_F} \zeta^{Le_F} + O(\varepsilon)$$

$$\tilde{Y}_O = \tilde{Y}_{O,f} (\xi^{Pr} = \varepsilon \tilde{x}^{1/3} \zeta / \tilde{Y}_{F0}) + \varepsilon \phi_O + O(\varepsilon^2) = \tilde{Y}_{O,\infty} [1 - (\varepsilon \tilde{x}^{1/3} \zeta / \tilde{Y}_{F0})^{Sc_O/Pr} / \tilde{x}^{1/3}]$$
$$| + \varepsilon \phi_O + O(\varepsilon^2) = \tilde{Y}_{O,\infty} + O(\varepsilon^{Le_O}; \varepsilon)$$

$$\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \zeta} \frac{\partial \zeta}{\partial \xi} = \frac{\tilde{Y}_{F0} Pr}{\varepsilon \tilde{x}^{1/3}} \xi^{Pr-1} \frac{\partial}{\partial \zeta}$$ therefore $$\xi \frac{\partial}{\partial \xi} = Pr \frac{\tilde{Y}_{F0}}{\varepsilon \tilde{x}^{1/3}} \xi^{Pr} \frac{\partial}{\partial \zeta} = Pr\, \zeta \frac{\partial}{\partial \zeta}$$ or

$$\frac{1}{Pr} \xi \frac{\partial}{\partial \xi} = \zeta \frac{\partial}{\partial \zeta}$$

$$\frac{\partial^2}{\partial \xi^2} = \frac{\partial}{\partial \xi}\left(\frac{\partial}{\partial \xi}\right) = \frac{\partial}{\partial \xi}\left(\frac{\tilde{Y}_{F0} Pr}{\varepsilon \tilde{x}^{1/3}} \xi^{Pr-1} \frac{\partial}{\partial \zeta}\right) = \frac{\tilde{Y}_{F0} Pr}{\varepsilon \tilde{x}^{1/3}}\left[(Pr-1)\xi^{Pr-2} \frac{\partial}{\partial \zeta} + \xi^{Pr-1} \frac{\partial}{\partial \xi}\left(\frac{\partial}{\partial \zeta}\right)\right]$$

$$= \frac{\tilde{Y}_{F0} Pr}{\varepsilon \tilde{x}^{1/3}}\left[(Pr-1)\xi^{Pr-2} \frac{\partial}{\partial \zeta} + \xi^{Pr-1} \frac{\tilde{Y}_{F0} Pr}{\varepsilon \tilde{x}^{1/3}} \xi^{Pr-1} \frac{\partial}{\partial \zeta}\left(\frac{\partial}{\partial \zeta}\right)\right] = \frac{Pr}{\xi^2}\left[Pr\, \zeta^2 \frac{\partial^2}{\partial \zeta^2} + (Pr-1)\zeta \frac{\partial}{\partial \zeta}\right]$$

$$\frac{1}{Pr} \xi^2 \frac{\partial^2}{\partial \xi^2} = Pr\, \zeta^2 \frac{\partial^2}{\partial \zeta^2} + (Pr-1)\zeta \frac{\partial}{\partial \zeta}$$

$$\frac{1}{Pr} \xi^2 \frac{\partial^2}{\partial \xi^2} + \left(\frac{1}{Pr} - 1\right) \xi \frac{\partial}{\partial \xi} = Pr\, \zeta^2 \frac{\partial^2}{\partial \zeta^2} + (Pr-1)\zeta \frac{\partial}{\partial \zeta} + \left(\frac{1}{Pr} - 1\right) Pr\, \zeta \frac{\partial}{\partial \zeta} = Pr\, \zeta^2 \frac{\partial^2}{\partial \zeta^2} \tag{3.18}$$

$$\frac{1}{Sc_j} \xi \frac{\partial}{\partial \xi} = \frac{Pr}{Sc_j} \zeta \frac{\partial}{\partial \zeta} = \frac{1}{Le_j} \zeta \frac{\partial}{\partial \zeta}$$

$$\frac{1}{Sc_j} \xi^2 \frac{\partial^2}{\partial \xi^2} + \left(\frac{1}{Sc_j} - 1\right) \xi \frac{\partial}{\partial \xi} = \frac{Pr}{Sc_j}\left[Pr\, \zeta^2 \frac{\partial^2}{\partial \zeta^2} + (Pr - 1)\zeta \frac{\partial}{\partial \zeta}\right] + \left(\frac{1}{Sc_j} - 1\right) Pr\, \zeta \frac{\partial}{\partial \zeta}$$
$$= \frac{Pr}{Sc_j}\left| Pr\, \zeta^2 \frac{\partial^2}{\partial \zeta^2} + (Pr - Sc_j)\zeta \frac{\partial}{\partial \zeta} \right|$$

$$= \frac{1}{Le_j}\left[Pr \zeta^2 \frac{\partial^2}{\partial \zeta^2} + Pr\left(1 - \frac{Sc_j}{Pr}\right)\zeta \frac{\partial}{\partial \zeta}\right] = \frac{Pr}{Le_j}\left[\zeta^2 \frac{\partial^2}{\partial \zeta^2} + (1 - Le_j)\zeta \frac{\partial}{\partial \zeta}\right] \tag{3.19}$$

$$\tilde{E} / \tilde{T} = \tilde{E} / [\tilde{T}_\infty + \varepsilon(\theta - \alpha \zeta) + O(\varepsilon^2)] = \tilde{E} / \{\tilde{T}_\infty [1 + (\varepsilon / \tilde{T}_\infty)(\theta - \alpha \zeta) + O(\varepsilon^2)]\}$$

$$= (\tilde{E} / \tilde{T}_\infty) - \varepsilon(\tilde{E} / \tilde{T}_\infty^{\,2})(\theta - \alpha \zeta) + (\tilde{E} / \tilde{T}_\infty) O(\varepsilon^2) = (\tilde{E} / \tilde{T}_\infty) - (\theta - \alpha \zeta) + O(\varepsilon)$$

$$\exp(-\tilde{E} / \tilde{T}) = \exp[-(\tilde{E} / \tilde{T}_\infty) + (\theta - \alpha \zeta) + O(\varepsilon)] = \exp(-\tilde{E} / \tilde{T}_\infty) \exp(\theta - \alpha \zeta) + O(\varepsilon) \tag{3.20}$$

(1) $\xi = 0$: $\zeta = 0$, $\tilde{T} = \tilde{T}_\infty$, $\tilde{Y}_F = 0$

$$\tilde{T}(\zeta = 0) = \tilde{T}_\infty + \varepsilon \theta(\zeta = 0) + O(\varepsilon^2) = \tilde{T}_\infty \quad \therefore \quad \theta(\zeta = 0) = 0$$

$$\tilde{Y}_F(\zeta=0)=\varepsilon^{Le_F}\phi_F(\zeta=0)+O(\varepsilon^{2\,Le_F})=0 \qquad \therefore \qquad \phi_F(\zeta=0)=0$$

(2)

$$4(1-\xi)\left[\frac{1}{Pr}\xi^2\frac{\partial^2\tilde{T}}{\partial\xi^2}+(\frac{1}{Pr}-1)\xi\frac{\partial\tilde{T}}{\partial\xi}\right]-\xi\left(\frac{2}{Pr}\xi\frac{\partial\tilde{T}}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)=-Da\,\tilde{x}^{4/3}\,\tilde{Y}_F^{\,n_F}\,\tilde{Y}_O^{\,n_O}\,\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$4[1-(\varepsilon\zeta)^{1/Pr}]\left[Pr\,\zeta^2\frac{\partial^2\tilde{T}}{\partial\zeta^2}+(Pr-1)\zeta\frac{\partial\tilde{T}}{\partial\zeta}+(\frac{1}{Pr}-1)Pr\,\zeta\frac{\partial\tilde{T}}{\partial\zeta}\right]-(\varepsilon\zeta)^{1/Pr}\left(\frac{2}{Pr}Pr\,\zeta\frac{\partial\tilde{T}}{\partial\zeta}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)$$

$$=-Da\tilde{x}^{4/3}[\varepsilon^{Le_F}(\tilde{Y}_{F0}/\tilde{x}^{1/3})^{1-Le_F}\zeta^{Le_F}+O(\varepsilon)]^{n_F}[\tilde{Y}_{O,\infty}+O(\varepsilon^{Le_O};\varepsilon)]^{n_O}[\tilde{T}_\infty+O(\varepsilon)]^{n_T-n_F-n_O+1}[\exp(-\tilde{E}/\tilde{T}_\infty)\exp(\theta-\alpha\zeta)+O(\varepsilon)]$$

$$=-Da\tilde{x}^{4/3}[\varepsilon^{Le_F}(\tilde{Y}_{F0}/\tilde{x}^{1/3})^{1-Le_F}\zeta^{Le_F}+O(\varepsilon)]^{n_F}[\tilde{Y}_{O,\infty}+O(\varepsilon^{Le_O};\varepsilon)]^{n_O}[\tilde{T}_\infty+O(\varepsilon)]^{n_T-n_F-n_O+1}[\exp(-\tilde{E}/\tilde{T}_\infty)\exp(\theta-\alpha\zeta)+O(\varepsilon)] \tag{3.21}$$

Take the leading order terms in ε

$$4\,Pr\,\zeta^2\frac{\partial^2\{\tilde{T}_\infty+\varepsilon[\theta-(\tilde{T}_\infty-\tilde{T}_0)\zeta/\tilde{x}^{1/3}]\}}{\partial\zeta^2}=4\varepsilon Pr\,\zeta^2\frac{\partial^2\theta}{\partial\zeta^2}$$

$$=-\varepsilon^{Le_Fn_F}Da\,\tilde{x}^{4/3}(\tilde{Y}_{F0}/\tilde{x}^{1/3})^{(1-Le_F)n_F}\,\tilde{Y}_{O,\infty}^{\;\;n_O}\,\tilde{T}_\infty^{\;n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_\infty)\,\zeta^{Le_Fn_F}\exp(\theta-\alpha\zeta)$$

$$\zeta^2\frac{\partial^2\theta}{\partial\zeta^2}=-\varepsilon^{Le_Fn_F-1}\frac{Da\,\tilde{Y}_{O,\infty}^{\;\;n_O}\,\tilde{T}_\infty^{\;n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_\infty)}{4\,Pr}\tilde{x}^{4/3}(\tilde{Y}_{F0}/\tilde{x}^{1/3})^{(1-Le_F)n_F}\,\zeta^{Le_Fn_F}\exp(\theta-\alpha\zeta)$$

Define $\tilde{D}a=\varepsilon^{Le_Fn_F-1}\dfrac{Da\,\tilde{Y}_{O,\infty}^{\;\;n_O}\,\tilde{T}_\infty^{\;n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_\infty)}{4\,Pr}\tilde{x}^{4/3}(\tilde{Y}_{F0}/\tilde{x}^{1/3})^{(1-Le_F)n_F}$ (3.22)

= Reduced Damköhler number

$$\zeta^2\frac{\partial^2\theta}{\partial\zeta^2}=-\tilde{D}a\,\zeta^{Le_Fn_F}\exp(\theta-\alpha\zeta) \tag{3.23}$$

(D) Matching

$$\tilde{T}=(\tilde{T}_\infty+\varepsilon a_T)-[(\tilde{T}_\infty-\tilde{T}_0)+\varepsilon a_T]\xi^{Pr}/\tilde{x}^{1/3}+O(\varepsilon^2)=(\tilde{T}_\infty+\varepsilon a_T)-[(\tilde{T}_\infty-\tilde{T}_0)+\varepsilon a_T](\varepsilon\zeta/\tilde{Y}_{F0})+O(\varepsilon^2)$$

$$=\tilde{T}_\infty+\varepsilon(a_T-\alpha\zeta)+O(\varepsilon^2)=\tilde{T}_\infty+\varepsilon(\theta-\alpha\zeta)+O(\varepsilon^2)\Big|_{\zeta\to\infty}$$

$\therefore \qquad \theta(\zeta\to\infty)=a_T \qquad$ or $\qquad (\partial\theta/\partial\zeta)_{\zeta\to\infty}=0$

(E) Summary

$$\zeta^2 \frac{\partial^2 \theta}{\partial \zeta^2} = -\tilde{D}a\, \zeta^{Le_F n_F} \exp(\theta - \alpha\zeta) \quad ; \quad \zeta = 0 \; : \quad \theta = 0 \quad ; \quad \zeta \to \infty \; : \quad \partial\theta/\partial\zeta \to 0 \quad ,$$

$$\theta \to a_T$$

$$\alpha = (\tilde{T}_\infty - \tilde{T}_0)/\tilde{Y}_{F,0} \quad , \quad \tilde{D}a = \varepsilon^{Le_F n_F - 1} \frac{Da\, \tilde{Y}_{O,\infty}{}^{n_O}\, \tilde{T}_\infty{}^{n_T - n_F - n_O + 1} \exp(-\tilde{E}/\tilde{T}_\infty)}{4\, Pr} \tilde{x}^{4/3} (\tilde{Y}_{F,0}/\tilde{x}^{1/3})^{(1-Le_F)n_F}$$

$$, \quad \varepsilon = \tilde{T}_\infty{}^2/\tilde{E}$$

Note: Since there is no differentiation with respect to $\tilde{x}$, the problem is locally similar and $\tilde{x}$ can be considered as a constant in the structure equation.

(F) Rescaling

when the change of α is by changing T_∞ or $Y_{F,0}$, or n_F or $\mathrm{Le_F}$ is varying

Define $\hat{T}_\infty$ as the reference value of $\tilde{T}_\infty$, $\hat{n}_F$ as the reference value of n_F ,

$\hat{Y}_{F,0}$ as the reference value of $\tilde{Y}_{F,0}$

$\hat{\varepsilon} = (\hat{T}_\infty)^2/\tilde{E}$ as the reference value of ε $\quad \Rightarrow \quad \hat{\varepsilon}/\varepsilon = (\hat{T}_\infty/\tilde{T}_\infty)^2$

$$\hat{D}a = \hat{\varepsilon}^{\hat{Le}_F \hat{n}_F - 1} [\, Da/(4\,\mathrm{Pr})\,] \tilde{Y}_{O,\infty}{}^{n_O}\, \hat{T}_\infty{}^{n_T - \hat{n}_F - n_O + 1} \exp(-\tilde{E}/\hat{T}_\infty)\, \tilde{x}^{4/3} (\hat{Y}_{F,0}/\tilde{x}^{1/3})^{(1-\hat{Le}_F)\hat{n}_F}$$

$$= (\hat{T}_\infty/\tilde{T}_\infty)^{n_T + (2\hat{Le}_F - 1)\hat{n}_F - n_O - 1} (\tilde{T}_\infty{}^2/\tilde{E})^{(\hat{Le}_F \hat{n}_F - Le_F n_F)}\, \tilde{T}_\infty{}^{n_F - \hat{n}_F} (\hat{Y}_{F,0}/\tilde{Y}_{F,0})^{(1-\hat{Le}_F)\hat{n}_F}$$
$$(\tilde{Y}_{F,0}/\tilde{x}^{1/3})^{(1-\hat{Le}_F)\hat{n}_F - (1-Le_F)n_F} \exp[\,\tilde{E}(\tilde{T}_\infty{}^{-1} - \hat{T}_\infty{}^{-1})\,]\, \tilde{D}a \tag{3.24}$$

$$\varepsilon a_T = \hat{\varepsilon}\hat{a}_T \quad \therefore \quad \hat{a}_T = (\varepsilon/\hat{\varepsilon})\, a_T = (\tilde{T}_\infty{}^2/\hat{T}_\infty{}^2)\, a_T$$

If only T_∞ is varying

$$\hat{D}a = (\hat{T}_\infty/\tilde{T}_\infty)^{n_T + (2Le_F - 1)n_F - n_O - 1} \exp[\,\tilde{E}(\tilde{T}_\infty{}^{-1} - \hat{T}_\infty{}^{-1})\,]\, \tilde{D}a \tag{3.25}$$

$$\hat{a}_T = (\tilde{T}_\infty{}^2/\hat{T}_\infty{}^2)\, a_T \tag{3.26}$$

In the calculations, we

(1) Choose a value of α as the reference value.

(2) Find the value of $\hat{T}_\infty$ based on this reference value of α. (need to specify $\tilde{T}_0$ and $\tilde{Y}_{F,0}$)

(3) For other values of α, determine $\tilde{T}_\infty$ using the same values of $\tilde{T}_0$ and $\tilde{Y}_{F,0}$.

(4) Use the values of $\hat{T}_\infty$ and $\tilde{T}_\infty$ to determine $\hat{D}a$.

If only n_F is varying, $\hat{D}a = (\tilde{T}_\infty^{\,2}/\tilde{E})^{Le_F(\hat{n}_F - n_F)}\,\tilde{T}_\infty^{\,n_F-\hat{n}_F}\,(\tilde{Y}_{F,0}/\tilde{x}^{1/3})^{(1-Le_F)(\hat{n}_F-n_F)}\,\tilde{D}a$ (3.27)

If only $Y_{F,0}$ is varying, $\hat{D}a = (\hat{Y}_{F,0}/\tilde{Y}_{F,0})^{(1-Le_F)n_F}\,\tilde{D}a$ (3.28)

If only Le_F is varying, $\hat{D}a = (\tilde{T}_\infty^{\,2}/\tilde{E})^{(\hat{Le}_F - Le_F)n_F}\,(\hat{Y}_{F,0}/\tilde{Y}_{F,0})^{(1-\hat{Le}_F)n_F}\,(\tilde{Y}_{F,0}/\tilde{x}^{1/3})^{(\hat{Le}_F+Le_F)n_F}\,\tilde{D}a$ (3.29)

3.3 Ignition Analysis II : T∞ > T_0 , $Le_F \approx 1$

As in I, ignition occurs at $\eta \to \infty$ if successful.

(A) Coordination Transformation and Outer Solutions (From Analysis I)

Define $\xi = \mathrm{sech}^2\eta$ then at $\eta = 0$, $\xi = 1$; as $\eta \to \infty$, $\xi = 0$

$$4(1-\xi)\left[\frac{1}{Pr}\xi^2\frac{\partial^2\tilde{T}}{\partial\xi^2}+\left(\frac{1}{Pr}-1\right)\xi\frac{\partial\tilde{T}}{\partial\xi}\right]-\xi\left(\frac{2}{Pr}\xi\frac{\partial\tilde{T}}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)=-Da\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$4(1-\xi)\left[\frac{1}{Sc_F}\xi^2\frac{\partial^2\tilde{Y}_F}{\partial\xi^2}+\left(\frac{1}{Sc_F}-1\right)\xi\frac{\partial\tilde{Y}_F}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_F}\xi\frac{\partial\tilde{Y}_F}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}\right)=Da\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$\xi = 0$: $\tilde{T} = \tilde{T}_\infty$, $\tilde{Y}_F = 0$

Outer solutions

$$\tilde{T} = (\tilde{T}_\infty + \varepsilon a_T) - [(\tilde{T}_\infty - \tilde{T}_0) + \varepsilon a_T]\,\xi^{Pr/\tilde{x}^{1/3}} + O(\varepsilon^2)$$

$$\tilde{Y}_F = \varepsilon a_F + (\tilde{Y}_{F,0} - \varepsilon a_F)\,\xi^{Sc_F/\tilde{x}^{1/3}} + O(\varepsilon^2)$$

$$\tilde{Y}_O = (\tilde{Y}_{O,\infty} + \varepsilon a_O)(1 - \xi^{Sc_O/\tilde{x}^{1/3}}) + O(\varepsilon^2)$$

(B) Inner Expansion

Define inner variable : $\xi^{Pr} = \varepsilon\zeta$ or $\zeta = \xi^{Pr}/\varepsilon$, $\varepsilon = \tilde{T}_\infty^{\,2}/\tilde{E}$;

$\xi = 0$: $\zeta = 0$

From Analysis I

$$\tilde{T} = \tilde{T}_\infty + \varepsilon[\theta - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] + O(\varepsilon^2) \quad ; \quad \tilde{Y}_F = \varepsilon^{Le_F}(\tilde{Y}_{F,0}\zeta^{Le_F}/\tilde{x}^{1/3}) + \varepsilon\phi_F + O(\varepsilon^2)$$

$$\frac{1}{Pr}\xi\frac{\partial}{\partial\xi} = \zeta\frac{\partial}{\partial\zeta} \quad ; \quad \frac{1}{Pr}\xi^2\frac{\partial^2}{\partial\xi^2} + (\frac{1}{Pr} - 1)\xi\frac{\partial}{\partial\xi} = Pr\zeta^2\frac{\partial^2}{\partial\zeta^2}$$

$$\frac{1}{Sc_F}\xi\frac{\partial}{\partial\xi} = \frac{1}{Le_F}\zeta\frac{\partial}{\partial\zeta} \quad , \quad \frac{1}{Sc_F}\xi^2\frac{\partial^2}{\partial\xi^2} + (\frac{1}{Sc_F} - 1)\xi\frac{\partial}{\partial\xi} = \frac{Pr}{Le_F}\left[\zeta^2\frac{\partial^2}{\partial\zeta^2} + (1 - Le_F)\zeta\frac{\partial}{\partial\zeta}\right]$$

$$4\varepsilon Pr\zeta^2\frac{\partial^2\theta}{\partial\zeta^2} = -Da\tilde{Y}_{O,\infty}^{\,n_O}\tilde{T}_\infty^{\,n_T - n_F - n_O + 1}\exp(-\tilde{E}/\tilde{T}_\infty)\tilde{x}^{4/3}[\varepsilon^{Le_F}(\tilde{Y}_{F,0}\zeta^{Le_F}/\tilde{x}^{1/3}) + \varepsilon\phi_F]^{n_F}\exp[\theta - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] + O(\varepsilon)$$

$\zeta = 0$: $\theta = 0$, $\phi_F = 0$

Expand Le_F as $Le_F = 1 + \varepsilon\ell_F + O(\varepsilon^2)$, then for any variable A

$$A^{Le_F} = \exp[\ell\text{n}(A^{Le_F})] = \exp(Le_F\,\ell\text{n}\,A) = \exp[(1 + \varepsilon\ell_F + \cdots)\ell\text{n}\,A]$$
$$= \exp(\ell\text{n}\,A)\exp(\varepsilon\ell_F\,\ell\text{n}\,A + \cdots) = A(1 + \varepsilon\ell_F\,\ell\text{n}\,A + \cdots) \tag{3.30}$$

Thus : $\tilde{Y}_F = \varepsilon^{Le_F}(\tilde{Y}_{F,0}\zeta^{Le_F}/\tilde{x}^{1/3}) + \varepsilon\phi_F + O(\varepsilon^2) = \varepsilon(\phi_F + \tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3}) + O(\varepsilon^2)$

$$\frac{1}{Sc_F}\xi^2\frac{\partial^2}{\partial\xi^2} + (\frac{1}{Sc_F} - 1)\xi\frac{\partial}{\partial\xi} = Pr\zeta^2\frac{\partial^2\tilde{Y}_F}{\partial\zeta^2} + O(\varepsilon) \tag{3.31}$$

(1) $4\varepsilon Pr\zeta^2\dfrac{\partial^2\theta}{\partial\zeta^2} = -Da\tilde{Y}_{O,\infty}^{\,n_O}\tilde{T}_\infty^{\,n_T - n_F - n_O + 1}\exp(-\tilde{E}/\tilde{T}_\infty)\tilde{x}^{4/3}$

$$[\varepsilon^{Le_F}(\tilde{Y}_{F,0}\zeta^{Le_F}/\tilde{x}^{1/3}) + \varepsilon\phi_F]^{n_F}\exp[\theta - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] + O(\varepsilon)$$

$$\zeta^2\frac{\partial^2\theta}{\partial\zeta^2} = -\frac{Da\,\tilde{Y}_{O,\infty}^{\,n_O}\tilde{T}_\infty^{\,n_T - n_F - n_O + 1}\exp(-\tilde{E}/\tilde{T}_\infty)}{4\varepsilon Pr}\tilde{x}^{4/3}$$
$$[\varepsilon(\phi_F + \tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3})]^{n_F}\exp[\theta - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] + O(\varepsilon)$$

$$= -\varepsilon^{n_F-1}\frac{Da\tilde{Y}_{O,\infty}{}^{n_O}\tilde{T}_\infty{}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_\infty)}{4Pr}\tilde{x}^{4/3}(\phi_F+\tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3})^{n_F}\exp[\theta+(\tilde{T}_0-\tilde{T}_\infty)\zeta/\tilde{x}^{1/3}]+O(\varepsilon) \qquad (3.32)$$

From Section 3.2, $\tilde{D}a = \varepsilon^{n_F-1}\frac{Da\tilde{Y}_{O,\infty}{}^{n_O}\tilde{T}_\infty{}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_\infty)}{4Pr}\tilde{x}^{4/3}$

The leading order terms are $\zeta^2\frac{\partial^2\theta}{\partial\zeta^2} = -\tilde{D}a(\phi_F+\tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3})^{n_F}\exp[\theta-(\tilde{T}_\infty-\tilde{T}_0)\zeta/\tilde{x}^{1/3}]$

(2) $\left\{4(1-\xi)\left[\frac{1}{Pr}\xi^2\frac{\partial^2\tilde{T}}{\partial\xi^2}+(\frac{1}{Pr}-1)\xi\frac{\partial\tilde{T}}{\partial\xi}\right]-\xi\left(\frac{2}{Pr}\xi\frac{\partial\tilde{T}}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)\right\}$

$+\left\{4(1-\xi)\left[\frac{1}{Sc_F}\xi^2\frac{\partial^2\tilde{Y}_F}{\partial\xi^2}+(\frac{1}{Sc_F}-1)\xi\frac{\partial\tilde{Y}_F}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_F}\xi\frac{\partial\tilde{Y}_F}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}\right)\right\}=0$

From Section 3.2,

$$4(1-\xi)\left[\frac{1}{Pr}\xi^2\frac{\partial^2\tilde{T}}{\partial\xi^2}+(\frac{1}{Pr}-1)\xi\frac{\partial\tilde{T}}{\partial\xi}\right]-\xi\left(\frac{2}{Pr}\xi\frac{\partial\tilde{T}}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right)=4\varepsilon Pr\zeta^2\frac{\partial^2\theta}{\partial\zeta^2}+O(\varepsilon^{1+(1/Pr)};\varepsilon^2)$$

$$4(1-\xi)\left[\frac{1}{Sc_F}\xi^2\frac{\partial^2\tilde{Y}_F}{\partial\xi^2}+(\frac{1}{Sc_F}-1)\xi\frac{\partial\tilde{Y}_F}{\partial\xi}\right]-\xi\left(\frac{2}{Sc_F}\xi\frac{\partial\tilde{Y}_F}{\partial\xi}+6\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}\right)$$

$$=4[1-(\varepsilon\zeta)^{1/Pr}]\frac{Pr}{Le_F}\left[\zeta^2\frac{\partial^2\tilde{Y}_F}{\partial\zeta^2}+(1-Le_F)\zeta\frac{\partial\tilde{Y}_F}{\partial\zeta}\right]-(\varepsilon\zeta)^{1/Pr}\left(\frac{2}{Le_F}\zeta\frac{\partial\tilde{Y}_F}{\partial\zeta}+6\tilde{x}\frac{\partial\tilde{Y}_F}{\partial\tilde{x}}\right)$$

$$=4Pr\zeta^2\frac{\partial^2[\varepsilon(\phi_F+\tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3})]}{\partial\zeta^2}+O(\varepsilon^2;\varepsilon^{1+(1/Pr)})=4\varepsilon Pr\zeta^2\frac{\partial^2\phi_F}{\partial\zeta^2}+O(\varepsilon^2;\varepsilon^{1+(1/Pr)})$$

Thus $4\varepsilon Pr\zeta^2\frac{\partial^2\theta}{\partial\zeta^2}+O(\varepsilon^{1+(1/Pr)})+4\varepsilon Pr\zeta^2\frac{\partial^2\phi_F}{\partial\zeta^2}+O(\varepsilon^2;\varepsilon^{1+(1/Pr)})=0$ or $\frac{\partial^2(\theta+\phi_F)}{\partial\zeta^2}=0$

$\Rightarrow \quad \theta+\phi_F = c\,\zeta + c_2$

$\zeta=0$: $\theta=\phi_F=0 \quad \therefore \quad c_2=0$ and $\theta+\phi_F=c\,\zeta$

(3) Summary

$\zeta^2\frac{\partial^2\theta}{\partial\zeta^2} = -\tilde{D}a(\phi_F+\tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3})^{n_F}\exp[\theta-(\tilde{T}_\infty-\tilde{T}_0)\zeta/\tilde{x}^{1/3}]$; $\zeta=0$: $\theta=0$

$\theta+\phi_F=c\,\zeta$ where c still needs to be determined.

(C) Matching

$$\tilde{T} = (\tilde{T}_\infty + \varepsilon a_T) - [(\tilde{T}_\infty - \tilde{T}_0) + \varepsilon a_T]\xi^{Pr/\tilde{x}^{1/3}} + O(\varepsilon^2) = (\tilde{T}_\infty + \varepsilon a_T) - [(\tilde{T}_\infty - \tilde{T}_0) + \varepsilon a_T](\varepsilon\zeta)^{/\tilde{x}^{1/3}} + O(\varepsilon^2)$$

$$= \tilde{T}_\infty + \varepsilon[a_T - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] + O(\varepsilon^2) = \tilde{T}_\infty + \varepsilon[\theta - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] + O(\varepsilon^2)\Big|_{\zeta\to\infty}$$

$$\therefore \quad \theta(\zeta\to\infty) = a_T \quad \text{or} \quad (\partial\theta/\partial\zeta)_{\zeta\to\infty} = 0$$

$$\tilde{Y}_F = \varepsilon a_F + (\tilde{Y}_{F,0} - \varepsilon a_F)\xi^{Sc_F/\tilde{x}^{1/3}} + O(\varepsilon^2) = \varepsilon a_F + (\tilde{Y}_{F,0} - \varepsilon a_F)(\xi^{Pr})^{Sc_F/Pr/\tilde{x}^{1/3}} + O(\varepsilon^2)$$

$$= \varepsilon a_F + (\tilde{Y}_{F,0} - \varepsilon a_F)(\varepsilon\zeta)^{Le_F/\tilde{x}^{1/3}} + O(\varepsilon^2) = \varepsilon a_F + (\tilde{Y}_{F,0} - \varepsilon a_F)(\varepsilon\zeta)[1 + \varepsilon\ell_F \ell n(\varepsilon\zeta) + \cdots]/\tilde{x}^{1/3} + O(\varepsilon^2)$$

$$= \varepsilon(a_F + \tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3}) + O(\varepsilon^2) = \varepsilon(\phi_F + \tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3}) + O(\varepsilon^2)\Big|_{\zeta\to\infty}$$

$$\therefore \quad \phi_F(\zeta\to\infty) = a_F$$

From (B) : $\theta + \phi_F = c\,\zeta$

$\zeta\to\infty$: $\theta\to a_T$, $\phi_F\to a_F$ $\therefore$ $a_T + a_F = c\,\zeta$ $\Rightarrow$ $a_T + a_F = c = 0$ or

$a_F = -a_T \Rightarrow$ $\theta + \phi_F = 0$ or $\phi_F = -\theta$

(E) Summary

$$\zeta^2\frac{\partial^2\theta}{\partial\zeta^2} = -\tilde{D}a(-\theta + \tilde{Y}_{F,0}\zeta/\tilde{x}^{1/3})^{n_F}\exp[\theta - (\tilde{T}_\infty - \tilde{T}_0)\zeta/\tilde{x}^{1/3}] \quad ; \quad \zeta = 0 : \quad \theta = 0 \quad ;$$

$\zeta\to\infty$: $d\theta/d\zeta\to 0$, $\theta\to a_T$

Rescaling

From Section 3.2, $\sigma = \tilde{Y}_{F,0}/\tilde{x}^{1/3}$, $\bar{\zeta} = \sigma\zeta$, $\beta = (\tilde{T}_\infty - \tilde{T}_0)/\tilde{Y}_{F,0}$, then

$$\bar{\zeta}^2\frac{\partial^2\theta}{\partial\bar{\zeta}^2} = -\tilde{D}a(-\theta + \bar{\zeta})^{n_F}\exp(\theta - \beta\bar{\zeta}) \quad ; \quad \bar{\zeta} = 0 : \quad \theta = 0 \quad ;$$

$\bar{\zeta}\to\infty$: $\partial\theta/\partial\bar{\zeta}\to 0$, $\theta\to a_T$

Note: Since there is no differentiation with respect to $\tilde{x}$, the problem is locally similar and $\tilde{x}$ can be considered as a constant in the structure equation.

3.4 Ignition Analysis III : $T_0 > T\infty$, $\tilde{x} \approx 1$, Thicker Reaction Region

Because spontaneous ignition is primarily controlled by temperature, ignition occurs near $\eta = 0$. This is the centerline of the jet.

(A) Outer Solutions

The outer solution is as follows

$$\tilde{T} = \tilde{T}_\infty + [(\tilde{T}_0 - \tilde{T}_\infty) + \varepsilon a_T](\text{sech}^{2Pr}\eta)/\tilde{x}^{1/3} + O(\varepsilon^2) \tag{3.33}$$

$$\tilde{Y}_F = (\tilde{Y}_{F,0} - \varepsilon a_F)(\text{sech}^{2Sc_F}\eta)/\tilde{x}^{1/3} + O(\varepsilon^2) \quad ; \tag{3.34}$$

$$\tilde{Y}_O = \tilde{Y}_{O,\infty} - (\tilde{Y}_{O,\infty} + \varepsilon a_O)(\text{sech}^{2Sc_O}\eta)/\tilde{x}^{1/3} + O(\varepsilon^2) \tag{3.35}$$

(B) Inner Expansion

If successful, ignition occurs in an inner region near $\eta = 0$ and $\tilde{x} \approx 1$

Since $d(\text{sech}\,\eta)/d\eta = 0$ at $\eta = 0$, it seems that the reaction region should be thicker than $O(\varepsilon)$.

Define inner variables $\eta = \sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\zeta$, $\tilde{x} = 1 + \varepsilon(3\xi/\tilde{Y}_{O,\infty})$, $\varepsilon = \tilde{T}_0^{\,2}/\tilde{E}$,

$\beta = (\tilde{T}_0 - \tilde{T}_\infty)/\tilde{Y}_{O,\infty}$; when $\eta = 0$: $\zeta = 0$

$$\Rightarrow \quad \eta^2 = \varepsilon\zeta^2/(Pr\tilde{Y}_{O,\infty}) \quad , \quad \partial\eta = \sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\partial\zeta \quad , \quad \partial\eta^2 = [\varepsilon/(Pr\tilde{Y}_{O,\infty})]\partial\zeta^2 \quad ,$$

$$\partial\tilde{x} = (3\varepsilon/\tilde{Y}_{O,\infty})\partial\xi$$

$$\text{sech}\,\eta = 1 - (\eta^2/2) + \cdots = 1 - \varepsilon[\zeta^2/(2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2)$$

$$\text{sech}^2\eta = \{1 - \varepsilon[\zeta^2/(2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2)\}^2 = 1 - 2\varepsilon[\zeta^2/[2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2) = 1 - \varepsilon[\zeta^2/(Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2)$$

$$\text{sech}^{2Pr}\eta = \{1 - \varepsilon[\zeta^2/(2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2)\}^{2Pr} = 1 - \varepsilon 2Pr[\zeta^2/(2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2) = 1 - \varepsilon(\zeta^2/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)$$

$$\text{sech}^{2Sc_i}\eta = \{1 - \varepsilon[\zeta^2/(2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2)\}^{2Sc_i} = 1 - \varepsilon 2Sc_i[\zeta^2/(2Pr\tilde{Y}_{O,\infty})] + O(\varepsilon^2)$$

$$= 1 - \varepsilon(Sc_i/Pr)(\zeta^2/\tilde{Y}_{O,\infty}) + O(\varepsilon^2) = 1 - \varepsilon Le_i(\zeta^2/\tilde{Y}_{O,\infty}) + O(\varepsilon^2) \tag{3.36}$$

$$\tanh\ \eta = \eta - (\eta^3/3) + \cdots = \sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\zeta + O(\varepsilon^{3/2}) \tag{3.37}$$

$$1/\tilde{x}^{1/3} = 1/[1+\varepsilon(3\xi/\tilde{Y}_{O,\infty})]^{1/3} = 1/[1+\varepsilon(\xi/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)] = 1-\varepsilon(\xi/\tilde{Y}_{O,\infty}) + O(\varepsilon^2) \tag{3.38}$$

$$\tilde{T} = \tilde{T}_f[\eta = \sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\zeta, \tilde{x} = 1+3\varepsilon(\xi/\tilde{Y}_{O,\infty})] + \varepsilon\theta + O(\varepsilon^2)$$

$$= \tilde{T}_\infty + (\tilde{T}_0 - \tilde{T}_\infty)[1-\varepsilon(\zeta^2/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)][1-\varepsilon(\xi/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)] + \varepsilon\theta + O(\varepsilon^2)$$

$$= \tilde{T}_0 + \varepsilon\{\theta - (\tilde{T}_0 - \tilde{T}_\infty)[(\zeta^2/\tilde{Y}_{O,\infty}) + (\xi/\tilde{Y}_{O,\infty})]\} + O(\varepsilon^2) = \tilde{T}_0 + \varepsilon\{\theta - [(\tilde{T}_0 - \tilde{T}_\infty)/\tilde{Y}_{O,\infty}](\zeta^2+\xi)\} + O(\varepsilon^2)$$

$$= \tilde{T}_0 + \varepsilon[\theta - \beta(\zeta^2+\xi)] + O(\varepsilon^2) \tag{3.39}$$

$$\tilde{Y}_F = \tilde{Y}_{F,f}[\eta = \sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\zeta, \tilde{x} = 1+3\varepsilon(\xi/\tilde{Y}_{O,\infty})] + \varepsilon\phi_F + O(\varepsilon^2)$$

$$= \tilde{Y}_{F,0}[1-\varepsilon Le_F(\zeta^2/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)][1-\varepsilon(\xi/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)] + \varepsilon\phi_F + O(\varepsilon^2) = \tilde{Y}_{F,0} + O(\varepsilon) \tag{3.40}$$

$$\tilde{Y}_O = \tilde{Y}_{O,f}[\eta = \sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\zeta, \tilde{x} = 1+3\varepsilon(\xi/\tilde{Y}_{O,\infty})] + \varepsilon\phi_O + O(\varepsilon^2)$$

$$= \tilde{Y}_{O,\infty}\{1-[1-\varepsilon Le_O(\zeta^2/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)][1-\varepsilon(\xi/\tilde{Y}_{O,\infty}) + O(\varepsilon^2)]\} + \varepsilon\phi_O + O(\varepsilon^2)$$

$$= \varepsilon\{\phi_O + \tilde{Y}_{O,\infty}[Le_O(\zeta^2/\tilde{Y}_{O,\infty}) + (\xi/\tilde{Y}_{O,\infty})]\} + O(\varepsilon^2) = \varepsilon(\phi_O + Le_O\zeta^2 + \xi) + O(\varepsilon^2) \tag{3.41}$$

$$\tilde{E}/\tilde{T} = \tilde{E}/\{\tilde{T}_0 + \varepsilon[\theta - \beta(\zeta^2+\xi)] + O(\varepsilon^2)\} = \tilde{E}/\langle\tilde{T}_0\{1+\varepsilon[\theta-\beta(\zeta^2+\xi)]/\tilde{T}_0 + O(\varepsilon^2)\}\rangle$$

$$= (\tilde{E}/\tilde{T}_0)\{1-\varepsilon[\theta-\beta(\zeta^2+\xi)]/\tilde{T}_0 + O(\varepsilon^2)\} = (\tilde{E}/\tilde{T}_0) - \varepsilon(\tilde{E}/\tilde{T}_0^2)[\theta-\beta(\zeta^2+\xi)] + (\tilde{E}/\tilde{T}_0)O(\varepsilon^2)$$

$$= (\tilde{E}/\tilde{T}_0) - [\theta - \beta(\zeta^2+\xi)] + O(\varepsilon)$$

$$\exp(-\tilde{E}/\tilde{T}) = \exp\{-(\tilde{E}/\tilde{T}_0) - [\theta-\beta(\zeta^2+\xi)] + O(\varepsilon)\} = \exp(-\tilde{E}/\tilde{T}_0)\exp[\theta-\beta(\zeta^2+\xi)] + O(\varepsilon) \tag{3.42}$$

(1) $\eta = 0$, $\tilde{x} = 1$: $\tilde{T} = \tilde{T}_0$, $\tilde{Y}_O = 0$ $\Rightarrow$ $\zeta = 0$, $\xi = 0$: $\theta = \phi_O = 0$

(2) $\eta = 0$, $\tilde{x} > 1$: $\partial\tilde{T}/\partial\eta = \partial\tilde{Y}_O/\partial\eta = 0$ $\Rightarrow$ $\zeta = 0$, $\xi > 0$:

$\partial\theta/\partial\zeta = \partial\phi_O/\partial\zeta = 0$

(3) $$\left[\frac{1}{Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}\right] + \left[\frac{1}{Sc_O}\frac{\partial^2\tilde{Y}_O}{\partial\eta^2} + 2(\tanh\eta)\frac{\partial\tilde{Y}_O}{\partial\eta} - 6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial\tilde{Y}_O}{\partial\tilde{x}}\right] = 0$$

$$\frac{1}{Pr}\frac{\partial^2\{\tilde{T}_0 + \varepsilon[\theta-\beta(\zeta^2+\xi)] + O(\varepsilon^2)\}}{[\varepsilon/(Pr\tilde{Y}_{O,\infty})]\partial\zeta^2} + 2[\sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\zeta + O(\varepsilon^{3/2})]\frac{\partial\{\tilde{T}_0 + \varepsilon[\theta-\beta(\zeta^2+\xi)] + O(\varepsilon^2)\}}{\sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\partial\zeta}$$

$$-6\{1-\varepsilon[\zeta^2/(Pr\tilde{Y}_{O,\infty})]+O(\varepsilon^2)\}[1+3\varepsilon(\xi/\tilde{Y}_{O,\infty})]\frac{\partial\{\tilde{T}_0+\varepsilon[\theta-\beta(\zeta^2+\xi)]+O(\varepsilon^2)\}}{(3\varepsilon/\tilde{Y}_{O,\infty})\partial\xi}$$

$$+\frac{1}{Sc_O}\frac{\partial^2[\varepsilon(\phi_O+Le_O\zeta^2+\xi)+O(\varepsilon^2)]}{[\varepsilon/(Pr\tilde{Y}_{O,\infty})]\partial\zeta^2}+2[\sqrt{\varepsilon/Pr}\,\zeta+O(\varepsilon^{3/2})]\frac{\partial[\varepsilon(\phi_O+Le_O\zeta^2+\xi)+O(\varepsilon^2)]}{\sqrt{\varepsilon/(Pr\tilde{Y}_{O,\infty})}\,\partial\zeta}$$

$$-6\{1-\varepsilon[\zeta^2/(Pr\tilde{Y}_{O,\infty})]+O(\varepsilon^2)\}[1+3\varepsilon(\xi/\tilde{Y}_{O,\infty})]\frac{\partial[\varepsilon(\phi_O+Le_O\zeta^2+\xi)+O(\varepsilon^2)]}{(3\varepsilon/\tilde{Y}_{O,\infty})\partial\xi}=0 \qquad (3.43)$$

The leading order terms are

$$\tilde{Y}_{O,\infty}\left\{\frac{\partial^2[\theta-\beta(\zeta^2+\xi)]}{\partial\zeta^2}-2\frac{\partial[\theta-\beta(\zeta^2+\xi)]}{\partial\xi}+\frac{Pr}{Sc_O}\frac{\partial^2(\phi_O+Le_O\zeta^2+\xi)}{\partial\zeta^2}-2\frac{\partial(\phi_O+Le_O\zeta^2+\xi)}{\partial\xi}\right\}=0$$

$$\frac{\partial^2\theta}{\partial\zeta^2}-2\beta-2\frac{\partial\theta}{\partial\xi}+2\beta+\frac{1}{Le_O}\left(\frac{\partial^2\phi_O}{\partial\zeta^2}+2Le_O\right)-2\frac{\partial\phi_O}{\partial\xi}-2=0 \quad \text{or}$$

$$\frac{\partial^2\theta}{\partial\zeta^2}-2\frac{\partial\theta}{\partial\xi}+\frac{1}{Le_O}\frac{\partial^2\phi_O}{\partial\zeta^2}-2\frac{\partial\phi_O}{\partial\xi}=0$$

(4) $$\frac{1}{Pr}\frac{\partial^2\tilde{T}}{\partial\eta^2}+2(\tanh\eta)\frac{\partial\tilde{T}}{\partial\eta}-6(\mathrm{sech}^2\eta)\tilde{x}\frac{\partial\tilde{T}}{\partial\tilde{x}}=-Da\tilde{x}^{4/3}\tilde{Y}_F^{n_F}\tilde{Y}_O^{n_O}\tilde{T}^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T})$$

$$\tilde{Y}_{O,\infty}\left[\frac{\partial^2\theta}{\partial\zeta^2}-2\frac{\partial\theta}{\partial\xi}+O(\varepsilon)\right]$$

$$=-Da[1+O(\varepsilon)]^{4/3}[\tilde{Y}_{F,0}+O(\varepsilon)]^{n_F}[\varepsilon(\phi_O+Le_O\zeta^2+\xi)+O(\varepsilon^2)]^{n_O}[\tilde{T}_0+O(\varepsilon)]^{n_T-n_F-n_O+1}$$

$$\cdot\exp(-\tilde{E}/\tilde{T}_0)\exp[\theta-\beta(\zeta^2+\xi)]+O(\varepsilon)$$

$$=-\varepsilon^{n_O}Da\,\tilde{Y}_{F,0}^{n_F}\tilde{T}_0^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_0)(\phi_O+Le_O\zeta^2+\xi)^{n_O}\exp[\theta-\beta(\zeta^2+\xi)]+O(\varepsilon)$$

Define $\tilde{D}a=\varepsilon^{n_O}Da(\tilde{Y}_{F,0}^{n_F}/\tilde{Y}_{O,\infty})\tilde{T}_0^{n_T-n_F-n_O+1}\exp(-\tilde{E}/\tilde{T}_0)$ (3.44)

= Reduced Damköhler number

Then : $$\frac{\partial^2\theta}{\partial\zeta^2}-2\frac{\partial\theta}{\partial\xi}=-\tilde{D}a(\phi_O+Le_O\zeta^2+\xi)^{n_O}\exp[\theta-\beta(\zeta^2+\xi)] \qquad (3.45)$$

(C) Matching

$$\tilde{T}=\tilde{T}_\infty+[(\tilde{T}_0-\tilde{T}_\infty)+\varepsilon a_T](\mathrm{sech}^{2Pr}\eta)/\tilde{x}^{1/3}+O(\varepsilon^2)$$

$$= \tilde{T}_\infty + [(\tilde{T}_0 - \tilde{T}_\infty) + \varepsilon a_T][1 - \varepsilon(\zeta^2 / \tilde{Y}_{O,\infty})][1 - \varepsilon(\xi / \tilde{Y}_{O,\infty})] + O(\varepsilon^2)$$

$$= \tilde{T}_0 + \varepsilon\{a_T - [(\tilde{T}_0 - \tilde{T}_\infty)/\tilde{Y}_{O,\infty}](\zeta^2 + \xi)\} + O(\varepsilon^2) = \tilde{T}_0 + \varepsilon[\theta - \beta(\zeta^2 + \xi)] + O(\varepsilon^2)\Big|_{\zeta\to\infty}$$

$$\therefore \quad \theta(\zeta \to \infty) \to a_T \quad \text{and} \quad (\partial\theta / \partial\zeta)_{\zeta\to\infty} \to 0$$

$$\tilde{Y}_O = \tilde{Y}_{O,\infty} - (\tilde{Y}_{O,\infty} + \varepsilon a_O)(\mathrm{sech}^{2Sc_O}\eta) / \tilde{x}^{1/3} + O(\varepsilon^2)$$
$$= \tilde{Y}_{O,\infty} - (\tilde{Y}_{O,\infty} + \varepsilon a_O)[1 - \varepsilon Le_O(\zeta^2 / \tilde{Y}_{O,\infty})][1 - \varepsilon(\xi / \tilde{Y}_{O,\infty})] + O(\varepsilon^2)$$

$$= \varepsilon(-a_O + Le_O\zeta^2 + \xi) + O(\varepsilon^2) = \varepsilon(\phi_O + Le_O\zeta^2 + \xi) + O(\varepsilon^2)\Big|_{\zeta\to\infty}$$

$$\therefore \quad \phi_O(\zeta \to \infty) \to -a_O \quad \text{and} \quad (\partial\phi_O / \partial\zeta)_{\eta\to\infty} \to 0$$

(D) Ignition Criterion

(1) Ignition is successful when $(\partial\tilde{T} / \partial\tilde{x})_{\eta=0} \geq 0$

Since $\eta = 0$ is in the inner, reactive region, the ignition condition becomes

$$(\partial\tilde{T}_{in} / \partial\xi)_{\zeta=0} \geq 0$$

$$(\partial\tilde{T}_{in} / \partial\xi)_{\zeta=0} = \langle \partial\{\tilde{T}_0 + \varepsilon[\theta - \beta(\zeta^2 + \xi)] + O(\varepsilon^2)\} / \partial\xi \rangle_{\zeta=0} = \varepsilon[(\partial\theta/\partial\xi)_{\zeta=0} - \beta] + O(\varepsilon^2) \geq 0$$

or $\quad (\partial\theta/\partial\xi)_{\zeta=0} \geq \beta$

(2) Ignition is successful when $\partial\tilde{T} / \partial\eta \geq 0$ at any $\tilde{x}$

In the inner, reactive region, the ignition condition becomes $\partial\tilde{T}_{in} / \partial\zeta \geq 0$ at any ξ

$$\partial\tilde{T}_{in} / \partial\zeta = \partial\{\tilde{T}_0 + \varepsilon[\theta - \beta(\zeta^2 + \xi)] + O(\varepsilon^2)\} / \partial\zeta = \varepsilon[(\partial\theta/\partial\zeta) - 2\beta\zeta] + O(\varepsilon^2) \geq 0$$

or $\quad \partial\theta/\partial\zeta \geq 2\beta\zeta \quad$ at any ξ

(E) Initial condition

At the nozzle exit, there is no reaction. Thus

$$\theta(\xi = 0) = \phi_O(\xi = 0) = 0$$

(F) Summary

$$\frac{\partial^2\theta}{\partial\zeta^2}-2\frac{\partial\theta}{\partial\xi}+\frac{1}{Le_O}\frac{\partial^2\phi_O}{\partial\zeta^2}-2\frac{\partial\phi_O}{\partial\xi}=0$$

$$\frac{\partial^2\theta}{\partial\zeta^2}-2\frac{\partial\theta}{\partial\xi}=-\tilde{D}a(\phi_O+Le_O\zeta^2+\xi)^{n_O}\exp[\theta-\beta(\zeta^2+\xi)]$$

$$\theta(\xi=0)=\phi_O(\xi=0)=0$$

$\zeta=0$, $\xi>0$: $\partial\theta/\partial\zeta=\partial\phi_O/\partial\zeta=0$

$\zeta\to\infty$: $\partial\theta/\partial\zeta\to 0$; $\partial\phi_O/\partial\zeta\to 0$

If $Le_O = 1$, we have $\phi_O=-\theta$ and the problem is reduced to

$$\frac{\partial^2\theta}{\partial\zeta^2}-2\frac{\partial\theta}{\partial\xi}=-\tilde{D}a(\zeta^2+\xi-\theta]^{n_O}\exp[\theta-\beta(\zeta^2+\xi)]$$

$\zeta=0$: $\xi=0$: $\theta=0$, $\xi>0$: $\partial\theta/\partial\zeta=0$; $\zeta\to\infty$: $\partial\theta/\partial\zeta\to 0$

Ignition criterion : $(\partial\theta/\partial\xi)_{\zeta=0}\geq\beta$ or $\partial\theta/\partial\zeta\geq 2\beta\zeta$ at any ξ

(G) Rescaling when the change of γ is by changing T_0 or $Y_{O,\infty}$, or n_O is varying

Define $\hat{T}_0$ as the reference value of $\tilde{T}_0$, $\hat{n}_O$ as the reference value of n_O ,

$\hat{Y}_{O,\infty}$ as the reference value of $\tilde{Y}_{O,\infty}$

$\hat{\varepsilon}=\hat{T}_0^{\,2}/\tilde{E}$ as the reference value of ε $\Rightarrow$ $\hat{\varepsilon}/\varepsilon=(\hat{T}_0/\tilde{T}_0)^2$

$$\hat{D}a=\hat{\varepsilon}^{\hat{n}_O}Da(\tilde{Y}_{F,0}^{\,n_F}/\hat{Y}_{O,\infty})\hat{T}_0^{\,n_T-n_F-\hat{n}_O+1}\exp(-\tilde{E}/\hat{T}_0)$$

$$=(\hat{T}_0/\tilde{T}_0)^{n_T-n_F+\hat{n}_O+1}(\tilde{T}_0/\tilde{E})^{\hat{n}_O-n_O}(\tilde{Y}_{O,\infty}/\hat{Y}_{O,\infty})\exp[\tilde{E}(\tilde{T}_0^{-1}-\hat{T}_0^{-1})]\tilde{D}a \quad (3.46)$$

If only T_0 is varying: $\hat{D}a=(\hat{T}_0/\tilde{T}_0)^{n_T-n_F+n_O+1}\exp[\tilde{E}(\tilde{T}_0^{-1}-\hat{T}_0^{-1})]\tilde{D}a$ (3.47)

In the calculations, we

(1) Choose a value of β as the reference value.

(2) Find the value of $\hat{T}_0$ based on this reference value of β. (need to specify $\tilde{T}_\infty$ and $\tilde{Y}_{O,\infty}$)

(3) For other values of β, determine $\tilde{T}_0$ using the same values of $\tilde{T}_\infty$ and $\tilde{Y}_{O,\infty}$.

(4) Use the values of $\hat{T}_0$ and $\tilde{T}_0$ to determine $\hat{D}a$.

If only n_O is varying : $\quad \hat{D}a = (\tilde{T}_0 / \tilde{E})^{\hat{n}_O - n_O}\, \tilde{D}a$ (3.47)

If only $Y_{O,\infty}$ is varying : $\quad \hat{D}a = (\tilde{Y}_{O,\infty} / \hat{Y}_{O,\infty})\tilde{D}a$ (3.48)

3.5 Analysis Scenarios

3.5.1 Cool jet flowing into a hot ambient ($T_\infty > T_0$)

(With reference to Section 3.2 Ignition Analysis I) In the presence of a weak reaction, the temperature is increased from its frozen value by a small, $O(\varepsilon)$ amount where $\varepsilon = \tilde{T}_\infty^{\,2} / \tilde{E}$ while the reactant concentrations are reduced from their respective frozen values by an $O(\varepsilon)$ amount. Because ignition is primarily controlled by temperature, ignition occurs near $\eta \to \infty$ if successful. Fig.3.1 shows a schematic of the inner and outer regions for the scenario.

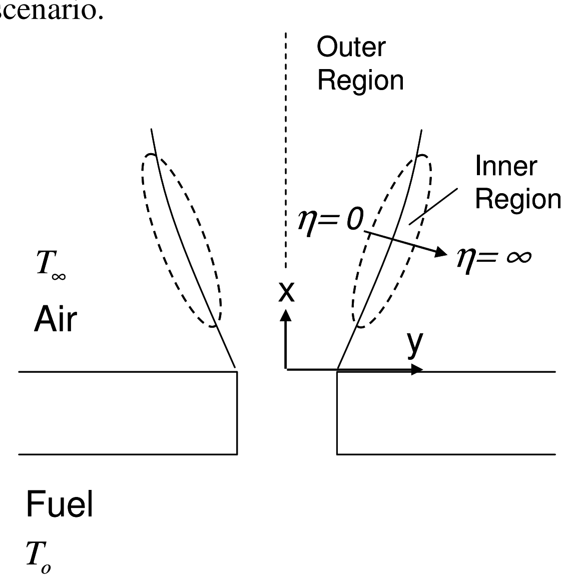

Fig. 3.1: Schematic of inner and outer regions for cool jet, hot ambient case.

Away from this high temperature region, the reaction is frozen. In the outer, chemically frozen region, the outer solutions are similar to Eqns. 3.4 – 3.6, but with an $O(\varepsilon)$ change in their values. In the inner, reactive region, defining a stretched inner variable as

$$\zeta = \tilde{Y}_{F,0}(\operatorname{sech}\eta)^{2Pr}/(\varepsilon\tilde{x}^{1/3}) \tag{3.49}$$

and substituting into Parts (C) to (E) of Ignition Analysis I, yields, when Le_F is sufficiently smaller than unity, as for hydrogen,

$$\zeta^2(\partial^2\theta/\partial\zeta^2) = -\tilde{D}a\,\zeta^{Le_F}\exp(\theta-\alpha\zeta) \quad , \tag{3.50}$$

where $\alpha = (\tilde{T}_\infty - \tilde{T}_0)/\tilde{Y}_{F,0}$ and the reduced Damköhler number is defined as

$$\tilde{D}a = Da\,\tilde{Y}_{O,\infty}\tilde{x}^{4/3}[\tilde{Y}_{F,0}/(\varepsilon\tilde{x}^{1/3})]^{1-Le_F}\exp(-\tilde{E}/\tilde{T}_\infty)/(4Pr\tilde{T}_\infty) \quad . \tag{3.51}$$

The boundary conditions required to solve this equation can be found by matching the inner and outer solutions as

$$\zeta = 0 : \quad \theta = 0 \quad ; \quad \zeta\to\infty : \quad \partial\theta/\partial\zeta \to 0 \quad , \quad \theta \to a_T \tag{3.52}$$

For the case of Le_F close to unity, Eqn. (3.2) is modified to

$$\zeta^2(\partial^2\theta/\partial\zeta^2) = -\tilde{D}a(\zeta-\theta)\exp(\theta-\alpha\zeta) \quad . \tag{3.53}$$

3.5.2 Hot jet flowing into a cool ambient ($T_0 > T_\infty$)

(With reference to Section 3.4 Ignition Analysis III) For the case of a hot jet issuing into a cold ambient, any ignition will occur near the jet centerline, η = 0. Fig.3.2 shows a schematic of the inner and outer regions for the scenario.

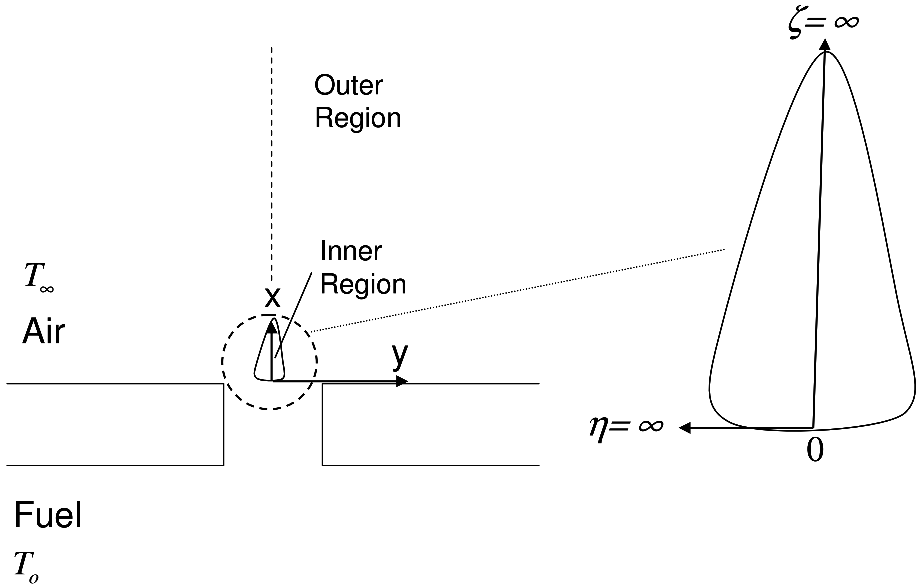

Fig. 3.2: Schematic of inner and outer regions for hot jet, cool ambient case.

Moreover, because the jet will be cooled by the cold ambient gas along the flow, ignition is expected to occur near the slot exit. The analysis is similar to that in Section 3.1, except that $\varepsilon = \tilde{T}_0^2 / \tilde{E}$ and the inner variables are defined as

$$\zeta = \eta \sqrt{Pr \tilde{Y}_{O,\infty} / \varepsilon} \quad , \quad \xi = \tilde{Y}_{O,\infty} (\tilde{x} - 1)/(3\varepsilon) \quad , \tag{3.54}$$

leading to

$$\frac{\partial^2 \theta}{\partial \zeta^2} - 2\frac{\partial \theta}{\partial \xi} + \frac{1}{Le_O}\frac{\partial^2 \phi_O}{\partial \zeta^2} - 2\frac{\partial \phi_O}{\partial \xi} = 0 \quad , \tag{3.55}$$

$$\frac{\partial^2 \theta}{\partial \zeta^2} - 2\frac{\partial \theta}{\partial \xi} = -\tilde{D}a(\phi_O + Le_O \zeta^2 + \xi)\exp[\theta - \beta(\zeta^2 + \xi)] \quad , \tag{3.56}$$

with the initial and boundary conditions

$$\theta(\xi = 0) = \phi_O(\xi = 0) = 0 \quad ,$$

$$\zeta = 0 \text{ and } \zeta \to \infty \ , \ \xi > 0 : \quad \partial\theta/\partial\zeta = \partial\phi_O/\partial\zeta = 0 \quad ,$$

where $\beta = (\tilde{T}_0 - \tilde{T}_\infty)/\tilde{Y}_{O,\infty}$ and the reduced Damköhler number is

$$\tilde{D}a = \varepsilon[Da\tilde{Y}_{F,0}/(\tilde{T}_0\tilde{Y}_{O,\infty})]\exp(-\tilde{E}/\tilde{T}_0) \quad . \tag{3.57}$$

Ignition is considered successful when the heat generation through reaction is sufficient to compensate the heat loss from the jet to the ambient at any location, and the ignition criterion is given by

$$(\partial\theta/\partial\xi)_{\zeta=0} \geq \beta \quad \text{or} \quad \partial\theta/\partial\zeta \geq 2\beta\zeta \text{ at any } \xi \quad . \tag{3.58}$$

Chapter 4: Results and Discussions

4.1 Recapitulation

Limits of spontaneous ignition were identified as functions of slot width, flow rate, and temperatures of the hydrogen jet and ambient air for the two scenarios of a cool jet flowing into a hot ambient and a hot jet flowing into a cool ambient. Specifically, Sections 3.2 (for the cool jet case) and 3.4 (for the hot jet case) were referenced for the analysis of hydrogen due to its low local Le_F of 0.6. Equations balancing diffusive terms with reaction terms were obtained for the cool jet case (Eqn. 3.50), and equations balancing the transverse diffusive, streamwise convective terms and reaction terms were obtained for the hot jet case (Eqn. 3.56). The solutions from the equations are discussed in greater detail in the following sections.

4.2 Cool jet flowing into a hot ambient ($T\infty > T_0$)

Equations (3.50) and (3.53), subject to Eqns. (3.51) – (3.52), were solved by a fourth order Runge-Kutta method (using computer codes). The results are shown in Fig. 4.1, a plot of the reaction temperature increase (a_T) versus reduced Damköhler number. This reveals the lower and middle branches of an S-curve [5]. In each such curve, there is a maximum value of $\tilde{D}a$ above which a solution does not exist. For values of $\tilde{D}a$ smaller than this ignition $\tilde{D}a$, there are two solutions. This represents the transition from weak reaction to vigorous burning, and is defined as the ignition state. The lower branch, showing an increase of temperature with higher reaction rate, is the physically realistic branch. The middle branch represents conditions that are not physically possible, owing to the negative slope. Spontaneous ignition is predicted for any $\tilde{D}a$ greater than this critical value.

Three curves are included in Fig. 4.1, each with a different value of α, where

$$\alpha = (\tilde{T}_\infty - \tilde{T}_0) / \tilde{Y}_{F,0} \tag{4.1}$$

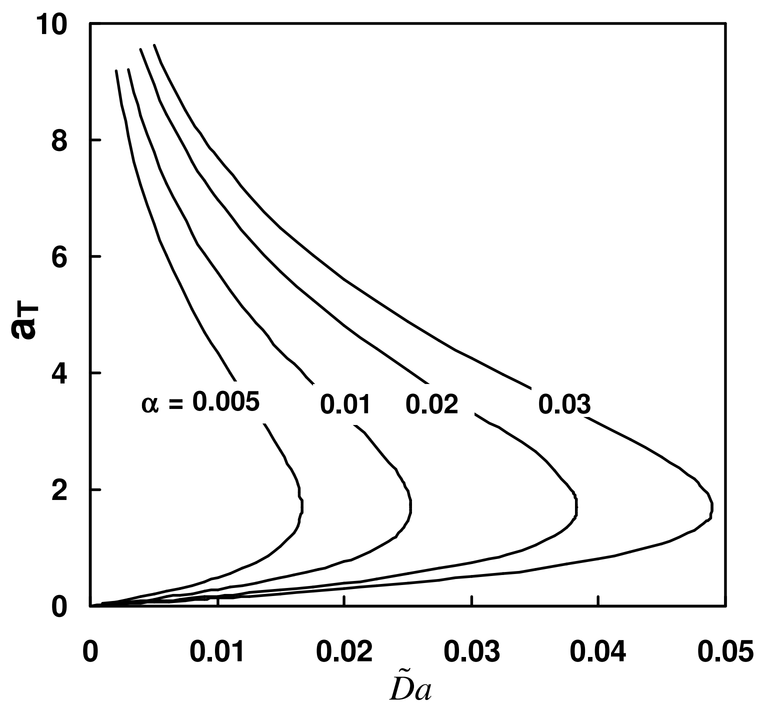

Fig. 4.1: a_T versus $\tilde{D}a$ for varying α (which is changed by variations in $\tilde{T}_0$ or $\tilde{Y}_{F,0}$) , with Le_F = 0.6 and constant $\tilde{T}_\infty$ = 0.0123, hot ambient. Definitions of $\tilde{D}a$ and a_T are in Section 3.2(Part C-2).

Fig. 4.1 indicates that a decrease in α reduces the critical $\tilde{D}a$ at ignition, which means that ignition is favored. Such a decrease can be accomplished either by increasing the reactant mass fraction in the fuel supply, $\tilde{Y}_{F,0}$, or by increasing the jet temperature, $\tilde{T}_0$. Both findings are physically realistic. A fuel such as hydrogen (which has Le_F of 0.6 or less in mixtures with N_2, is hence more ignitable as compared to fuels such as isooctane and methane (which have higher Le_F, under the same conditions). Table 1 lists the typical values of α and q_F for hydrogen and 2 other fuels.

Properties/Fuel	**Hydrogen (H_2)**	**Methane (CH_4)**	**Iso-octane (C_8H_{18})**
Typical α	0.0064	0.024	0.024
q_F (kJ/g)	120.9	54.8	46.4

Table 1: Values of α and specific heat of combustion (q_F) from [4].

Parameter α also can be changed by variations in the ambient temperature, $\tilde{T}_\infty$, but this changes $\tilde{D}a$ simultaneously. To investigate the effects of $\tilde{T}_\infty$ variations at fixed $\tilde{D}a$ requires a rescaling. The rescaling is performed here by specifying a reference value of $\tilde{T}_\infty$ as $\hat{T}_\infty$, defining rescaled parameters:

$$\hat{\varepsilon} = (\hat{T}_\infty)^2 / \tilde{E}, \tag{4.2}$$

$$\hat{a}_T = (\tilde{T}_\infty^{\,2} / \hat{T}_\infty^{\,2}) a_T \text{ and} \tag{4.3}$$

$$\hat{D}a = \tilde{D}a \tilde{Y}_{O,\infty} \tilde{x}^{4/3} [\tilde{Y}_{F,0} / (\hat{\varepsilon} \tilde{x}^{1/3})]^{(1-Le_F)} \exp(-\tilde{E} / \hat{T}_\infty) / (4 Pr \hat{T}_\infty) \tag{4.4}$$

and plotting the results in terms of rescaled variables $\hat{a}_T$ and $\hat{D}a$. The results are shown in Fig. 4.2. Here an increase in $\tilde{T}_\infty$, which increases α without changing $\hat{D}a$, is seen to favor ignition. This also is physically realistic because more heat is transferred to the cold fuel flow at a higher rate when the ambient is at a higher temperature. By the same reason, when the kinetic data are unchanged, an increased $\tilde{T}_\infty$ yields ignition to occur nearer the edge of the jet. Note that the Damköhler number shown is a function of the axial distance from the virtual origin of the jet (see Eqn. 2.50).

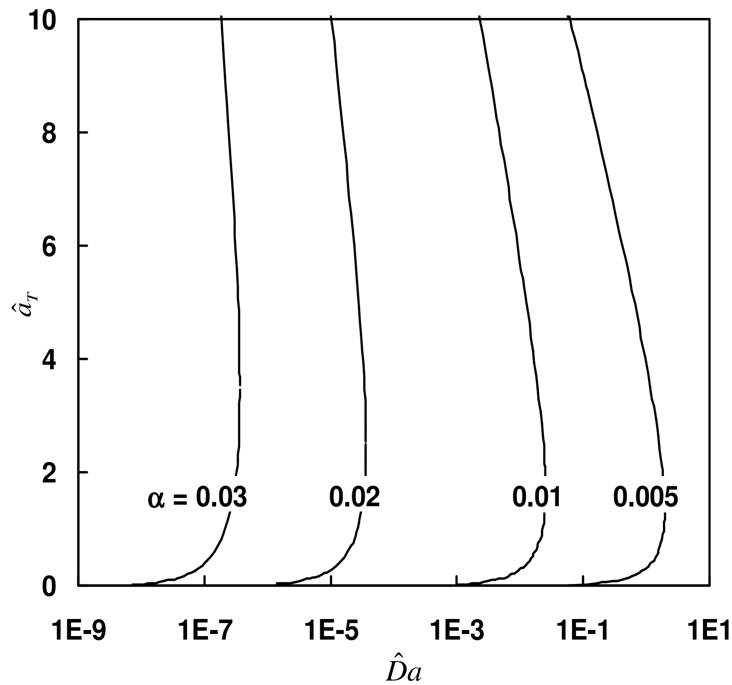

Fig. 4.2: Rescaled plot of $\hat{a}_T$ versus $\hat{D}a$ (rescaled $\tilde{D}a$ values due to changes in $\tilde{T}_\infty$) for varying α (which is changed by variations in $\tilde{T}_\infty$), with Le_F = 0.6, $\tilde{T}_0$ = 0.00226, $\tilde{E}$ = 1.79, $\tilde{Y}_{F,0}$ = 1, and α = 0.01 as reference, hot ambient.

The influence of reactant Lewis number on ignition is considered in Fig. 4.3. Here Le_F is defined as the mixture thermal diffusivity divided by the mass diffusivity of fuel into the mixture. A decrease in Le_F for fixed $\hat{D}a$ is seen to favor ignition. This occurs because a smaller Le_F implies that fuel species diffuse more quickly into the hot oxidizer. A fuel such as a mixture of hydrogen and nitrogen has a small Le_F, is hence easier to ignite than other fuels of higher Le_F at the same conditions. Nayagam and Williams [23] found that in a one-dimensional model of steady motion of edges of reaction sheets, increasing the Lewis number decreases the propagation velocity at small Damköhler numbers.

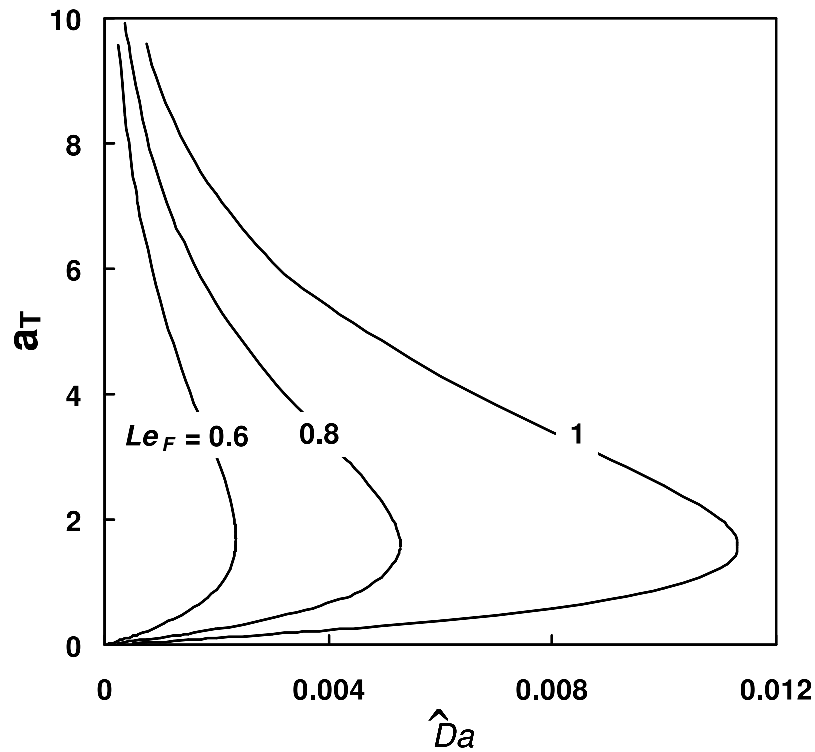

Fig. 4.3: a_T versus $\hat{Da}$ (rescaled $\tilde{D}a$ values due to changes in Le_F) for varying Le_F, with $\alpha = 0.02$ $\tilde{T}_0 = 0.00226$, $\tilde{E} = 1.79$, hot ambient.

4.2.1 Ignition states that separate the ignitable and non-flammable regions

Plots of ignition $\hat{D}a$ versus α under several conditions for the cool jet scenario are shown in Figs. 4.4 - 4.6. In Fig. 4.4, ignition $\hat{D}a$ versus α is plotted for varying Le_F, with Le_F =1 as the reference. The plot shows that as the Le_F decreases, ignition is favored (similar to explanation for Fig. 4.3) for decreasing α (at fixed $\tilde{T}_\infty$), resulting in a larger ignitable region. This is consistent with the findings shown in Fig. 4.2.

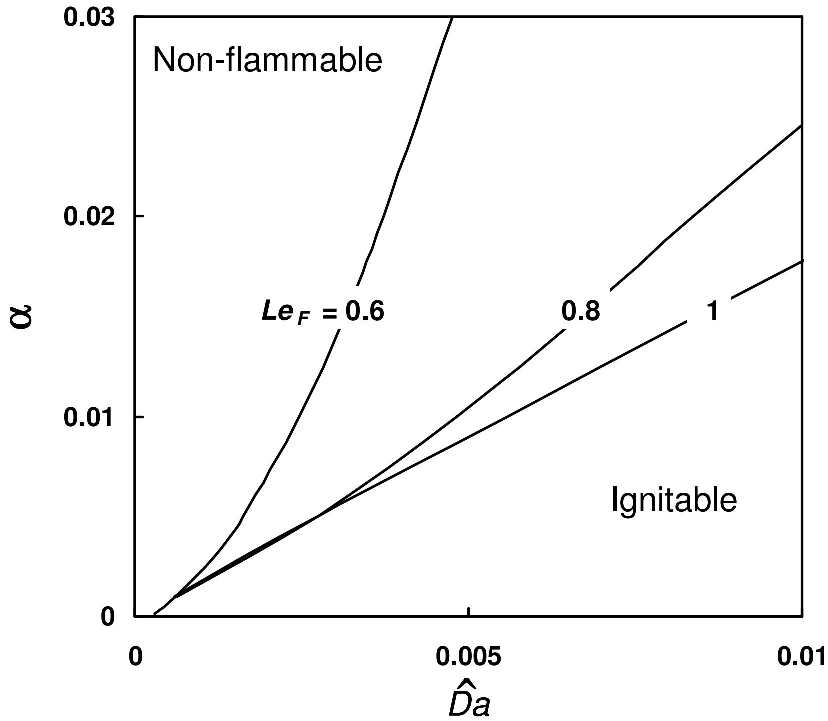

Fig. 4.4: α (which is changed by variations in $\tilde{T}_0$ or $\tilde{Y}_{F,0}$) versus $\hat{Da}$ (rescaled $\tilde{Da}$ values due to changes in Le_F) for varying Le_F, with Le_F = 1 as reference and constant $\tilde{T}_\infty$ = 0.0123, hot ambient.

In Fig. 4.5, ignition $\hat{Da}$ versus α is plotted for varying Le_F. The plot shows that as the Le_F decreases, ignition is favored (similar to explanation for Fig. 4.3) for increasing α (due to increases in $\tilde{T}_\infty$), resulting in a larger ignitable region, which is physically realistic.

In Fig. 4.6, ignition $\hat{Da}$ versus α is plotted for varying n_F. The plot shows that as the n_F increases, ignition is favored due to an increased reaction rate, resulting in a larger ignitable region. The effect of increasing n_F on ignition, however, is weaker as compared to the effects of reducing Le_F or increasing $\tilde{T}_\infty$.

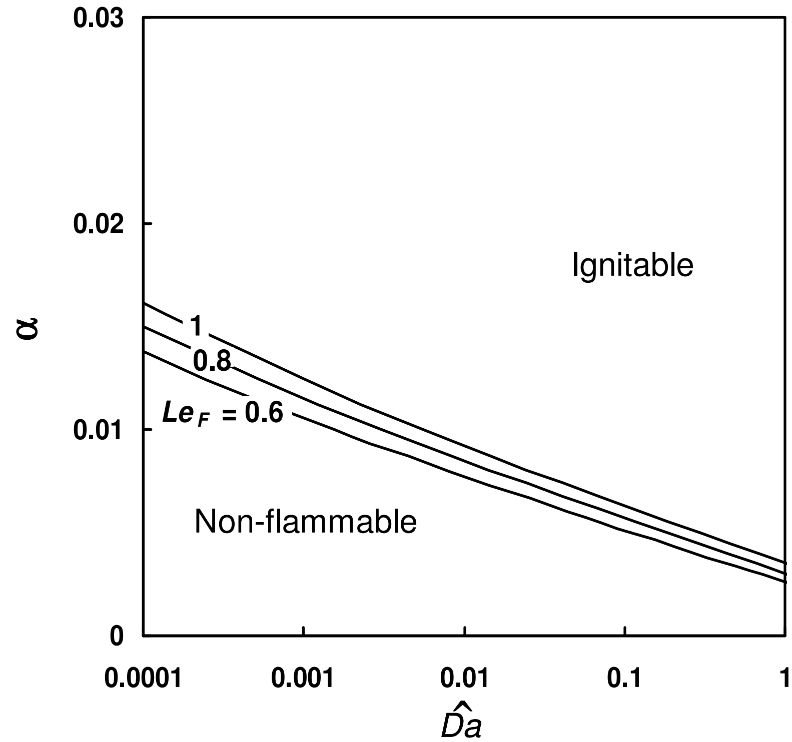

Fig. 4.5: α (which is changed by variations in $\tilde{T}_\infty$) versus $\hat{Da}$ (rescaled $\tilde{Da}$ values due to changes in $\tilde{T}_\infty$) for varying Le_F, and $\tilde{T}_0$ = 0.00226, hot ambient.

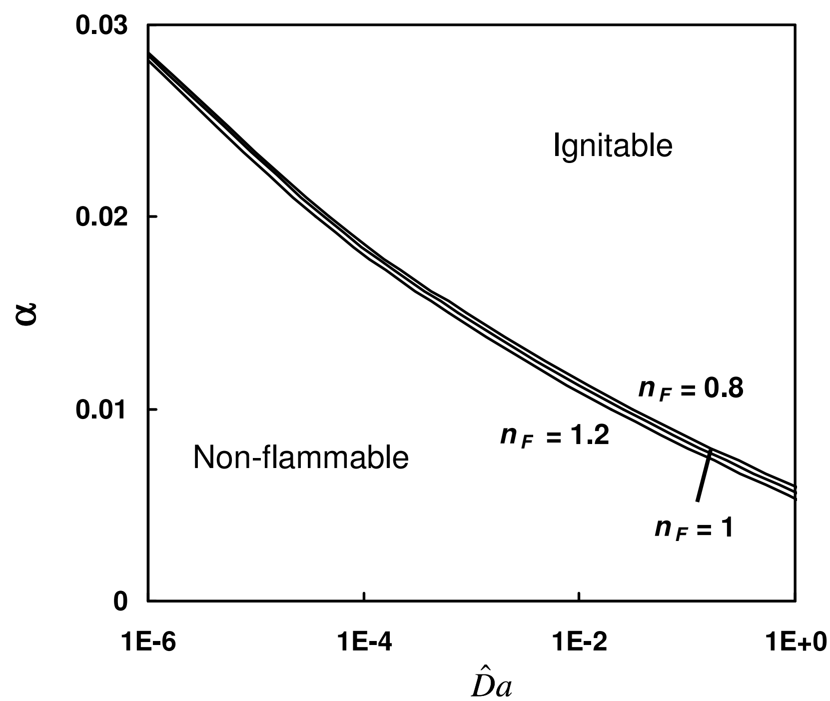

Fig. 4.6: α (which is changed by variations in $\tilde{T}_\infty$) versus $\hat{Da}$ (rescaled $\tilde{Da}$ values due to changes in $\tilde{T}_\infty$) for varying n_o at Le_F = 0.6, and $\tilde{T}_0$ = 0.00226, hot ambient.

4.3 Hot jet flowing into a cool ambient ($T_0 > T\infty$)

Eqns. (3.55) – (3.56) were solved by the Crank-Nicholson method and the resulting matrix was inverted by LU decomposition (using computer codes). Selected results are shown in Figs. 4.7 and 4.8. In Fig. 4.7, θ_{max} represents the maximum value of temperature increase through reaction before ignition occurs. The corresponding ignition location, X, is shown in Fig. 4.8.

Three curves are included in Figs. 4.7 and 4.8, each with a different value of β, where

$$\beta = (\tilde{T}_0 - \tilde{T}_\infty) / \tilde{Y}_{O,\infty} \tag{4.5}$$

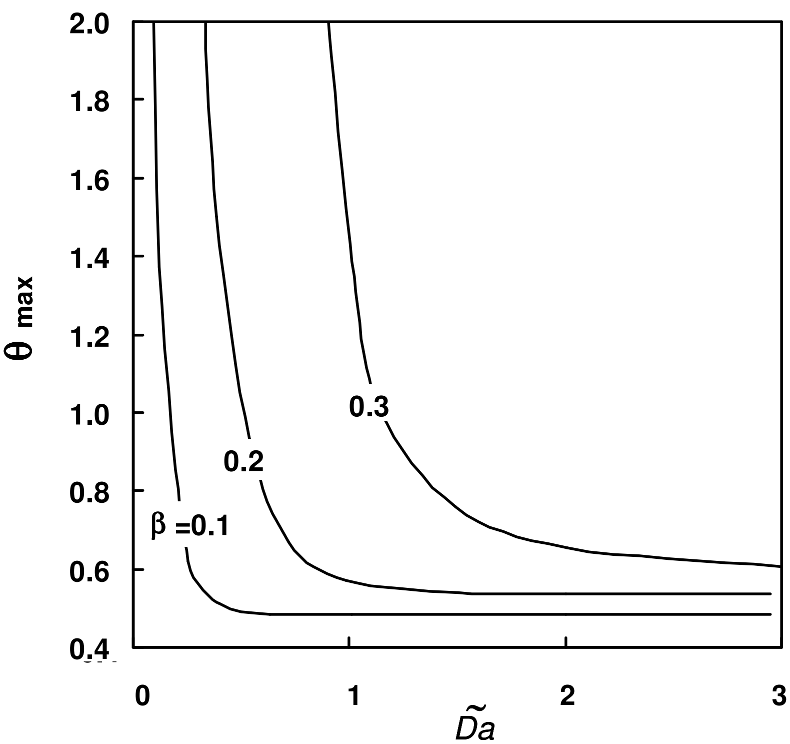

Fig. 4.7: θ_{max} versus $\tilde{Da}$ for varying β (which is changed by variations in $\tilde{T}_\infty$ or $\tilde{Y}_{O,\infty}$) at Le_o = 1, and constant $\tilde{T}_0$ = 0.0388, hot jet.

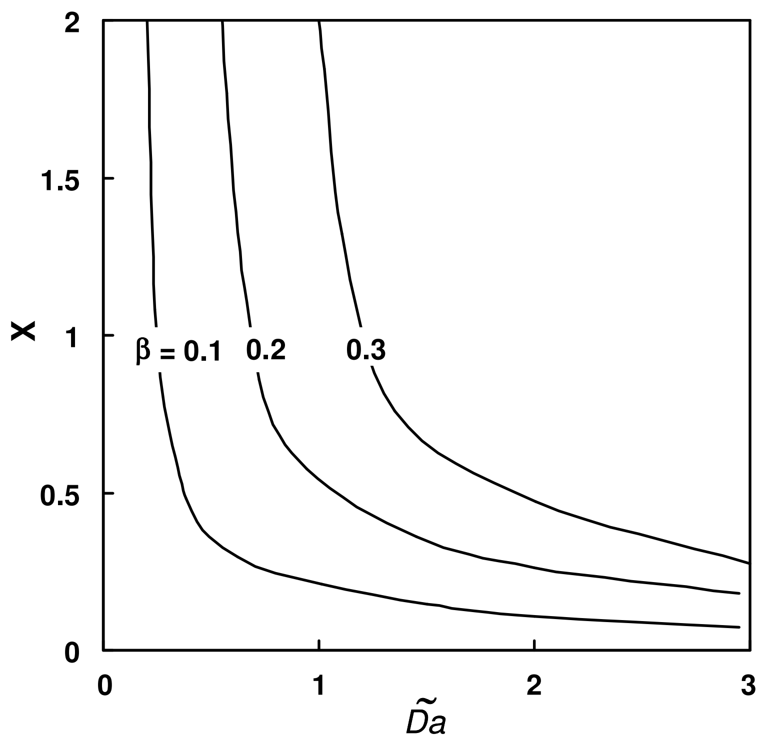

Fig. 4.8: X versus $\tilde{Da}$ for varying β (which is changed by variations in $\tilde{T}_\infty$ or $\tilde{Y}_{O,\infty}$) at Le_o = 1, and constant $\tilde{T}_0$ = 0.0388, hot jet.

These curves do not have the shape of an S-curve because the solutions are derived from a partial differential equation (since it is dependent on both transverse and streamwise stretched coordinates), in contrast to the ordinary differential equation of the cool jet (which is only dependent on the transverse diffusive term). On each curve, by increasing the reaction rate, $\tilde{Da}$, a smaller temperature increase and a shorter ignition location is observed before ignition, as is reasonable to expect. A higher value of $\tilde{Da}$ yields an increased heat generation rate, which compensates for some heat loss from the hot jet to the cold ambient, favors ignition, and moves the point of ignition closer to the jet exit. In contrast, a reduction in $\tilde{Da}$ weakens the reaction and makes ignition more difficult such that both $\theta_{\max}$ and X increase.

Although an increase of X provides longer residence time for the reaction so that ignition can occur at a smaller $\tilde{D}a$, the reaction rate decreases with X because the jet is cooled by the cold ambient, as can be seen from the reaction term of Eq. (3.56). A sharp increase in $\theta_{\max}$ and X, as shown the low $\tilde{D}a$ side of the curves in Figs. 4.7 and 4.8, means that the reduction of reaction rate dominates over the residence time increase, and defines the smallest $\tilde{D}a$ for which ignition occurs.

Figures 4.7 and 4.8 also indicate that a decrease in β for any fixed $\tilde{D}a$ favors ignition, as ignition occurs at a lower temperature increase, $\theta_{\max}$, and at a shorter ignition location, X. More importantly, a decrease in β permits ignition at a lower value of $\tilde{D}a$. Such a decrease can be accomplished either by increasing the reactant mass fraction in the oxidizer supply, $\tilde{Y}_{O,\infty}$, or by increasing the ambient temperature, $\tilde{T}_\infty$. Both findings are physically realistic.

Parameter β also can be changed by variations in the jet temperature, $\tilde{T}_0$, but this changes $\tilde{D}a$ simultaneously. To investigate the effects of $\tilde{T}_0$ variations at fixed $\tilde{D}a$ requires a rescaling similar to that performed for the cool jet scenario. The rescaling is performed here by specifying a reference value of $\tilde{T}_0$ as $\hat{T}_0$, defining rescaled parameters :

$$\hat{\varepsilon} = (\hat{T}_0)^2/\tilde{E}, \tag{4.6}$$

$$\hat{\theta}_{\max} = (\tilde{T}_0/\hat{T}_0)^2\theta_{\max} \text{ and} \tag{4.7}$$

$$\hat{D}a = \hat{\varepsilon}[Da\tilde{Y}_{F,0}/(\hat{T}_0\tilde{Y}_{O,\infty})]\exp(-\tilde{E}/\hat{T}_0) \tag{4.8}$$

and plotting the results in terms of rescaled variables $\hat{\theta}_{\max}$ and $\hat{D}a$. The results are shown in Figs. 4.9 and 4.10. Here an increase in $\tilde{T}_0$, which increases β without changing $\hat{D}a$, is seen to favor ignition because ignition can occur at a lower reaction rate, or lower $\hat{D}a$. This also is physically realistic. Ignition is predicted to occur near the centerline if the fuel is hotter than the air because this is where the highest temperature is attained.

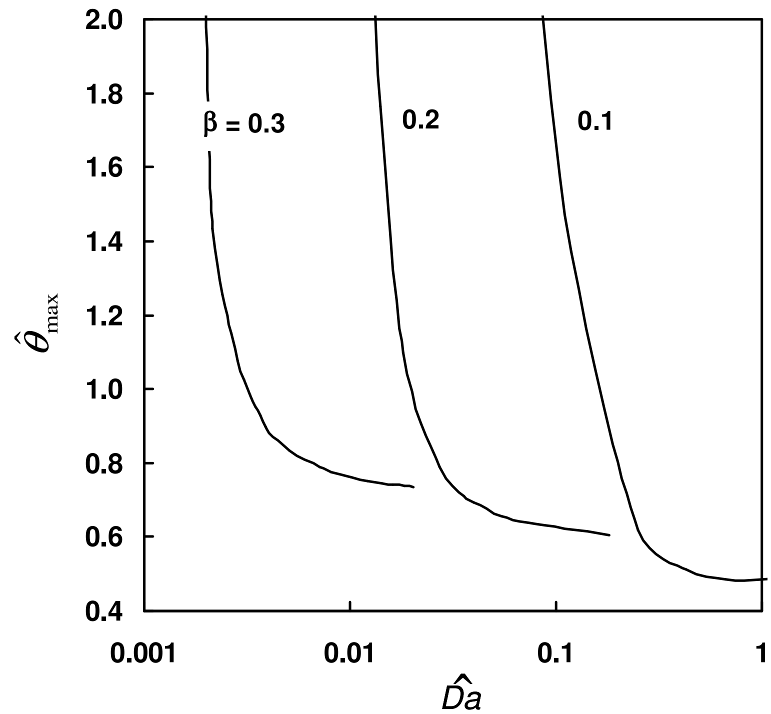

Fig. 4.9: Rescaled plot of $\hat{\theta}_{\max}$ versus $\hat{D}a$ (rescaled $\tilde{D}a$ values due to changes in $\tilde{T}_0$) for varying β (which is changed by variations in $\tilde{T}_0$), with Le_o = 1, $\tilde{T}_\infty$ = 0.0358, $\tilde{E}$ = 1.79, $\tilde{Y}_{O,\infty}$ = 0.029, and β = 0.1 as reference value, hot jet.

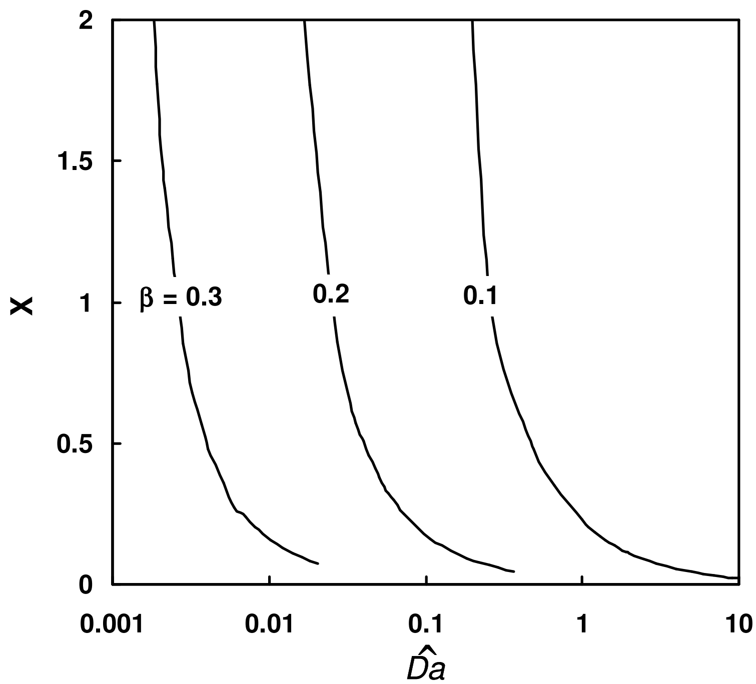

Fig. 4.10: X versus $\hat{Da}$ (rescaled $\tilde{Da}$ values due to changes in $\tilde{T}_0$) for varying β (which is changed by variations in $\tilde{T}_0$), with $Le_o = 1$, $\tilde{T}_\infty = 0.0358$, $\tilde{E} = 1.79$, $\tilde{Y}_{O,\infty} = 0.029$, and β = 0.1 as reference value, hot jet.

The effects of oxidizer Lewis number on spontaneous ignition are considered in Fig. 4.11. This plot shows that decreased Le_O makes ignition more difficult. For an increase in the mass diffusivity of the oxidizer (or a decreased Le_O) at a fixed value of $\tilde{Da}$, $\theta_{\max}$ increases. In addition, the minimum $\tilde{Da}$ for ignition increases with decreased Le_O. This differs from the ignition behavior with respect to fuel Lewis number in the cool jet case (Fig. 4.3). In a cool jet, there is unlimited heat transfer from the hot ambient gas to preheat the fuel so that a higher fuel diffusion rate (lower

Le_F) results in a higher fuel concentration in the reaction region, more heat generation through the reaction and, hence, easier ignition.

In the hot jet, only limited heat is available from the fuel flow. An increased oxidizer mass diffusivity increases the transport rate of oxidizer to the center of the jet, thus requiring more heat to preheat the oxidizer, decreasing the temperature in the hot zone, and making ignition more difficult. Furthermore, unlike the cool jet case, the Lewis number of the oxidizer only has a weak effect on the ignition state (see Fig. 4.11) because ignition occurs near the jet exit if successful. In the reaction region, the flow velocity is high such that streamwise convection dominates over transverse diffusion. Moreover, because Le_O is close to unity for oxygen in air, the effect of Le_O in a hot-hydrogen cold-air system is secondary. As in Fig. 4.10, the effect of Le_O on the ignition location is similar to that on the ignition state, shown in Fig. 4.12.

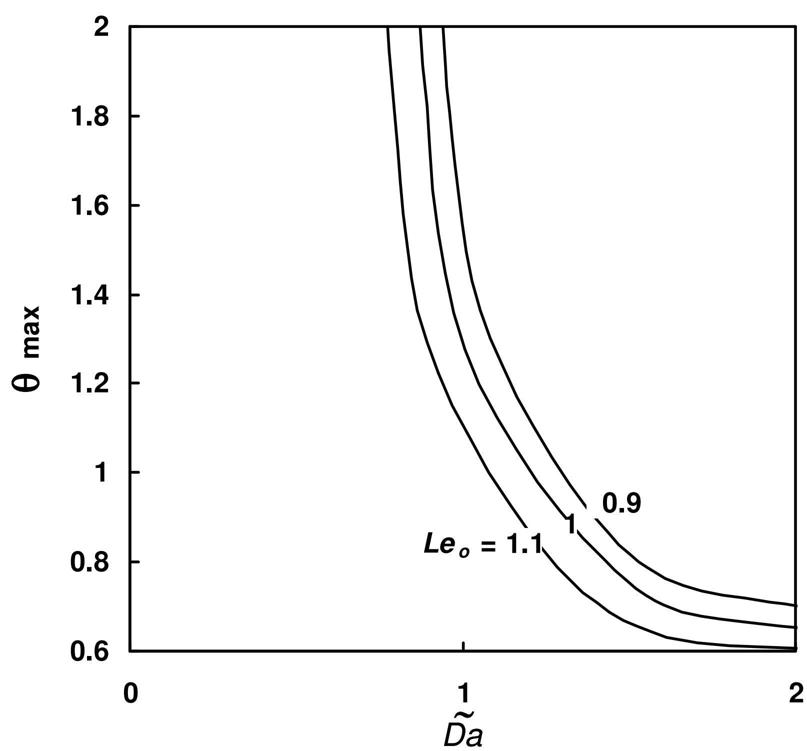

Fig. 4.11: θ_{max} versus $\tilde{Da}$ for varying Le_o, with β = 0.3 and constant $\tilde{T}_0$ = 0.0388, hot jet.

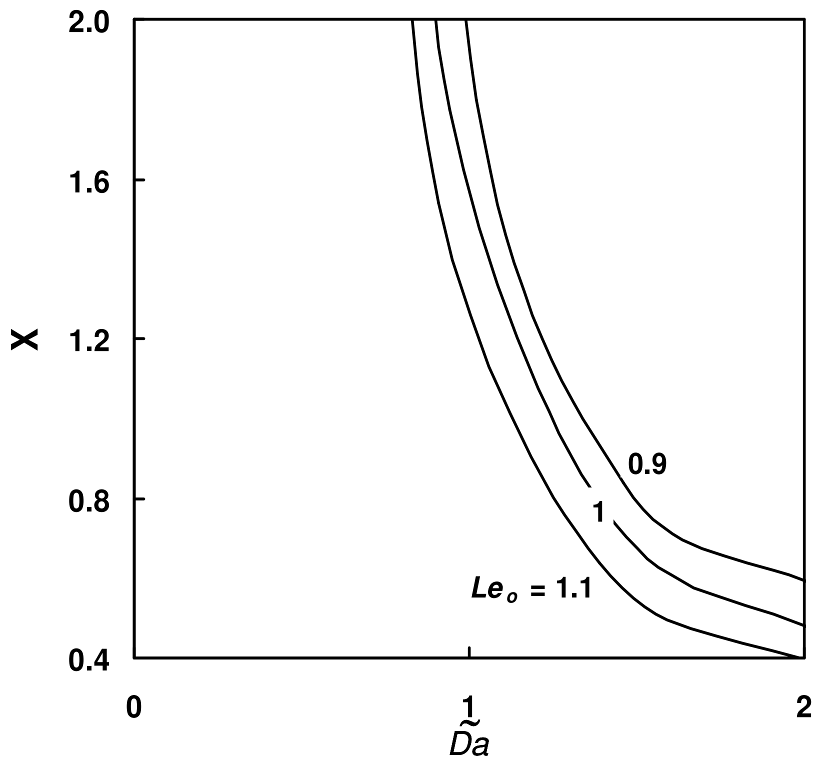

Fig. 4.12: X versus $\tilde{Da}$ for varying Le_o, with β = 0.3 and constant $\tilde{T}_0$ = 0.0388, hot jet.

<u>*4.3.1 Ignition states that separate the ignitable and non-flammable regions*</u>

Plots of ignition $\hat{D}a$ versus β under several conditions for the hot jet scenario are shown on Figs. 4.13 – 4.14. In Fig. 4.13, ignition $\hat{D}a$ versus β was plotted for varying n_o and constant $\tilde{T}_0$. The plot shows that as the oxidizer reaction order increases, ignition is favored, resulting in a larger ignitable region, which is physically realistic.

In Fig. 4.14, ignition $\hat{D}a$ versus β was plotted for varying n_o and $\tilde{T}_0$. The plot shows that as the n_o and $\tilde{T}_0$ increases, ignition is favored, resulting in a larger ignitable region covering lower values of $\hat{D}a$.

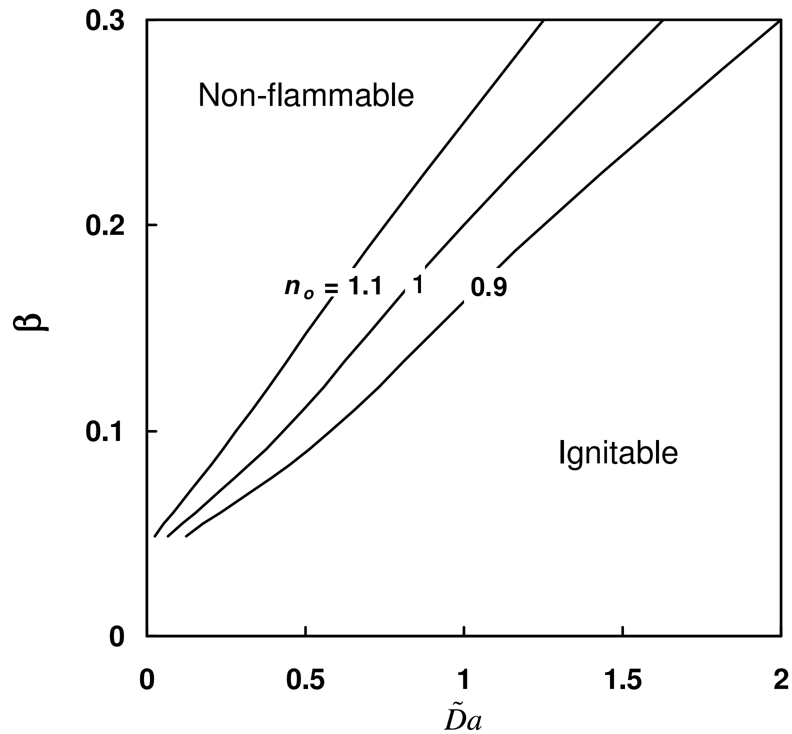

Fig. 4.13: β (which is changed by variations in $\tilde{T}_\infty$ or $\tilde{Y}_{O,\infty}$) versus $\tilde{D}a$ for varying n_o, and constant $\tilde{T}_0$ = 0.0388, hot jet.

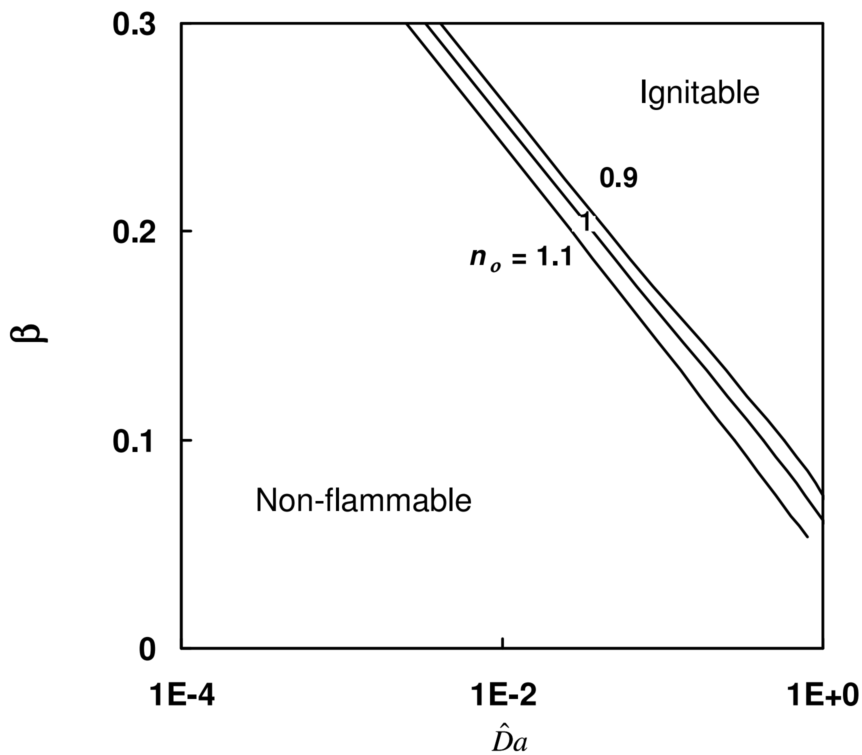

Fig. 4.14: β (which is changed by variations in $\tilde{T}_0$) versus $\hat{D}a$ (rescaled $\tilde{D}a$ values due to changes in $\tilde{T}_0$) for varying n_o, with Le_o = 1, $\tilde{T}_\infty$ = 0.0358, $\tilde{E}$ = 1.79, $\tilde{Y}_{O,\infty}$ = 0.029, and β = 0.1 as reference value, hot jet.

Chapter 5: Conclusions

5.1 Conclusions

The spontaneous ignition of a hydrogen jet emanating from a slot into air has been considered analytically. A similarity solution of the flowfield was obtained for the scenario of cool jet flowing into hot ambient, which was then combined with the species and energy conservation equations. Solutions were found using activation energy asymptotics.

The analysis yielded limiting conditions for spontaneous ignition of fuel jets. For a cool jet flowing into a hot ambient, ignition is found to be a strong function of ambient temperature and fuel Lewis number. Ignition was favored by an increase in ambient temperature or a decrease in Lewis number. For the hot jet scenario, ignition was significantly affected by the jet temperature, but only weakly affected by the oxidizer Lewis number.

Because spontaneous ignition is very sensitive to temperature, ignition is predicted to occur near the edge of the jet if the fuel is cooler than the air and on the centerline if the fuel is hotter than the air.

The value of the mixture fraction Z at which ignition occurs can be extracted from the AEA solutions as $Z = \dfrac{\sigma Y_F + (Y_{o,\infty} - Y_o)}{\sigma Y_{F,o} + Y_{o,\infty}}$.

In the first scenario of cool jet flowing into a hot ambient, ignition occurs at $Z \rightarrow 0$ since it occurs at the jet edge where $\tilde{Y}_O \rightarrow \tilde{Y}_{O,\infty}$ and Y_F is very small and of the order ε. In the second scenario of the hot jet, ignition occurs at the jet centerline, where $Z \rightarrow 1$ since $\tilde{Y}_O \rightarrow 0$ and $Y_F \rightarrow Y_{F,0}$.

The present model can be extended to studies of flame extinction and to circular jet configurations. When experimental data becomes available, parametric comparisons can also be made to establish reaction rates for use in the present model.

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