Abstract

The effects of an externally applied field are studied for a single isolated droplet flame under the spherically symmetric 1-D configuration. A reduced 3-step chemical kinetic mechanism is proposed to capture the production and destruction of ions inside the flame, which is then used for conducting analytical and numerical investigations. Large activation energy asymptotics were used to study the flame structure in the absence of the external field. The effect of the electric field is modelled using the Ionic Wind and Ohmic Heating. Furthermore, two distinguished limits of weak and strong field are studied to understand the charge redistribution in both cases. Based on the numerical results, an increase in the mass burning rate is observed with increasing potential. However, maximum flame temperature doesn’t seem to be effected with the external field. Ohmic Heating effects are used to explain these observations.
To the Almighty
Acknowledgments

Foremost, I would like to express my sincere gratitude to my advisor Prof. Moshe Matalon, who was always there to guide and help me specially in times of great confusion. I also want to sincerely thank Prof Kyritsis whose insightful discussions were extremely helpful in materializing ideas. This project would not have been possible without my colleagues and friends, Dr. Zhangbin Lu, Navin Fogla and Arjun Krishnan who tolerated my innumerable questions and had the patience to answer every one of them. I am also deeply indebted to the Department of Mechanical Sciences and Engineering for providing me with funding in the form of Teaching Assistantships. Last but not the least, I would like to thank my family for being there with me in times of happiness and despair.
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Chapter 1

Introduction

With increasing demand for more efficient combustion processes, alternative processes like application of magnetic and electric fields for modification of combustion have offered possible solutions. The effects of an externally applied electric field on combustion had been first noticed by researchers as early as the 1600’s. For the next 300 years, most of the work was concentrated in establishing that flames by nature produce electrically charged particles. In one of the early works by Lewis [1], a systematic measurement was made to identify the effect of external fields on flame deflection. He conducted experiments on various hydrocarbon fuels at different equivalence ratios to observe the conditions when the flame would get extinguished. Based on his experiments, it was concluded that for every type of fuel, the flame seemed to have an electrically charged behaviour. In general, these flames seemed to get deflected towards the positive electrode with the amount of deflection depending upon the strength of the field. He also found that each of these flames could be extinguished if the field was strengthened beyond a particular value. It was suggested that extinction was caused by removal of the charged species completely from the flame. The extinction limit depended on the type of fuel that was used and its equivalence ratio. Both these observations pointed to the conclusion that the charged species played an important role in the combustion of the fuel and by manipulating them, certain characteristics of the flame could be changed.

In order to investigate the reason for the creation of these ions, Calcote [2] wrote a review paper on the mechanisms believed to be the cause of these ions. He mentioned three main mechanisms thought to be responsible for the charged species in flames, namely thermal ionization (due to impurities, carbon particles, equilibrium and non-equilibrium species), ionization due to translational energy and chemi-ionization. Based on experimental results, it was concluded that chemi-ionization or cumulative excitation was the main reason for the production of these charged particles. This conclusion was verified by a number of similar studies conducted since then [3, 4, 5, 6]. In the late 1900’s, Goodings et.al. [7, 8] performed one of the first extensive experimental works detailing the mechanism of charge creation and the different type of positive as well as negative ions produced in fuel-lean and rich methane flames. The authors also suggested chemi-ionization to be the dominant mechanism for generation of charged species. In the review papers by Fialkov [9] and
Heinsohn et.al. [10], the impact of utilizing these ionic species to modify flame characteristics were reviewed. It was shown that external fields could be used not only to extinguish flames, but also to stabilize them, modify flame speeds, use electrolytically charged fluids in fire-fighting etc.

Over the years, a lot of work has been done to review the effects of external electric fields for both premixed as well as diffusion flames. Jaggers and Von Engel [11] used transverse electric fields to modify the flame speed of various premixed air-fuel mixtures. Belhi et.al. [12] numerically simulated the effects longitudinal DC fields and observed a reduction in the flame lift-off heights and stabilization for premixed flames. Papac and Rankin [13] performed a numerical simulation on a diffusion flame to demonstrate the usage of electric fields to counteract the buoyant force. Ueda et.al. [14], Okai et.al. [15] and Yuan et.al. [16] studied the effect of these fields on flame shape modification under microgravity. Work done by Ueda et.al. [14] also showed the possibility of a change in the mass burning rate of the fuel for sooting and non-sooting fuels. Yamashita et.al. [17] used experimental data along with numerical simulation to show the increase in the burning rate constant for diffusion flames. Anderson et.al. [18] performed experiments on droplet combustion and observed the coupling of electrostatics with combustion chemistry.

Now, while it is important to understand the possible effects of electric fields on flames, it is also essential to be able to identify the main mechanisms behind these effects since the end goal of all investigations is to be able to manipulate the observed effects for practical applications. In the work done by all the authors mentioned above, it was identified that an external field can have two major effects, namely kinetic and body force; both of which arise due to manipulation of the fraction of ions in the system. The kinetic effects are believed to be caused by the changes occurring to the chemical mechanism when charged species are affected using external fields. The body forces on the other hand can affect the system in two ways. The first is through the momentum equation, called the ionic wind. The second way is through the energy equation where the electric field can appear as positive/negative work done on the system. This term has been referred to by different names by different authors. In the present work, we would refer to this by Ohmic heating. In practical terms, the ionic wind primarily modifies the pressure field depending upon the relative charge concentration in the system, whereas the Ohmic heating can act as a heat source or sink depending upon the system.

There have been different views as to the main mechanisms responsible for the modification of flame behaviour. Jaggers and Von Engel [11] believed that the change in flame behaviour was caused due to the kinetic effects. They suggested that the activation of reactions due to the collision of neutral species with the charged ones was responsible for the modification of flames speeds. Pedersen and Brown [3] also suggested the ionic wind effect to be negligible in their work on premixed methane flames. However, almost
all of the work by other researchers suggest the role of body force effects for the observed changes in flame characteristics. Most of the authors who worked on the modification of flame shape [13, 14, 16, 17, 18] suggested the ionic wind to be responsible for the observed effects. Belhi et.al. [12] believed this to be the main reason behind flame stabilization. It is also worthwhile to mention that in most of the above work, the flame was observed to be partially positive in nature. It was reasoned that for weak and moderate fields, electrons were the majority negative charge carriers. Now, since electrons have a negligible mass as compared to the other species generated in the flames, they would instantaneously get removed from the flame upon production. This would give the flame a partial positive charge and thus it would generally tend to get deflected towards the negative electrode. As far as the effect of Ohmic heating is concerned, Belhi et.al. [12] and Papac and Runkin [13] suggested that it would practically be negligible in most cases.

The main reason for the discrepancy noticed above may be the lack of a simplified framework to investigate each of these effects one at a time. The usage of complicated chemical kinetic mechanisms and different hydrocarbon fuels makes it difficult to logically point out the exact mechanism responsible for the observed electric field effects and thereby remove the discrepancies. It is therefore the aim of this work to use a simplified reduced model independent of the fuel used to understand the effect of an externally applied electric field on diffusion flames. For the same, a spherically symmetric field is used to develop an analytical framework which would on one hand preserve the physics involved in the problem and on the other hand limit the system variables to the least possible. An isolated droplet configuration is chosen for this study because this problem is very well understood and documented in the absence of the electric field. Also, in the one dimensional version of this problem since the pressure field doesn’t play an active role in determining the system characteristics, it can be determined a posteriori. This gives us opportunity to answer the question about what would happen fundamentally to a system where ionic wind doesn’t play an active role in stabilizing of the system. Also, since the only remaining effects would be the kinetic and Ohmic heating, it would be possible to investigate how they effect the flame.
2.1 General Equations

The conservation equations of a chemically-reacting gas mixture can be written as follows:-

*Continuity*

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \]

*Poisson’s Equation*

\[ \nabla^2 \phi = -\frac{e}{\epsilon_o} (n^+ - n^-) \]

*Species Conservation*

\[ \rho \frac{D Y_i}{D t} = w_i - \nabla \cdot (\rho Y_i \mathbf{V}_i) \]

*Momentum Conservation*

\[ \rho \frac{D \mathbf{v}}{D t} = -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^{N} Y_i \mathbf{f}_i \]

*Energy Conservation*

\[ \rho \frac{D e}{D t} = -\nabla \cdot \mathbf{q} - \mathbf{P} : (\nabla \mathbf{v}) + \rho \sum_{i=1}^{N} Y_i \mathbf{f}_i \cdot \mathbf{V}_i \]

where,

‘i’ = identifies the chemical species including ionic

φ = Electrical potential of the system

Y_i = Mass fraction of species ‘i’

v = Bulk velocity of the gas mixture

V_i = Diffusion velocity of species ‘i’

f_i = Body force vector

e = Specific internal energy of the gas mixture
\[ P = \left[ p + \left( \frac{2}{3} \mu + \kappa \right)(\nabla \cdot \mathbf{v})\right] \mathbf{I} - \mu \left[ (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T \right] = \text{Pressure tensor} \]

\[ \mathbf{q} = -\lambda \nabla T + \rho \sum_{i=1}^{N} h_i Y_i \mathbf{v}_i = \text{Heat flux vector} \]

\[ n^\pm = \sum_{i=1}^{N} n^\pm_i = \text{Total positive/negative ion number densities respectively} \]

### 2.2 Governing Equations

Following assumptions have been made for the governing equations of our problem:

1. Mixture of Ideal Gases
2. Radiation and thermal diffusion effects in the heat flux vector \( \mathbf{q} \) are neglected
3. Dilute mixture is taken for which Fick’s Law of binary-diffusion applies

Now, each of the conservation equations can be modified by adding specific terms and the above assumptions to suit our given problem. This is done as follows:

#### Ideal Gas Law

\[ p = \rho RT/W \]

(2.2.1)

where,

\( W = \text{Average molecular weight of the gas mixture} \)

\( R = \text{Universal gas constant} \)

#### Continuity

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \]

(2.2.2)

#### Poisson’s Equation

\[ \nabla^2 \phi = -\frac{q}{\epsilon_o} (n^+ - n^-) \]

(2.2.3)

#### Species Conservation

The Stefen-Maxwell relations after neglecting the Soret and pressure gradient effects are as follows:-

\[ \nabla X_i = \sum_{j=1}^{N} \left( \frac{X_i X_j}{D_{ij}} \right) (\mathbf{v}_j - \mathbf{v}_i) + \left( \frac{\rho}{p} \right) \sum_{j=1}^{N} Y_i Y_j (f_i - f_j) \]
Here, $f_i$ is the differential body force due to the electric field and is given as,

$$f_i = s_i q E N_A / W_i$$  \hspace{1cm} (2.2.4)

where, ‘$s_i$’ is used to take care of the charge of the ionic species and is defined as,

$$s_i = \begin{cases} 
+1 & \text{if } i = \text{positively charged species} \\
-1 & \text{if } i = \text{negatively charged species} \\
0 & \text{if } i = \text{neutral species}
\end{cases}$$

Now, assuming a dilute mixture with ‘$\hat{N}$’ representing the species present in majority, we get the following relation:

$$\nabla X_i = -\frac{X_i V_i}{D_{i\hat{N}}} + \frac{\rho}{\rho} Y_i (f_i - f_N)$$

$$\Rightarrow \nabla X_i = -\frac{X_i V_i}{D_{i\hat{N}}} + \frac{q N_A W_i}{RT W_i} Y_i E$$

$$\Rightarrow Y_i V_i = -\frac{D_{i\hat{N}}}{\hat{N}} \nabla Y_i + \frac{q N_A D_{i\hat{N}} Y_i}{RT} E$$

In the above analysis, we have used the following relations as a result of the dilute mixture assumption:

- $Y_{\hat{N}} \approx 1$
- $W = \sum_{i=1}^{N} X_i W_i \approx W_{\hat{N}}$
- $Y_i = \frac{X_i W_i}{W_{\hat{N}}}$

Now, we use the following relationship between diffusivity and mobility known as the Einstein relation\(^1\):

$$\frac{D_{ij}}{\tilde{\mu}_{ij}} = \frac{k_b T}{q}$$

where, $k_b = \text{Boltzmann constant} = R/N_A$. Therefore, Fick’s law can be written as:

$$\rho Y_i V_i = -\rho D_{i\hat{N}} \nabla Y_i + \rho s_i \tilde{\mu}_{i\hat{N}} Y_i E$$  \hspace{1cm} (2.2.5)

$$\Rightarrow \rho Y_i V_i = -\rho D_{i\hat{N}} \nabla Y_i - \rho s_i \tilde{\mu}_{i\hat{N}} Y_i \nabla \phi$$  \hspace{1cm} (2.2.6)

\(^{1}\text{For ionic mobilities, the convention is to put a positive or negative sign when using it in the expression for drift velocity depending upon the charge of the ionic species. However, we use a } s_i \text{ to denote this for maintaining consistency as shown in eq 2.2.4}\)
where, \( E = -\nabla \phi \).

If we look closely at eq (2.2.5), we can see that the external electric field increases the net diffusive flux for the negative ions and decreases it for positive ions. The above expression\(^2\) is then substituted into the species equation to get (after dropping the ‘N’ in the subscripts)\(^3\):

\[
\rho \frac{DY_i}{Dt} = w_i + \nabla \cdot (\rho D_i \nabla Y_i) + s_i \nabla \cdot (\rho Y_i \hat{\mu}_i \nabla \phi)
\]  
(2.2.7)

where, \( w_i = W_i (\nu''_i - \nu'_i) w \)

and, \( w = \) species independent reaction rate

**Momentum Equation**

The term \( \rho \sum_{i=1}^{N} Y_i f_i \) in the momentum equation signifies the effect of a body force per unit mass. This body force in our case arises due to gravity and Coulomb’s force. The force generated because of induced magnetic fields is usually due to very small current densities produced as a result of chemi-ionization (except during electrical breakdown) \([19]\) . Therefore, the net body force is the sum of the buoyancy force and the individual body force of the ions derived from eq (2.2.4) as shown below :-

\[
\rho g + \rho \sum_{i=1}^{N} Y_i f_i = \rho g + q (-\nabla \phi) \left( \sum_{i=1}^{N^+} n_i^+ - \sum_{i=1}^{N^-} n_i^- \right)
\]

where,

- \( n_i = N_A \left( \frac{\rho Y_i}{W_i} \right) \)

- \( n^\pm = \sum_{i=1}^{N^\pm} n_i^\pm = \) Total positive/negative ion number densities respectively

- \( N^\pm = \) Total number of positively/negatively charged species

Substituting the above relation for the body force vector into the momentum equation, we get;

\[
\rho \frac{DV}{Dt} = -\nabla p - \nabla \cdot \tau + \rho g + q (-\nabla \phi) \left( n^+ - n^- \right)
\]  
(2.2.8)

where,

\[
\tau = \left[ \left( \frac{2}{3} \mu - \kappa \right) (\nabla \cdot v) - \mu \left\{ (\nabla v) + (\nabla v)^T \right\} \right] = \text{Viscous stress tensor}
\]

\(^2\)A similar expression can also be found in \([3]\)

\(^3\)Note that ‘N’ is dropped from here onwards only for ease of representation. The mobilities and diffusivities are still binary w.r.t the abundant species
**Energy Equation**

We use the relations

\[ e = h - p/\rho \]
\[ h = \sum_{i=1}^{N} Y_i h_i \]
\[ h_i = h_i^o + h_i^s \]

Also, the contribution of the electric field term can be expressed using eq (2.2.6) as follows:

\[
\rho \sum_{i=1}^{N} Y_i f_i \cdot V_{i,\text{drift}} + \rho \sum_{i=1}^{N} Y_i f_i \cdot V_{i,\text{diff}}
\]

\[
= qE \left( \sum_{i=1}^{N^+} n_i^+ V_{i,\text{drift}}^+ - \sum_{i=1}^{N^-} n_i^- V_{i,\text{drift}}^- \right) - qE \rho N_A \left( \sum_{i=1}^{N^+} \frac{D_i^+}{W_i} \nabla Y_i^+ - \sum_{i=1}^{N^-} \frac{D_i^-}{W_i} \nabla Y_i^- \right)
\]

\[
= (\nabla \phi)^2 \left( \sum_{i=1}^{N^+} n_i^+ \mu_i^+ + \sum_{i=1}^{N^-} n_i^- \mu_i^- \right) + q(\nabla \phi) \rho N_A \left( \sum_{i=1}^{N^+} \frac{D_i^+}{W_i} \nabla Y_i^+ - \sum_{i=1}^{N^-} \frac{D_i^-}{W_i} \nabla Y_i^- \right)
\]

Substituting these relations in the energy equation, we get:

\[
\rho \frac{\partial h}{\partial t} + \rho v \cdot \nabla h + \rho \sum_{i=1}^{N} h_i Y_i V_i - \nabla \cdot (\lambda \nabla T) = \frac{Dp}{Dt} + \Phi
\]

\[
\text{Ohmic Heating}
\]

\[
+ q(\nabla \phi)^2 \left( \sum_{i=1}^{N^+} n_i^+ \mu_i^+ + \sum_{i=1}^{N^-} n_i^- \mu_i^- \right) + q(\nabla \phi) \rho N_A \left( \sum_{i=1}^{N^+} \frac{D_i^+}{W_i} \nabla Y_i^+ - \sum_{i=1}^{N^-} \frac{D_i^-}{W_i} \nabla Y_i^- \right)
\]

where, \( \Phi = \text{Viscous dissipation} \)

Now, multiply the species equation with \( h_i^o \), sum over all possible species and subtract it from the above energy equation to get:

\[
\rho \frac{\partial h^o}{\partial t} + \rho v \cdot \nabla h^o + \rho \sum_{i=1}^{N} h_i^o Y_i V_i - \nabla \cdot (\lambda \nabla T) = \frac{Dp}{Dt} + \Phi - \sum_{i=1}^{N} h_i^o w_i + q(\nabla \phi)^2 \left( \sum_{i=1}^{N^+} n_i^+ \mu_i^+ + \sum_{i=1}^{N^-} n_i^- \mu_i^- \right)
\]

\[
+ q(\nabla \phi) \rho N_A \left( \sum_{i=1}^{N^+} \frac{D_i^+}{W_i} \nabla Y_i^+ - \sum_{i=1}^{N^-} \frac{D_i^-}{W_i} \nabla Y_i^- \right)
\]
We now assume $c_{p,i} \equiv c_p$, which gives that $h_i^s \equiv h^s$. Also,

$$h^s = \int_T^{T_o} c_p(T) \, dT = c_p(T - T_o)$$

Replacing $w_i$ with the species-independent reaction rate gives us the final energy equation as:

$$c_p \left( \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T \right) - \nabla \cdot \left( \lambda \nabla T \right) = \frac{D_p}{D_t} + \Phi - \sum_{i=1}^{N} h_i^s w_i + q(\nabla \phi) \left\{ \sum_{i=1}^{N^+} n_i^+ \dot{\mu}_i^+ + \sum_{i=1}^{N^-} n_i^- \dot{\mu}_i^- \right\}$$

$$+ q(\nabla \phi) \rho N_A \left\{ \sum_{i=1}^{N^+} \frac{D_i^+}{W_i} \nabla Y_i^+ - \sum_{i=1}^{N^-} \frac{D_i^-}{W_i} \nabla Y_i^- \right\} \quad (2.2.9)$$

Now, as can be seen in the above equation, the Ohmic heating can act as a heat source when it is positive and a heat sink when it is negative. It contains two terms; the first term represents the positive work done by the electric field on each of the species by “pushing” them in the same direction as their drift velocities. The second term represents the work done by the electric field in moving each of the ionic species in the direction of the field, but negating the effect of diffusion in the system. This work is can be either positive or negative in different regions of the system. It is considered positive/negative since when the external field forces the species to always move in the direction of their charge which may counteract the natural state of the system to diffuse away species after they are created in the reaction zone. However, it will be later shown in the results section that the net work done by this term is generally negative.

### 2.3 Model Configuration

The configuration used for the current model includes two electrodes, one at the surface of the droplet (similar to a mesh used to apply the potential around the surface of a porous sphere) and the other situated far away such that it doesn’t interfere with the combustion process. The potential (positive or negative) is applied at the inner electrode with the outer one being grounded such that we obtain a spherically symmetric electric field. This configuration is shown in Fig. 2.1.
2.4 Non-Dimensionalization

The various non-dimensional variables to be used in the conservation equations are defined as follows:

\[ r^* = \frac{r}{r_o} \quad \rho^* = \frac{\rho}{\rho\infty} \quad v^* = \frac{v}{(D_{th}/r_o)} \quad t^* = \frac{t}{(r_o/\bar{u})} \]

\[ \phi^* = \frac{\phi}{V} \quad T^* = \frac{T}{T\infty} \quad \Phi^* = \frac{\Phi}{(\mu_s \bar{u}^2/r_o^2)} \quad \dot{W} = \frac{W_s}{W_-} \]

During non-dimensionalization, we will assume that \( c_p, \lambda, \rho D_i, \rho \mu_i \) are constant. Substituting these expressions, we can non-dimensionalize our governing equations as shown below:

**Ideal Gas Law**

\[ p^* = \rho^* T^* \]
Continuity

Multiply eq (2.2.2) by \(r_0/ (\rho_\infty \bar{u})\) to get;

\[
\frac{\partial \rho^*}{\partial t^*} + \nabla^* \cdot (\rho^* \mathbf{v}^*) = 0
\]

Poisson’s Equation

Multiply eq (2.2.3) by \((r_0^2/\bar{V})\) to get;

\[
\nabla^2 \phi^* = - \left\{ \frac{qr_0^2 N_\Lambda \rho_\infty}{\epsilon_o} \frac{(W_+ \bar{V})}{(W_+ \bar{V} + r_o \rho_\infty \bar{u})} \right\} \left( Y^{**} - \hat{W} Y^{-*} \right) \rho
\]

Species Equation

Multiply eq (2.2.7) by \(r_0/ (\rho_\infty \bar{u})\) to get;

\[
\rho^* \frac{\partial Y_i}{\partial t^*} + \rho^* \mathbf{v}^* \cdot \nabla^* Y_i = \sum_{j=1}^{\text{reactions}} w_{i,j} + \left( \frac{\nabla^*}{\rho_\infty \bar{u}} \right) \cdot \left[ \rho D_i \left\{ \nabla Y_i + s_i \left( \frac{\hat{\mu}_i \bar{V}}{D_i} \right) Y_i \nabla \phi \right\} \right]
\]

Momentum

Multiply eq (2.2.8) by \(r_0/ (\rho_\infty \bar{u}^2)\) to get;

\[
\rho^* \frac{\partial \mathbf{v}^*}{\partial t^*} + \rho^* \mathbf{v}^* \cdot \nabla^* \mathbf{v}^* = - \left( \frac{p_\infty}{\rho_\infty \bar{u}^2} \right) \nabla^* p^* + \left( \frac{\mu}{\rho_\infty \bar{u} r_o} \right) \nabla^* \cdot \tau^* + \left( \frac{r_o}{\rho_\infty \bar{u}} \right) \rho g - \left( \frac{qr_0 N_\Lambda}{\rho_\infty \bar{u}^2} \right) \left( Y^{**} - \hat{W} Y^{-*} \right) \rho
\]

Writing each non-dimensional group in terms of earlier defined “numbers”;

\[
\rho^* \frac{\partial \mathbf{v}^*}{\partial t^*} + \rho^* \mathbf{v}^* \cdot \nabla^* \mathbf{v}^* = - \frac{1}{\gamma M^2} \nabla^* p^* + \frac{\rho^*}{Fr} \hat{\varepsilon}_g + \frac{1}{Re} \nabla^* \cdot \tau^* - Pr \left\{ \frac{|q| V N_\Lambda \rho_\infty}{\nu \rho D_{th} / r_o^3} \right\} (Y^{**} - \hat{W} Y^{-*}) \rho
\]

where, \(Re = \frac{\rho_\infty \bar{u} r_o}{\mu}\) reduces to the \(Pr^{-1}\) due to our choice of the diffusion velocity for \(\bar{u}\).
Energy Equation

Multiply eq (2.2.9) by \( \frac{r_o}{(\bar{u}_\infty T_\infty c_p)} \) and open the pressure tensor to get;

\[
\rho_0 \frac{\partial T^*}{\partial t^*} + \rho^* \mathbf{v}^* \cdot \nabla^* T^* - \nabla^* \cdot \nabla^* = \frac{p_\infty}{\rho_\infty c_p T_\infty} \left( \frac{Dp^*}{Dt^*} \right) + \sum_{k=1}^{\text{reactions}} q_k \bar{u}_k + \left( \frac{\mu \bar{u}^2}{\rho_\infty c_p T_\infty \bar{u}_o^2} \right) \Phi^* \\
+ \left( \frac{r_o q \bar{V} \rho_\infty N_A}{W_+ \rho_\infty c_p T_\infty \bar{u}_o^2} \right) (\nabla^* \phi^*)^2 \left[ \sum_{i=1}^{N^+} \frac{\mu_i^+ Y_i^+}{D_{ih}} + \sum_{i=1}^{N^-} \frac{\mu_i^- Y_i^-}{D_{ih}} \right] \rho \\
+ \left( \frac{r_o q \bar{V} \rho_\infty N_A}{W_+ \rho_\infty c_p T_\infty \bar{u}_o^2} \right) (\nabla^* \phi^*) \left[ \sum_{i=1}^{N^+} \frac{\nabla Y_i^+}{Le_i^+} - \sum_{i=1}^{N^-} \frac{\nabla Y_i^-}{Le_i^-} \right] \rho
\]

where, \( W_+ \) and \( W_- \) are mass fraction averaged weights of total positive and negative ion densities respectively.

Again, introducing the non-dimensional numbers, we get;

\[
\rho_0 \frac{\partial T^*}{\partial t^*} + \rho^* \mathbf{v}^* \cdot \nabla^* T^* - \nabla^* \cdot \nabla^* = \frac{\gamma - 1}{\gamma} \left( \frac{Dp^*}{Dt^*} \right) + \frac{(\gamma - 1) M^2}{Re} \Phi^* + \sum_{k=1}^{\text{reactions}} q_k \bar{u}_k \\
+ \left\{ \frac{q \bar{V}}{\rho_\infty c_p T_\infty W_+ / (N_A \rho_\infty)} \right\} (\nabla^* \phi^*)^2 \left[ \sum_{i=1}^{N^+} \frac{\mu_i^+ \bar{V}}{D_{ih}} Y_i^+ + \sum_{i=1}^{N^-} \frac{\mu_i^- \bar{V}}{D_{ih}} Y_i^- \right] \rho \\
+ \left\{ \frac{q \bar{V}}{\rho_\infty c_p T_\infty W_+ / (N_A \rho_\infty)} \right\} (\nabla^* \phi^*) \left[ \sum_{i=1}^{N^+} \frac{\nabla Y_i^+}{Le_i^+} - \sum_{i=1}^{N^-} \frac{\nabla Y_i^-}{Le_i^-} \right] \rho
\]

Therefore, the non-dimensional parameters found in these equations are:

\[
\alpha_+ = \left\{ \frac{q r_o^2 N_A \rho_\infty}{\epsilon_o} \right\} = \text{Permittivity of "medium" / Permittivity of vacuum}
\]

\[
\eta_+ = \left( \frac{\bar{u}_+ \bar{V}}{D_i} \right) = \text{Electrical Diffusivity / Mass Diffusivity}
\]

\[
\beta_+ = Pr \left\{ \frac{q \bar{V} N_A \rho_\infty}{\nu D_{ih} / r_o^3} \right\} = Pr \left\{ \text{Electric force per unit volume / Viscous force per unit volume} \right\}
\]

\[
\chi_+ = \left\{ \frac{q \bar{V}}{\rho_\infty c_p T_\infty W_+ / (N_A \rho_\infty)} \right\} = \text{Enthalpy of Electric Field / Enthalpy of Cold Surroundings}
\]

\[
Le_i = \frac{D_{ih}}{D_i} = \text{Thermal Diffusivity / Mass Diffusivity}
\]

\[
M = \frac{\bar{u}}{c_\infty} = \text{Velocity of object in medium / Velocity of sound in medium}
\]

\[
Fr = \frac{\bar{u}^2}{gr_o} = \text{Bouyancy Force / Viscous Force}
\]
\[ Pr = \frac{\nu}{D_{th}} = \text{Momentum Diffusivity} / \text{Thermal Diffusivity} \]

The last parameter used in the energy equation is related to parameter occurring in the species equation as

\[ \eta_i = Le_i \times \left( \frac{\hat{\mu}_i \bar{V}}{D_{th}} \right) \]

## 2.5 Approximations

### 2.5.1 Non-Dimensional Parameters

Based on experimentally found values of a few of the parameters used and approximation of gas properties using nitrogen has as the abundant species, estimates of the non-dimensional parameters defined earlier have been found. It has been found that in diffusion flames, \( H_3O^+ \) ions make up for a large portion of positive ions and therefore have been used to estimate the value for the ionic properties. The values used for these parameters are as follows (with ‘I’ denoting the positive \( H_3O^+ \) ion):

- \( T_\infty = 300 \text{ K} \)
- \( r_o = 1 \text{ mm} \)
- \( |\bar{V}| = 3 \text{ kV (high) or 3 V (low)} \)
- \( |q| = e = 1.6 \times 10^{-19} \text{ C} \)
- \( \epsilon_o = 8.854 \times 10^{-12} \text{ CV}^{-1} \text{m}^{-1} \)
- \( \hat{\mu}_i = 2.9 \times 10^{-4} \text{ m}^2 \text{V}^{-1} \text{sec}^{-1} \) [13]
- \( D_i = 2 \times 10^{-4} \text{ m}^2 \text{V}^{-1} \text{sec}^{-1} \) [19]
- \( D_{th} = 22.1 \times 10^{-6} \text{ m}^2 \text{sec}^{-1} \) [20]
- \( \rho_\infty = 1.123 \text{ kg m}^{-3} \) [13]
- \( c_p = 1041 \text{ J kg}^{-1} \text{K}^{-1} \) [13]
- \( \lambda = 25.9 \times 10^{-3} \text{ Wm}^{-1} \text{K}^{-1} \) [13]
- \( \mu = 1.99 \times 10^{-5} \text{ kg m}^{-1} \text{sec}^{-1} \)
- \( W_i = 19 \times 10^{-3} \text{ kg/mol} \)
\[ N_A = 6.022 \times 10^{23} \text{ molecules/mol} \]

Substituting these values gives us

1. \( \alpha_I = 2.144 \times 10^8 \) (high) or \( = 2.144 \times 10^{11} \) (low)
2. \( \eta_I = 4.35 \times 10^3 \) (high) or \( = 4.35 \) (low)
3. \( \beta_I = 3.11 \times 10^{13} \) (high) or \( = 3.11 \times 10^{10} \) (low)
4. \( \chi_I = 4.87 \times 10^4 \) (high) or \( = 4.87 \times 10^1 \) (low)
5. \( Le_I = 0.112 \)
6. \( Pr = 0.707 \)
7. \( Fr = 0.051 \)
8. \( M^2 = 4.23 \times 10^{-9} \)

### 2.5.2 Low Mach Number

Most of the combustion phenomenon take place in low-speed environments which makes application of the low Mach number approximation possible. The consequence of this approximation is that from the momentum equation, we can observe that pressure can now be expressed as,

\[
p(r, t) \sim P(t) + \gamma M^2 \hat{p}(r, t)
\]

where, \( P(t) = 1 \) in non-dimensional terms. While applying this limit, care must be taken that \( \left( \frac{\beta_I}{1/\gamma M^2} \right) \ll 1 \) for the above expansion to be valid. From here on, we will also drop the ‘\(*\)’ sign for non-dimensionalized numbers giving us the following non-dimensionalized reactions:

**Ideal Gas Law**

\[
\rho T = 1
\]

**Continuity**

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0
\]

**Poisson’s Equation**

\[
\nabla^2 \phi = -\alpha_+ \left( Y^+ - \bar{W} Y^- \right) \rho
\]
Species Conservation

\[ \rho \frac{\partial Y_i}{\partial t} + \rho v \cdot \nabla Y_i = \sum_{j=1}^{\text{reactions}} w_{i,j} + \frac{1}{Le_i} \nabla \cdot [\nabla Y_i + s_i \eta_i Y_i \nabla \phi] \]

Momentum Equation

\[ \rho \frac{\partial v}{\partial t} + \rho v \cdot \nabla v = -\nabla \hat{p} + \rho \frac{\beta}{Fr} + \rho \nabla \cdot \tau - \beta_+ (\nabla \phi) \left( Y^+ - \hat{W} Y^- \right) \rho \]

Energy Conservation

\[ \rho \frac{\partial T}{\partial t} + \rho v \cdot \nabla T - \nabla^2 T = \sum_{k=1}^{\text{reactions}} q_k \hat{w}_k + \chi_+ (\nabla \phi)^2 \left[ \sum_{i=1}^{N^+} \eta_i Y_i^+ + \sum_{i=1}^{N^-} \hat{W} \eta_i Y_i^- \right] + \chi_+ (\nabla \phi) \rho \left[ \sum_{i=1}^{N^+} \frac{\nabla Y_i^+}{Le_i} - \sum_{i=1}^{N^-} \frac{\nabla Y_i^-}{Le_i} \right] \]

2.6 Radial Coordinates

Studying the electric field effect for a spherically symmetric configuration with the added assumption of no gravity gives us the final equations in radial coordinates as:

Ideal Gas Law

\[ \rho T = 1 \]  \hspace{1cm} (2.6.1)

Continuity

\[ \frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho v \right) = 0 \]  \hspace{1cm} (2.6.2)

Poisson’s Equation

\[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \phi}{\partial r} \right) = -\alpha_+ \left( Y^+ - \hat{W} Y^- \right) \rho \]  \hspace{1cm} (2.6.3)

Species Conservation

\[ \rho \frac{\partial Y_i}{\partial t} + \rho v \frac{\partial Y_i}{\partial r} = \sum_{k=1}^{\text{reactions}} w_{i,k} + \frac{1}{Le_i} \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_i}{\partial r} \right] \]  \hspace{1cm} (2.6.4)

\[ \rho \frac{\partial Y_j}{\partial t} + \rho v \frac{\partial Y_j}{\partial r} = \sum_{k=1}^{\text{reactions}} w_{j,k} + \frac{1}{Le_j} \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_j}{\partial r} + s_j \eta_j r^2 Y_j \frac{\partial \phi}{\partial r} \right] \]  \hspace{1cm} (2.6.5)
where,

‘i’ = Fuel, Oxidizer, Products

‘j’ = Ionic Species - positive and negative

**Momentum Equation**

\[
\rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial r} = -\frac{\partial \hat{p}}{\partial r} + Pr \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 r) - \beta_+ \left( \frac{\partial \phi}{\partial r} \right) \left( Y^+ - \hat{W} Y^- \right) \rho
\]  

(2.6.6)

**Energy Conservation**

\[
\rho \frac{\partial T}{\partial t} + \rho v \frac{\partial T}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) = \sum_{k=1}^{\text{reactions}} q_k \hat{w}_k + \chi_+ \left( \frac{\partial \phi}{\partial r} \right)^2 \rho \left[ \sum_{i=1}^{N^+} \eta_i Y_i^+ + \sum_{i=1}^{N^-} \hat{W} \eta_i Y^- \right] + \chi_+ \left( \frac{\partial \phi}{\partial r} \right) \rho \left[ \sum_{i=1}^{N^+} \frac{1}{Le_i} \frac{\partial Y_i^+}{\partial r} - \sum_{i=1}^{N^-} \frac{\hat{W}}{Le_i} \frac{\partial Y_i^-}{\partial r} \right]
\]  

(2.6.7)
Chapter 3

Chemical Mechanism

3.1 Background

While studying the effect of the ions on the combustion characteristics of a diffusion flame, it behoves us to understand the mechanism of formation of these ions and thus to explore a more detailed kinetic mechanism as compared to the one-step chemistry. Since, the full kinetic mechanisms are usually too large to allow some kind of analytical analysis, the accepted method is to generally represent the system by a smaller number of equations which in essence cover the physical aspect of the problem. For example, Peters\(^1\) provided a 4-step systematically-reduced mechanism for the combustion of methane using a series of steady-state and partial-equilibrium assumptions. This mechanism shown below has been used to study the structure of methane-air flames asymptotically.

\[
\begin{align*}
&\text{1. } CH_4 + 2H + H_2O \rightarrow CO + 4H_2 \\
&\text{2. } CO + H_2O \rightleftharpoons CO_2 + H_2 \\
&\text{3. } 2H + M \rightarrow H_2 + M \\
&\text{4. } O_2 + 3H_2 \rightleftharpoons 2H_2O + 2H \\
\end{align*}
\]

Here, the first reaction represents the oxidation of methane to get CO. The second reaction is a culmination of the chain branching reactions while the third reaction signifies the chain branching in the combustion of methane. Lastly, the fourth reaction represents the conversion of CO to CO\(_2\) and thus the major part of the heat release in the entire mechanism. It can be shown that a general 4-step mechanism can also be written to show the combustion of any hydrocarbon, the caveat in that case being that as the hydrocarbon gets more complex, the assumptions of steady-state and partial-equilibrium may no longer be appropriate. This in turn would affect the accuracy of the solution.

3.2 Ionic Species

Now, the above system of reactions was written without considering the possibility of any electric species inside the flame. In a paper written by Calcote [2], it was logically argued and shown that amongst the different sources of creation of ions inside flames, chemi-ionization is the dominant mode.

There has been some work in the past to determine the dominant reactions for the ionic species and it was found that the CH radical was the main precursor to these reactions. Research in this direction has led to the identification of the following three main reactions for the existence of ions [12]

A \[ CH + O \rightarrow HCO^+ + e^- \]

B \[ HCO^+ + H_2O \rightarrow CO + H_3O^+ \]

C \[ H_3O^+ + e^- \rightarrow H_2O + H \]

In the above set of reactions, though \( HCO^+ \) seems to be main ion which is formed from the \( CH \) radical, however it has been experimentally found that its \( H_3O^+ \) which is the dominant positive ion. As far as the negative ions are concerned, its believed that inside the flame region electrons form the majority of negative species [19]. Species like \( O_2^- \) also exist, but for majority of the cases, their number concentrations are much lesser that electrons. It is possible that for extremely high external fields, the collisions of electrons with neutral particles may result in a considerable percentage of other negative ions. Now, once we take into account the above three equations for ions and do a steady-state approximation similar to that of Peters, we get the following system of equations for any general hydrocarbon :

1. \[ C_nH_m + aH + nH_2O \rightarrow nCO + \left( \frac{m + a + 2n}{2} \right) H_2 \]
2. \[ C_nH_m + a'H + b'O_2 \rightarrow nCO + \left( \frac{m + a' + 3n - 6b'}{2} \right) H_2 + \left( 2b' - n \right) (H_3O^+ + e^-) \]
3. \[ CO + H_2O \Leftrightarrow CO_2 + H_2 \]
4. \[ 2H + M \rightarrow H_2 + M \]
5. \[ O_2 + 3H_2 \Leftrightarrow 2H_2O + 2H \]
6. \[ H_3O^+ + e^- \rightarrow H_2O + H \]

It has been observed that the since reactions 1 & 2 represent the oxidation of the hydrocarbon, therefore these reactions highlight the role of varied radicals during the oxidation process. During this time, there is a competition for the fuel between these radicals which causes a part of the fuel to oxidise to \( CO \) and the
other part to lead to the formation of ionic species by following up the CH radical. Thus, based on this, the following general three step reaction mechanism has been proposed to represent the kinetic mechanism for a hydrocarbon:

\[ \text{I } \nu_F F + \nu_O O \rightarrow X_1 + X_2 \]

\[ \text{II } X_2 \rightarrow p + n \]

\[ \text{III } p + n + X_1 \rightarrow (\nu_F + \nu_O) P \]

where,

\( F = \text{Fuel} \)

\( O = \text{Oxidizer} \)

\( P = \text{Product} \)

\( X_1 = \text{Radicals responsible for oxidation of fuel to CO} \)

\( X_2 = \text{Radicals responsible for formation of positive (p) and negative (n) ionic species} \)

From the above reaction, it is observed that the key property separating the radicals \( X_1 \) and \( X_2 \) is that the latter mostly originates from the fuel and so is dependant on the fuel type. The reasoning for this goes from reactions A-C discussed before. It is seen from these reactions that for the formation of ionic species, the crucial element is the CH radical. Since, the carbon atom in this radical has to originate from the fuel, therefore this shows that the involvement of the fuel is essential for \( X_2 \). \( X_1 \) on the other hand can be formed from a combination of both the fuel and the oxidizer.

Also, comparing the above general set of equations and the 6-step mechanism, we observe that the Eqs. 1 & 2 are partly represented by Eqs. I & II, which show the creation of two sets of radicals representing the combustion process with and without the ionic species. The group of radicals \( X_1 \) represent the radicals in Eqs. 3-5 which lead to oxidation of fuel to mainly CO and then the subsequent reduction to \( \text{CO}_2 \). Whereas, the group of radicals \( X_2 \) represents consist among them the \( \text{CH} \) and \( \text{HCO}^+ \) radicals which are responsible for the creation of \( p \) & \( n \). The last equation in the general mechanism, Eq. III is a combination of Eqs. 3-6 leading to the formation of the product.

Another assumption made in this mechanism that it is only in the first and third steps of the mechanism, where the maximum amount of heat is liberated. The justification for this comes from the fact that step 2

\(^2\)Note that \( \text{HCO}^+ \) is a part of the reactions which lead to the formation of \( p \) and so, \( X_2 \) doesn’t contain any ions itself.
II behaves like a chain propagation step responsible only for the creation of ions. As far as the activation energy is concerned, we assume that the first and last reactions have very high activation energies, with the former step having the higher one. Step II is assumed to have a zero activation energy.
Chapter 4

Asymptotic Solution

4.1 Modified Governing Equations

Having discussed a reduced kinetic mechanism for the droplet with an external electric field, it now behoves us to modify our governing equations to explicitly include these reactions. Recall, the proposed mechanism:

I \[ \nu F + \nu O \xrightarrow{k_1} X_1 + X_2 \]

II \[ X_2 \xrightarrow{k_2} p + n \]

III \[ p + n + X_1 \xrightarrow{k_3} (\nu F + \nu O) P \]

Now, the species-independent reactions rates to be used in the species equations can be expressed as follows:\(^1\):

- \[ \dot{\hat{\omega}}_F = -D_1 \rho^2 Y_F Y_O e^{(\beta_1/T_f - \beta_1/T)} \]
- \[ \dot{\hat{\omega}}_O = -\nu D_1 \rho^2 Y_F Y_O e^{(\beta_1/T_f - \beta_1/T)} \]
- \[ \dot{\hat{\omega}}_{X_1} = D_1 W_1 \rho^2 Y_F Y_O e^{(\beta_1/T_f - \beta_1/T)} - D_3 W_2 \rho^3 Y_p X_n Y_{X_1} e^{(\beta_3/T_f - \beta_3/T)} \]
- \[ \dot{\hat{\omega}}_{X_2} = D_1 W_1 \rho^2 Y_F Y_O e^{(\beta_1/T_f - \beta_1/T)} - D_2 \rho Y_{X_2} \]
- \[ \dot{\hat{\omega}}_p = \left( D_2 \frac{W_1}{W_2 W_3} \right) \rho Y_{X_2} - D_3 \rho^3 Y_p X_n Y_{X_1} e^{(\beta_3/T_f - \beta_3/T)} \]
- \[ \dot{\hat{\omega}}_n = \left( D_2 \frac{W_1}{W_2 W_3} \right) \rho Y_{X_2} - \left( \frac{D_3}{W} \right) \rho^3 Y_p X_n Y_{X_1} e^{(\beta_3/T_f - \beta_3/T)} \]

where,

\(^1\)Note that \( X_n \) represents the mass fraction of the negative ions similar to \( Y_p \).
\[ \nu = \frac{\nu_o W_o}{\nu_W} \]
\[ W = \frac{W_p}{W_n} \]
\[ W_3 = \frac{W_{x_3}}{W_p} \]
\[ \beta_1 = E_1 / RT_\infty \]
\[ \beta_2 = E_2 / RT_\infty = 0 \]
\[ \beta_3 = E_3 / RT_\infty \]
\[ \hat{\dot{D}}_1 = \frac{\nu_p \beta_3^2 B_1 e^{-\beta_3/T_f}}{(\lambda/C_p) W_o} \]
\[ \hat{\dot{D}}_2 = \frac{\rho_\infty r_0^2 B_2}{(\lambda/C_p)} \]
\[ \hat{\dot{D}}_3 = \frac{\rho_\infty^2 r_0^2 B_3 e^{-\beta_3/T_f}}{(\lambda/C_p) W_n W_{x_3}} \]

We will assume unity Lewis numbers and molecular ratios for all species. We will additionally ignore the momentum equation which can be solved for pressure a posteriori. Another motive of doing this is that we intend to investigate whether the interaction between the external electric field and the flame in terms of the work done called Ohmic Heating is important relative to the Ionic Wind. This will highlight the most basic effect the electric field has on the flame. Since, the pressure in this case only plays a passive role in the system, therefore any stabilization effect offered by the Ionic Wind can be later studied by perturbing the flame. Thus, substituting the above expressions in our governing equations in radial coordinates through eqs (2.6.1) to (2.6.7), we get following modified equations for a steady-state :

\[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \phi}{\partial r} \right) = -\alpha_p (Y_p - X_n) \rho \quad (4.1.1) \]
\[ \rho \frac{\partial Y_e}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_e}{\partial r} \right] = -\hat{\dot{D}}_1 \rho^2 Y_e Y_o e^{(\beta_1/T_f - \beta_1/T)} \quad (4.1.2) \]
\[ \rho \frac{\partial Y_o}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_o}{\partial r} \right] = -\hat{\dot{D}}_1 \rho^2 Y_e Y_o e^{(\beta_1/T_f - \beta_1/T)} \quad (4.1.3) \]
\[ \rho \frac{\partial Y_{x_1}}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_{x_1}}{\partial r} \right] = \hat{\dot{D}}_1 \rho^2 Y_e Y_o e^{(\beta_1/T_f - \beta_1/T)} - \hat{\dot{D}}_3 \rho^3 Y_p X_n Y_{x_1} e^{(\beta_3/T_f - \beta_3/T)} \quad (4.1.4) \]
\[ \rho \frac{\partial Y_{x_2}}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_{x_2}}{\partial r} \right] = \hat{\dot{D}}_1 \rho^2 Y_e Y_o e^{(\beta_1/T_f - \beta_1/T)} + \hat{\dot{D}}_3 \rho^3 Y_p X_n Y_{x_1} e^{(\beta_3/T_f - \beta_3/T)} \quad (4.1.5) \]
\[ \rho \frac{\partial Y_p}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_p}{\partial r} \right] = D_2 \rho Y_{x_2} - \hat{\dot{D}}_3 \rho^3 Y_p X_n Y_{x_1} e^{(\beta_3/T_f - \beta_3/T)} + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ \eta_p r^2 Y_p \frac{\partial \phi}{\partial r} \right] \quad (4.1.6) \]
\[ \rho \frac{\partial X_n}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial X_n}{\partial r} \right] = D_2 \rho Y_{x_2} - \hat{\dot{D}}_3 \rho^3 Y_p X_n Y_{x_1} e^{(\beta_3/T_f - \beta_3/T)} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ \eta_n r^2 X_n \frac{\partial \phi}{\partial r} \right] \quad (4.1.7) \]
\[
\rho v^2 \frac{\partial T}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) = Q_1 \tilde{D}_1 \rho^2 Y_p Y_o e^{(\beta_1 / T_f - \beta_1 / T)} + Q_3 \tilde{D}_3 \rho^3 Y_p X_n Y_{x_1} e^{(\beta_3 / T_f - \beta_3 / T)}
+ \chi_p \left( \frac{\partial \phi}{\partial r} \right)^2 \rho (\eta_p Y_p + \eta_n X_n) + \chi_p \left( \frac{\partial \phi}{\partial r} \right) \rho \left( \frac{\partial Y_p}{\partial r} - \frac{\partial X_n}{\partial r} \right)
\] (4.1.8)

where,

\[Y_p \text{ & } X_n = \text{Mass fractions of positive and negative ions respectively}\]

\[M = r^2 \rho v = \text{Derived from the continuity equation}\]

\[Q_1 = \frac{q_1}{c_p T_\infty W_p}\]

\[Q_3 = \frac{q_3}{c_p T_\infty W_p}\]

Having a look at the above equations we observe that the electric field can effect the flame characteristics in two ways :-

1. **Kinetic Effects** : These effects generally result due to the repartition of the various species as a consequence of the external field and appear in the energy and species equations.

2. **Body Force Effects** : These kind of effects are a result of the work done by the electrostatic or Coulomb forces on the ionic species. Recall that the amount of effect the body force has on the energy equation depends upon the balance between the positive and negative work done by this force as explained before.

Therefore, we will first try and understand the nature of the solution without the electric field and then analyse the effects caused by the aforementioned effects.

### 4.2 Flame Structure

From here onwards, we try to tackle the problem using activation energy asymptotics. But, we will do this in steps by making certain assumptions about the structure of the problem using \(\beta_1, \beta_3\) and \(D_2\).

1. The first set of assumption is that \(\beta_1 \gg 1\), which is similar to the case of the classical problem. In doing so, we note that \(w_1\) exists only inside the reaction zone (near \(r_f\)) which has a thickness of \(O(\beta_1^{-1})\).

We call this reaction zone as the consumption layer. Everywhere else, the problem exists with both \(w_2\) and \(w_3\) occurring everywhere.
2. Now, we assume that the second step of the mechanism occurs extremely fast; i.e; \( D_2 \gg 1 \). Note that the following operator has been used for ease of presentation:

\[
\mathcal{L}_i = \frac{M}{r^2} \frac{d}{dr} - \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right)
\]

where, \( i = \) any species in the system.

Using eq (4.1.5), we get that as long as that \( \frac{D_2}{\hat{D}_1} e^{(\beta_1/T_f - \beta_1/T)} \sim O(1) \) or \( \ll 1 \);

\[
\mathcal{L}_{X_2} = \hat{D}_1 e^{(\beta_1/T_f - \beta_1/T)} \left\{ \rho^2 Y_F Y_O - \frac{D_2}{\hat{D}_1} e^{(\beta_1/T_f - \beta_1/T)} \rho Y_{X_2} \right\} \atop \approx 0
\]

\[
\therefore \quad Y_{X_2} = \rho \left( \frac{\hat{D}_1 e^{(\beta_1/T_f - \beta_1/T)}}{D_2} \right) Y_F Y_O
\]

This means that \( Y_{X_2} = 0 \) everywhere except inside the flame zone at least to the leading order. The only place where \( Y_{X_2} \) occurs is inside the consumption layer. The structure at this stage is depicted in Fig. 4.1.

![Figure 4.1: Flame structure using large \( \beta_1 \) and \( D_2 \)](image)

3. The problem at this stage is still too complicated to solve analytically. We go one step further and assume that \( \beta_3 \gg 1 \). This results in \( w_3 = 0 \) everywhere except near the reaction zone which has a thickness of \( O(\beta_3^{-1}) \). We call this layer as the intermediate layer which has the consumption layer embedded in it. The problem now has no reaction occurring everywhere else outside this zone. The scenario after this stage is depicted in Fig. 4.2.

\[\text{Note that } w_i \text{ here refers to } w_i, \text{ for } i = 1, 2, 3\]

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4.3 Outer Flame Structure

Now, given the aforementioned assumptions, the outer structure reduces to the following set of equations:

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \phi}{\partial r} \right) = -\alpha_p (Y_p - X_n) \rho \quad (4.3.1)
\]

\[
\frac{M}{r^2} \frac{\partial Y_p}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_p}{\partial r} \right] = 0 \quad (4.3.2)
\]

\[
\frac{M}{r^2} \frac{\partial Y_O}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_O}{\partial r} \right] = 0 \quad (4.3.3)
\]

\[
\frac{M}{r^2} \frac{\partial Y_{X_1}}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_{X_1}}{\partial r} \right] = 0 \quad (4.3.4)
\]

\[
Y_{X_2} = 0 \quad (4.3.5)
\]

\[
\frac{M}{r^2} \frac{\partial Y_p}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial Y_p}{\partial r} \right] = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ \eta_p r^2 Y_p \frac{\partial \phi}{\partial r} \right] \quad (4.3.6)
\]

\[
\frac{M}{r^2} \frac{\partial X_n}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial X_n}{\partial r} \right] = -\frac{1}{r^2} \frac{\partial}{\partial r} \left[ \eta_n r^2 X_n \frac{\partial \phi}{\partial r} \right] \quad (4.3.7)
\]

\[
\frac{M}{r^2} \frac{\partial T}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) = X_p \left( \frac{\partial \phi}{\partial r} \right)^2 \rho (\eta_p Y_p + \eta_n X_n) + X_p \frac{\partial \phi}{\partial r} \rho \left( \frac{\partial Y_p}{\partial r} - \frac{\partial X_n}{\partial r} \right) \quad (4.3.8)
\]

The jump conditions across the flame zone are described below:

\[
\left[ \frac{\partial Y_p}{\partial r} \right]_{r_f^+} - \frac{1}{\nu} \left[ \frac{\partial Y_O}{\partial r} \right]_{r_f^-} = 0
\]
\[ \left[ \frac{\partial Y_{x_1}}{\partial r} \right]_{\xi}^+ - \left[ \frac{\partial Y_{x_2}}{\partial r} \right]_{\xi}^+ - \left[ \frac{\partial Y_{p}}{\partial r} \right]_{\xi}^+ = -\eta_p \left[ \frac{\partial \phi}{\partial r} \right]_{\xi}^+ \]

\[ \left[ \frac{\partial Y_{p}}{\partial r} \right]_{\xi}^+ - \left[ \frac{\partial X_n}{\partial r} \right]_{\xi}^+ = -\eta_n \left[ X_n \frac{\partial \phi}{\partial r} \right]_{\xi}^+ + \eta_p \left[ \frac{\partial \phi}{\partial r} \right]_{\xi}^+ \]

\[ \frac{1}{Q_3} \left[ \frac{\partial T}{\partial r} \right]_{\xi}^+ + \left[ \frac{\partial Y_{p}}{\partial r} \right]_{\xi}^+ + \left( 1 + \frac{Q_1}{Q_3} \right) \left[ \frac{\partial Y_{F}}{\partial r} \right]_{\xi}^+ = -\eta_p \left[ \frac{\partial \phi}{\partial r} \right]_{\xi}^+ \]

### 4.4 Inner Flame Structure

Recall, the inner structure of our system has two layers of different scales. The inner most layer is called the consumption layer where the heat release due to step I occurs. This layer is embed inside a bigger intermediate layer, where the heat release due to the step III occurs.

#### 4.4.1 Equations in the Consumption Layer

We expand the consumption layer as the following asymptotic series :-

\[ r \sim r_f + \epsilon \xi \]
\[ T \sim T_a + \epsilon \tau_1 \]
\[ \phi \sim \phi^* + \epsilon \phi_1 \]
\[ Y_p \sim 0 + \epsilon \phi_p \]
\[ Y_o \sim 0 + \epsilon y_o \]
\[ Y_{x_1} \sim 0 + \epsilon y_{x_1} \]
\[ Y_{x_2} \sim 0 + \epsilon y_{x_2} \]
\[ Y_p \sim y_p^* + \epsilon y_p \]
\[ X_n \sim x_n^* + \epsilon x_n \]

where, \( \epsilon = T_a^2 / \beta_1 = D_2^{-1/2} \)

\[ \frac{\partial^2 \phi_1}{\partial \xi^2} = 0 \]  \hspace{1cm} (4.4.1)

\[ \frac{\partial^2 y_p}{\partial \xi^2} = \Lambda_1 y_p y_o e^\tau \]  \hspace{1cm} (4.4.2)

\[ \frac{\partial^2 y_o}{\partial \xi^2} = \nu \Lambda_1 y_p y_o e^\tau \]  \hspace{1cm} (4.4.3)

\[ \frac{\partial^2 y_{x_1}}{\partial \xi^2} = -\Lambda_1 y_p y_o e^\tau \]  \hspace{1cm} (4.4.4)

\[ \frac{\partial^2 y_{x_2}}{\partial \xi^2} = -\Lambda_1 y_p y_o e^\tau + \Lambda_2 y_{x_2} \]  \hspace{1cm} (4.4.5)

\[ \frac{\partial^2 y_p}{\partial \xi^2} = -\Lambda_2 y_{x_2} - \Lambda_3 \frac{\partial^2 \phi_1}{\partial \xi^2} \]  \hspace{1cm} (4.4.6)
\[
\frac{\partial^2 x_n}{\partial \xi^2} = -\Lambda_2 y_{x_2} + \Lambda_4 \frac{\partial^2 \phi_1}{\partial \xi^2} \tag{4.4.7}
\]

\[
\frac{\partial^2 \tau}{\partial \xi^2} = -Q_1 \Lambda_1 y_{x_1} e^\tau \tag{4.4.8}
\]

where,

\[
\Lambda_1 = \rho_n^2 \quad \Lambda_2 = \rho_n \\
\Lambda_3 = \eta_p y_p^* \quad \Lambda_4 = \eta_n x_n^*
\]

### 4.4.2 Equations in the Intermediate Layer

We expand the intermediate layer as the following asymptotic series :

\[
\begin{align*}
  r & \sim r_f + \delta \zeta \\
  T & \sim T_f + \delta \hat{\Theta}_1 \\
  \phi & \sim \hat{\phi} + \delta \hat{\phi}_1 \\
  Y_F & \sim 0 + \delta \hat{y}_F \\
  Y_O & \sim 0 + \delta \hat{y}_O \\
  Y_{X_2} & \sim 0 + \delta \hat{y}_{X_2} \\
  Y_p & \sim \hat{y}_p + \delta \hat{y}_p \\
  X_n & \sim \hat{x}_n + \delta \hat{x}_n
\end{align*}
\]

where, \( \delta \sim T_f^2/\beta_3 \)

\[
\begin{align*}
  \frac{\partial^2 \hat{\phi}_1}{\partial \zeta^2} & = 0 \tag{4.4.9} \\
  \frac{\partial^2 \hat{y}_p}{\partial \zeta^2} & = 0 \tag{4.4.10} \\
  \frac{\partial^2 \hat{y}_O}{\partial \zeta^2} & = 0 \tag{4.4.11} \\
  \frac{\partial^2 \hat{y}_{X_1}}{\partial \zeta^2} & = \left( \frac{\Delta_1}{Q_3} \right) e^{\hat{\phi}_1} \tag{4.4.12} \\
  \frac{\partial^2 \hat{y}_{X_2}}{\partial \zeta^2} & = 0 \tag{4.4.13} \\
  \frac{\partial^2 \hat{y}_p}{\partial \zeta^2} & = \left( \frac{\Delta_1}{Q_3} \right) e^{\hat{\phi}_1} - \Delta_2 \frac{\partial^2 \hat{\phi}_1}{\partial \zeta^2} \tag{4.4.14} \\
  \frac{\partial^2 \hat{x}_n}{\partial \zeta^2} & = \left( \frac{\Delta_1}{Q_3} \right) e^{\hat{\phi}_1} + \Delta_3 \frac{\partial^2 \hat{\phi}_1}{\partial \zeta^2} \tag{4.4.15} \\
  \frac{\partial^2 \hat{\Theta}_1}{\partial \zeta^2} & = -\Delta_1 e^{\hat{\phi}_1} \tag{4.4.16}
\end{align*}
\]

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where,

\[ \Delta_1 = \delta^2 \hat{D}_3 \rho h \hat{y}_p \hat{x}_n \hat{y} \hat{y} \hat{x}_1 \]
\[ \Delta_2 = \eta_p \hat{y}_p \]
\[ \Delta_3 = -\eta_n \hat{x}_n \]

These equations are valid only for \(-\infty < \zeta < 0\) and \(0 < \zeta < \infty\)

### 4.5 Boundary Conditions

The boundary conditions for our system can be summarized as follows:

**Conditions due to the flame structure:**

This condition gives us that to the leading order, as \(r \to r_f\), \(Y_p = Y_o = 0\)

**Boundary Conditions as \(r \to 1\):**

- \(T = T_s\)
- \(MY_p - \frac{\partial Y_p}{\partial r} = M\)
- \(MY_o - \frac{\partial Y_o}{\partial r} = 0\)
- \(MY_{X_1} - \frac{\partial Y_{X_1}}{\partial r} = 0\)
- \(MY_{X_2} - \frac{\partial Y_{X_2}}{\partial r} = 0\)
- \(MY_p - \frac{\partial Y_p}{\partial r} = M\psi_p\)
- \(MX_n - \frac{\partial X_n}{\partial r} = M\psi_n\)
- \(\frac{\partial T}{\partial r} - ML_v = 0\)
- \(\phi = 1\)

**Boundary Conditions as \(r \to \infty\):**

- \(T = 1\)
- \(Y_o = Y_{o\infty}\)
- \(Y_p = Y_p = X_n = Y_{X_1} = Y_{X_2} = \phi = 0\)
We now modify the boundary conditions for the ionic species using the following justifications:

1. Practically, there would be a buffer layer very near the droplet surface where the ions and electrons would react with the potential at the surface and cause it to drop a little. In order to maintain the potential at a constant value, we would need to keep on supplying extra current from the source and it is this current which gives us $\psi_p$ and $\psi_n$.

2. We assume that for moderate and strong external fields, the effect of this current on the external field supplied is very small or zero to the leading order. Therefore, the boundary conditions for the positive and negative ions at the surface reduce to no flux.

Therefore, the new boundary conditions for the ionic species at the droplet surface become:

- $MY_p - \frac{\partial Y_p}{\partial r} = 0$
- $MX_n - \frac{\partial X_n}{\partial r} = 0$

### 4.6 Coupling Functions

We can formulate a few coupling functions for our system which will be later used to derive jump conditions across the flame zone. These functions can be summarized as follows:

\[ \mathcal{L}_p - \frac{\mathcal{L}_\phi}{\nu} = 0 \]  
\[ \mathcal{L}_{x_1} - \mathcal{L}_{x_2} - \mathcal{L}_{y_p} = -\frac{1}{r^2} \frac{\partial}{\partial r} \left\{ \eta_p r^2 Y_p \frac{\partial \phi}{\partial r} \right\} \]  
\[ \mathcal{L}_{y_p} - \mathcal{L}_{x_n} = \frac{1}{r^2} \frac{\partial}{\partial r} \left\{ \eta_n r^2 X_n \frac{\partial \phi}{\partial r} \right\} - \frac{1}{r^2} \frac{\partial}{\partial r} \left\{ \eta_p r^2 Y_p \frac{\partial \phi}{\partial r} \right\} \]  
\[ \frac{\mathcal{L}_r}{Q_3} + \mathcal{L}_p + \mathcal{L}_{x_2} + \mathcal{L}_{y_p} \left( 1 + \frac{Q_1}{Q_3} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} \left\{ \eta_p r^2 Y_p \frac{\partial \phi}{\partial r} \right\} \]

where,

\[ \mathcal{L}_i \equiv \frac{M}{r^2} \frac{d}{dr} - \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) \]

### 4.7 Solution Procedure in the Absence of Electric Field

Using the above S-Z equations, we will not explicitly solve for $Y_p$, $X_n$ and $Y_{x_1}$ in the inner layers and calculate them later from these relations applying the appropriate boundary conditions. To calculate the profile for
temperature for which we need to solve for it inside the intermediate layer and match these solutions to those obtained for the outer layer. Also, inside the intermediate layer, we will use the following jump conditions across the consumption layer so that we can get a solution without actually solving for the system inside the consumptions layer:

**Conditions across the Consumption layer**

- All variables are continuous across the reaction zone.
- \( \left[ \frac{\partial \hat{y}_F}{\partial \zeta} \right]_0^{+} = \frac{1}{\nu} \left[ \frac{\partial \hat{y}_O}{\partial \zeta} \right]_0^{-} \)
- \( \left[ \frac{\partial \hat{\Theta}_I}{\partial \zeta} \right]_0^{+} + Q_1 \left[ \frac{\partial \hat{y}_F}{\partial \zeta} \right]_0^{-} = 0 \)
- \( \left[ \frac{\partial \hat{y}_x^2}{\partial \zeta} \right]_0^{+} = 0 \)

### 4.7.1 Solving for Temperature and \( M \)

The general solution for temperature in the outer layer is given as:

\[
T = A + Be^{-M/r}
\]

Applying the boundary conditions at \( r \to 1 \) and \( r \to \infty \) gives us:

\[
T(r) = \begin{cases} 
C_{1l} + L_{v}e^{M(1-1/r)} & \text{if } r < r_f \\
C_{1r} + (1 - C_{1r})e^{-M/r} & \text{if } r > r_f 
\end{cases}
\]

(4.7.1)

Similarly, solving eq 4.4.16 in the intermediate layer gives the general solutions of temperature as:

\[
\hat{\Theta}_1(\zeta) = \begin{cases} 
C_{3l} + 2 \ln \left[ \text{sech} \left( \sqrt{\frac{\Delta_1 e^{C_{3l}}}{2}} (\zeta - C_{4l}) \right) \right] & \text{if } \zeta < 0 \\
C_{3r} + 2 \ln \left[ \text{sech} \left( \sqrt{\frac{\Delta_1 e^{C_{3r}}}{2}} (\zeta - C_{4r}) \right) \right] & \text{if } \zeta > 0 
\end{cases}
\]

(4.7.2)

Now, we will use the boundary condition for temperature as \( r \to 1 \) along with the jump conditions for \( \hat{\Theta}(\zeta) \) across the consumption layer to solve for \( C_{4l} \) and two of the four constants from the intermediate layer. Then, we will match the slopes of the solution in the intermediate layer to the slopes from the outer layer to solve for one more constant and \( M \). We will use the continuity of the temperature from the outer layer across
the two inner layers to solve for one more constant. We will also shift our coordinates of the intermediate layer towards infinity to fix $C_{4r}$. This is done as follows:

$$T \bigg|_{r \to 1} = T_s$$

This conditions gives us the value of $C_{4l}$ as:

$$C_{4l} = T_s - L_v$$  \hspace{1cm} (4.7.3)\]

$[T] = 0$

This condition refers to the continuity of the temperature across the two inner layers and gives us $C_{1r}$ as:

$$T \bigg|_{r \to r_f^-} = T \bigg|_{r \to r_f^+} \Rightarrow C_{1r} = \frac{C_{4l} + e^{-M/r_f} (1 - L_v e^M)}{e^{-M/r_f} Y_{O \infty} / \nu}$$  \hspace{1cm} (4.7.4)$$

$$\frac{\partial T}{\partial r} \bigg|_{r \to r_f^-} = \frac{\partial \hat{\Theta}}{\partial \zeta} \bigg|_{\zeta \to -\infty}$$

This condition matches the slope of the outer solution with that of the intermediate on left side of the domain and gives $\lambda_l$:

$$\lambda_l = L_v e^{M (1 - 1/r_f)} \frac{M}{2 r_f^2}$$  \hspace{1cm} (4.7.5)$$

where, $C_{3l} = e^{(2 \lambda_l^2 / \Delta_1)}$

$$\frac{\partial T}{\partial r} \bigg|_{r \to r_f^+} = \frac{\partial \hat{\Theta}}{\partial \zeta} \bigg|_{\zeta \to \infty}$$

This condition matches the slope of the outer solution with that of the intermediate on right side of the domain and gives $\lambda_r$:

$$\lambda_r = (C_{1r} - 1) e^{-M/r_f} \frac{M}{2 r_f^2}$$  \hspace{1cm} (4.7.6)$$

where, $C_{3r} = e^{(2 \lambda_r^2 / \Delta_1)}$
\[ \hat{\Theta}_1 = 0 \]

This condition refers to the continuity of temperature across the consumption layer and provides us \( C_{4l} \):

\[ \hat{\Theta}_1 \bigg|_{\zeta \to 0^+} = \hat{\Theta}_1 \bigg|_{\zeta \to 0^-} \]
\[ \Rightarrow \quad C_{4l} = \text{sech}^{-1} \left\{ \frac{\text{sech} (\lambda_r C_{4r} e^{C_{3r} - C_{4l}/2})}{\lambda_l} \right\} \quad (4.7.7) \]

\[ \left[ \frac{\partial \hat{\Theta}_1}{\partial \zeta} \right]_{0^+} + Q_1 \left[ \frac{\partial y_F}{\partial \zeta} \right]_{0^-} = 0 \]

This condition relates the jump in the slope of temperature across the consumption layer with that of the fuel. The assumption being made here is that \(|\gamma| \leq 1\). This relation provides us an expression for \( M \):

\[ \left[ \frac{\partial \hat{\Theta}_1}{\partial \zeta} \right]_{0^+} + Q_1 \left[ \frac{\partial y_F}{\partial \zeta} \right]_{0^-} = 0 \]
\[ \Rightarrow \quad \{ \lambda_r \tanh (\lambda_r C_{4r}) - \lambda_l \tanh (\lambda_l C_{4l}) \} = -Q_1 \left( 0 + \frac{M r_f^2}{r_f^2} \right) \]
\[ \Rightarrow \quad M = \frac{\lambda_r \tanh (\lambda_r C_{4r}) - \lambda_l \tanh (\lambda_l C_{4l})}{Q_1 r_f^2} \quad (4.7.8) \]

Using eqs 4.7.3 - 4.7.7 and 4.7.8 simultaneously, we can solve for the mass burning rate and temperature in the intermediate as well as the outer layer. The profile for \( T \) based on the above solution is shown in Fig. 4.3.

**4.7.2 Solving for \( Y_F, Y_O \) and \( r_f \)**

To solve for \( Y_F \) and \( Y_O \) we use the boundary conditions at \( r \to 1 \) and \( r \to \infty \) coupled with continuity across the entire flame zone. This gives us the following relations:

\[ Y_F = \begin{cases} 1 - e^M \left( \frac{1}{r_f} - \frac{1}{r} \right) & \text{if } r < r_f \\ 0 & \text{if } r > r_f \end{cases} \quad (4.7.9) \]

\[ Y_O = \begin{cases} 0 & \text{if } r < r_f \\ \nu \left[ e^M \left( \frac{1}{r_f} - \frac{1}{r} \right) - 1 \right] & \text{if } r > r_f \end{cases} \quad (4.7.10) \]
To solve for $r_f$, we integrate (eq 4.6.1) across the flame zone and apply continuity of fuel and oxidizer. This gives us the following relation from which we can formulate $r_f$:

$$
\left[ \frac{\partial Y_F}{\partial r} \right]_{r_f}^r = \frac{1}{\nu} \left[ \frac{\partial Y_O}{\partial r} \right]_{r_f}^r
\Rightarrow r_f = \frac{M}{\ln(1 + Y_{O\infty}/\nu)}
$$

The profiles for $Y_F$ and $Y_O$ based on the above solution are shown in Fig. 4.4.

### 4.7.3 Solving for $Y_p$

The general solution for the positive ions in the outer layer is given as:

$$Y_p = C + De^{-M/r}$$

We then use coupling function in eq (4.6.4) and apply the boundary conditions as $r \to 1$ and $r \to \infty$ along with continuity across the entire zone. We also use integrate this equation to get an additional jump
condition across the flame zone as:

\[
\frac{1}{Q_3} \left[ \frac{\partial T}{\partial r} \right]_r^{r_f} + \left[ \frac{\partial Y_p}{\partial r} \right]_r^{r_f} + \left( 1 + \frac{Q_1}{Q_3} \right) \left[ \frac{\partial Y_F}{\partial r} \right]_r^{r_f} = 0
\]

Applying all these conditions gives the solution for \( Y_p \) as:

\[
Y_p = \begin{cases} 
C \left( 1 - e^{M/r_f} \right) e^{-M/r} & \text{if} \quad r < r_f \\
C \left( e^{-M/r} - 1 \right) & \text{if} \quad r > r_f
\end{cases}
\] (4.7.12)

where, \( C = \frac{e^{-M/r_f}}{Q_3} \left[ C_1 + \frac{Q_1}{Q_3} \right] - \left( 1 + \frac{Q_1}{Q_3} \right) \) The profile for \( Y_p \) based on the above solution is shown in Fig. 4.5.
4.7.4 Solving for $Y_{X_1}$ and $X_n$

We use coupling functions in eqs (4.6.2) & (4.6.4) and apply the boundary conditions at $r \to 1$ and $r \to \infty$ along with continuity across the flame zone. We also integrate these across the entire flame zone to get the following jump relations

$$\left[ \frac{\partial Y_{X_1}}{\partial r} \right]_{r_f^-}^{r_f^+} = \left[ \frac{\partial Y_p}{\partial r} \right]_{r_f^-}^{r_f^+}$$

$$\left[ \frac{\partial Y_p}{\partial r} \right]_{r_f^-}^{r_f^+} = \left[ \frac{\partial X_n}{\partial r} \right]_{r_f^-}^{r_f^+}$$

Applying these conditions gives us that:

$$Y_{X_1} = X_n = Y_p \quad (4.7.13)$$

Comparison of Model with Classical Solution

It now becomes essential to ensure that the new model is able to capture the physics of the classical droplet case. Given the above relations, we can find out the mass burning rate and the profiles of all the variables in our system. With regards to the solution of $M$, since we need to solve a system of algebraic equations
simultaneously to get this value, therefore it is very difficult to represent it with a transfer number like in classical solution of the one-step mechanism and then compare them. To overcome this difficulty, we use the classical definition of the transfer number to find one of the variables involved say, $L_v$ in our case and then use this value to estimate the burning rate of our system.

After going through the above exercise, the results for a range of transfer numbers were found out and plotted for comparison in Fig. 4.6. We can observe that even though the developed model physically overestimates the burning rate, it captures the trend of the mass burning rate. It will also be to see through the numerical solution in the next chapter that the flame structure of our model boils down to the classical case if we compare our fuel consumption layer with the flame zone of the known one-step droplet solution.
Chapter 5

Results and Discussion

In this section, we will use numerical methods to discuss the results of applying an external electric field across the droplet since addition of the electric field terms in the system makes solving it analytically difficult. The effects of this external electric field will be discussed in two limiting regimes:

- **Strong Field Limit:** In this limit the externally applied field will be presumed to be strong enough such that there is almost no effect of the internal charge distribution due to the ionic species on it.

- **Weak Field Limit:** In this limit the internal charge redistribution will be considered to be at least of the order of the externally applied field.

Before we proceed further, we need to explain the means by which the above two limits are achieved. In our model, the strong/weak limits are based on a comparison of whether the internal charge distribution due to the ionic species is strong enough to effect the external field distribution or not. If we look at the Poisson’s equation eq (4.1.1),

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \phi}{\partial r} \right) = -\alpha_p (Y_p - X_n) \rho
\]

We notice that the magnitude of the parameter \( \alpha_p \) defines the impact of the internal field on the externally applied field. Consider the following two cases:

1. If \( \alpha_p \to 0 \), the above equation points out that the internal field isn’t strong enough to effect the external one. In other words, the external field is relatively stronger. Numerically, we take this limit by substituting \( \alpha_p = 0 \).

2. If \( \alpha_p \to \infty \), the above equation points that the both the ionic species are proportional and the field distribution will need to be calculated from the species equations. In other words, if we take \( \alpha_p \) to be a large number, then the Poisson’s equation can be interpreted to be in the limit of a weak external field such that the internal field can affect it significantly. Numerically, we take this limit
by substituting $\alpha_p \rightarrow 10^5$, where the large number is estimated from non-dimensional estimates and numerical experimentation.

3. Care must be taken while interpreting these two limits. These limits primarily establish a link between the externally applied field and the internal field due to the ionic species. Going from the weak field to the strong field limit doesn’t indicate that the state has been achieved by only strengthening the external field. All it entails is making changes to the system such that there is no effect of the internal field on the external one. Comparison of these two limits becomes necessary because they define the effective charge at any point in the field. And, since the Ionic Wind and the negative work done by the external field depend only on the effective charge at each system in the field, therefore having knowledge of the behaviour of the system in these extreme limits can shed light on the impact of the aforementioned body force effects.

At this stage, it is worthwhile mentioning that a closer look of the governing equations will show us that our system is symmetric w.r.t the applied potential. What that means is that if we apply a negative potential at the droplet surface in contrast to a positive, there will be almost no change in our solution. This is so because when we change the sign of the potential, due to our assumption of unity Lewis numbers and molecular ratios and also equal mobilities, the positive and negative ions merely switch places. Also, since wherever the electric field terms occur in our equations, they are accompanied by the difference of the mass fractions of the ionic species, the resulting effect is that the system becomes exactly symmetric. Practically however, since in a large number of situations the electrons form the majority of the negative charge carriers, therefore given the departure of the Lewis numbers, molecular ratios and electrical mobilities, the flame starts to behave differently depending upon the sign of the applied potential.

5.1 Numerical Methodology

In order to solve the system of equations with the application of an external field at steady state, a time relaxation finite difference code was written. A 4th order explicit central difference scheme was used for spatial calculations with a 4th order forward/backward scheme at the leftmost and rightmost boundaries respectively. The discretization used is shown below with the nomenclature that $r_1$ is the leftmost point and $r_2$ is the rightmost point of the mesh :-

1. Left edge for the first point :

$$\left( \frac{\partial f}{\partial r} \right)_{r_1} = \frac{-3f_{r_1+4} + 16f_{r_1+3} - 36f_{r_1+2} + 48f_{r_1+1} - 25f_{r_1}}{12\Delta r}$$
2. **Left edge for the second point:**
\[
\left( \frac{\partial f}{\partial r} \right)_{r_{1+1}} = \frac{-3f_{r_1} - 10f_{r_1+1} + 18f_{r_1+2} - 6f_{r_1+3} + f_{r_1+4}}{12\Delta r}
\]

3. **Central region:** For \(i = r_1 + 2\) to \(r_2 - 2\),
\[
\left( \frac{\partial f}{\partial r} \right)_i = \frac{-f_{i+2} + 8f_{i-1} + f_{i-2}}{12\Delta r}
\]

4. **Right edge for the penultimate point:**
\[
\left( \frac{\partial f}{\partial r} \right)_{r_2-1} = \frac{-3* f_{r_2} - 10f_{r_2-1} + 18f_{r_2-2} - 6f_{r_2-3} + f_{r_2-4}}{12\Delta r}
\]

5. **Right edge for the last point:**
\[
\left( \frac{\partial f}{\partial r} \right)_{r_2} = \frac{-3f_{r_2-4} + 16f_{r_2-3} - 36f_{r_2-2} + 48f_{r_2-1} - 25f_{r_2}}{12\Delta r}
\]

As far as the time relaxation scheme is concerned, we used an explicit 4th order Runge-Kutta method to integrate in time for achieving the steady state. For the calculation of the results, a grid spacing of \(\Delta r = 0.2\) was used with \(\Delta t = 10^{-4}\). The grid spacing conforms with the approximate width of the consumption layer in the system which was approximately \(O(\epsilon) \approx 0.1\) (\(\delta\) was taken to be 0.5). The convergence criteria was based on a tolerance percentage of 0.5%. The way this tolerance was executed is shown below:

- Since, the time step size taken was \(10^{-4}\), therefore it is logical to reason that our non-dimensional time based on the diffusion time scale would ideally change by \(O(1)\) in \(10^4\) iterations or one physical unit of time.
- Therefore, every \(10^4\) iterations, we compare the answer of say the temperature array with that of its previous value \(10^4\) iterations back.
- We then find the percentage change of this array and choose the maximum of the absolute value of the percentage changes at each grid point as the maximum error value for that entire array.
- The process is repeated for all the arrays being calculated in the system and each of their maximum errors is noted.
- Once we have these values, the maximum amongst this array of errors is selected and the convergence criteria is set to have this final error as less than our prescribed tolerance percentage, which was 0.5% in our case.
5.2 Weak Field Limit

This limit is applicable when the internal field due to the ionic species is sufficiently large in magnitude to effect the externally applied electric field. The results presented in this section are for a large value of $\alpha_p \rightarrow 10^5$. In this limit, it is interesting to see how would all the species and temperature profiles along with the mass burning rate vary if we were to increase the magnitude to the electric field. This increase is achieved in the weak field limit by fixing $\alpha_p$ and varying $\eta$ and $\chi$. Since, $\chi$ can be related to $\eta$ by a group of known constants, therefore for the following study, we only varied $\eta$ independently. To do this we assume that both the ionic species have the same mobilities and molecular weights. Therefore, this gives us that:

- $\eta_p = \eta_n$

Given these additional assumptions, Figs. 5.1 - 5.12 show the effect of increasing external field in the weak field limit.

We will now try to explain the above results:

1. As can be seen Fig. 5.1, the mass burning rate increases quite appreciably as the field strengthens. To
Figure 5.2: Variation of $\phi$ in the weak field limit

Figure 5.3: Variation of $T$ in the weak field limit
Figure 5.4: Variation of $Y_\rho$ in the weak field limit

Figure 5.5: Variation of $Y_\sigma$ in the weak field limit
Figure 5.6: Variation of $Y_{x_2}$ in the weak field limit

Figure 5.7: Variation of $Y_{x_1}$ in the weak field limit
Figure 5.8: Variation of $Y_p$ in the weak field limit

Figure 5.9: Variation of $X_n$ in the weak field limit
Figure 5.10: Variation of $Y_p$ and $X_n$ in the weak field limit for $\eta = 2.0$

Figure 5.11: Variation of $w_1$ in the weak field limit
deduce the reason for this, let us reconsider eq 4.3.8:

\[
\frac{M \partial T}{r^2 \partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) = \chi_p \left( \frac{\partial \phi}{\partial r} \right)^2 \rho \left( \eta_p Y_p + \eta_n X_n \right) + \chi_p \left( \frac{\partial \phi}{\partial r} \right) \rho \left( \frac{\partial Y_p}{\partial r} - \frac{\partial X_n}{\partial r} \right)
\]

The energy equations involves two terms, the first which “pushes” the ions in the same direction as that of their drift velocity and thus does positive work on the system. This term behaves as a heat source. The second term applies electrostatic force on the ions which may perform positive or negative work on the system. This term is seen to generally behave as a heat sink. It is the balance between these two terms which determines the net effect on the system. Looking at Fig 5.1, we can safely conclude that the net effect of the electric field is to act as a heat source for the system, which thereby increases the mass burning rate.

2. Another effect of the increase in the mass burning rate is the increase in the flame position. This is clear from eq (4.7.11),

\[
r_f = \frac{M}{\ln (1 + Y_{O\infty}/\nu)}
\]

The flame position was defined as the point of maximum reaction rate of the fuel consumption step (Step I). The shift in the reaction layers can be seen is Figs. 5.11 and 5.12.
3. The change in flame position accounts for the changes in the profiles for temperature, fuel, oxidizer and the neutral radicals. It is observed that the flame temperature (defined as the maximum temperature of the system) stays almost constant. The slight change observed is of the same order as the system tolerance and therefore cannot be considered. What this indicates physically is that the most basic effect of the electric field is to change the fuel burning rate. Though this field interacts with the ions and therefore impacts the chemistry in the flame, but it effectively doesn’t change the thermodynamics of the system and therefore the flame temperature observed remains approximately the same.

4. If we now look at Fig. 5.2, we see an appreciable change in the field because the internal field resulting from the charge distribution of the ionic species is strong enough to effect the external field.

5. As far as the ionic species are concerned, if we look closely at Fig. 5.10, we will notice that there is barely any difference in the mass fractions of the positive and negative ions for a given value of $\eta$. Now, the reason we see a change in their individual mass fractions with $\eta$, but not on a relative scale is because when we vary $\eta$, the mass burning rate changes. So, not only is the flame position changing but there is also an effect of the drift velocity on the ions. However, this effect which by definition is opposite between positive and negative ions is very weak for a given value of $\eta$ due to the weak field limit and thus the ionic species appear to be almost indistinguishable.

6. Given the above explanations, we can infer that for the weak electric field limit, all of the effect of the field is limited to a heat source term in the energy equation which increases mass burning rate and flame position.

5.3 Strong Field Limit

This is described as the limit when the external electric field is too strong as compared to the internal field arising from the ionic species. The results presented in this section are achieved by taking the the value of $\alpha_p \rightarrow 0$. Similar to the previous section, we will try and understand how the system gets effected if we increase the strength of the external field, which is achieved by increasing $\eta$ and $\chi$. As mentioned before, $\chi$ can be related to $\eta$ by a group of known constants; therefore for the following study, we only varied $\eta$ independently. We will again assume equal mobilities and molecular weights for the ions. Figs. 5.13 - 5.24 depict the result of the increasing field in this limit :-

We will now try to explain the above results and point out the differences with respect to the previous section :-
Figure 5.13: Variation of $M$ in the strong field limit

Figure 5.14: Variation of $\phi$ in the strong field limit
Figure 5.15: Variation of $T$ in the strong field limit

Figure 5.16: Variation of $Y_F$ in the strong field limit
Figure 5.17: Variation of $Y_o$ in the strong field limit

Figure 5.18: Variation of $Y_{x_2}$ in the strong field limit
Figure 5.19: Variation of $Y_{X_1}$ in the strong field limit

Figure 5.20: Variation of $Y_p$ in the strong field limit
Figure 5.21: Variation of $X_n$ in the strong field limit

Figure 5.22: Variation of $Y_p$ and $X_n$ in the strong field limit for $\eta = 2.0$
Figure 5.23: Variation of $w_1$ in the strong field limit

Figure 5.24: Variation of $w_3$ in the strong field limit
1. Similar to the weak field limit, the mass burning rate again increases due to the net effect of a heat source in the energy equation. The increase as will be shown later to be almost similar to the previous case. Initially, one may expect that since the heat sink term is dependant upon the electric field, therefore in the strong field limit, the overall effect may be negative. However, since the source is also dependant upon the square of the field, the net effect still remains that of a positive work.

2. Again, the increase in the mass burning rate leads to an increase in the flame position as seen from Figs. 5.23 and 5.24.

3. The change in flame position accounts for the changes in the profiles for temperature, fuel, oxidizer and the neutral radicals. Similar to before, it is observed that the flame temperature stays almost constant.

4. If we look at Fig. 5.14, we now see no change in the field because in this limit the value of $\alpha \to 0$ signifies that the external field is too strong to be effected by the internal electric field.

5. Coming to the ionic species, if we look closely at Fig. 5.22, we will now notice that there is an appreciable difference in the mass fractions of the positive and negative ions for a given value of $\eta$. This is so because for a strong field, the effect of the drift velocity is now appreciable enough to cause a substantial relative change between the positive and negative ions. As was described before, if we examine eq (2.2.5), we can see that the electric field on one hand strengthens the diffusive flux for negative ions; whereas on the other hand it weakens it for the positive ions. As a result, the negative ions diffuse out more strongly once they are produced at the flame as compared to the positive ions. It can also be seen that near the boundary, the positive ions would logically feel a repulsive force due to the positive potential applied, due to which we observe a higher fraction of negative ions present near the droplet surface. The reason for the change in the individual profiles as well in this case is that due to our application of the strong field limit, not only does the flame position change, but now the effect of the drift velocity also becomes appreciable.

5.4 Comparison of the two limits

This section essentially aims to summarize our previous observations about the similarities and differences between the two limiting cases of a very strong and a very weak field. This is done by comparing the calculated quantities at the two limits for $\eta \to 2.0$ in Figs. 5.25 - 5.32.

We conclude from these graphs that :-
Figure 5.25: Variation of $M$ in the two limiting cases

Figure 5.26: Variation of $T$ in the two limiting cases
Figure 5.27: Variation of $Y_F$ in the two limiting cases

Figure 5.28: Variation of $Y_O$ in the two limiting cases
Figure 5.29: Variation of $Y_{X_2}$ in the two limiting cases

Figure 5.30: Variation of $Y_{X_1}$ in the two limiting cases
Figure 5.31: Variation of $Y_p$ in the two limiting cases

Figure 5.32: Variation of $X_n$ in the two limiting cases
• The mass burning rate behaves in almost the same way between the two limiting cases. The primary reason for not observing a higher or a lower value for a stronger field is that the increased heat provided by the heat source term in the energy equation is in this case now balanced by the larger loss due to the negative work done on the system.

• Due to the similarity in the mass burning rate, the flame position also remains nearly same. The result is that there is a negligible change in the profiles of the neutral species.

• The only substantial change is observed in the case of the ionic species because in the strong field limit, the contribution of the drift velocity becomes appreciable to cause a noticeable change in the charge distribution.
Chapter 6

Conclusions and Future Work

The effect of an externally applied electric field on a diffusion flame in the single droplet configuration was studied. A 3-step reduced kinetic mechanism was proposed to study the effect of the charged species on the combustion characteristics. For the same, large activation energy asymptotics were used to investigate the flame structure of the system. A spherically symmetric configuration was applied because in such a condition, the body force effects on the pressure field only played a passive role in the system. As a result of this, the most basic effects of the external field could be investigated.

The system of equations in the model were solved analytically in the absence of the electric field. By comparing the trend of the mass burning rate with the transfer number and the flame structure for the new model with the classical droplet solution, it was observed that the proposed chemical model was able to capture the physics of the classical solution. To examine the effects of the external electric field, two distinguished limits were concerned, the weak and strong field limits. These limits primarily differentiated the two extreme states of the system when the internal field due to the charged species was able to effect the external field (weak field limit) and when it wasn’t (strong field limit). The summary of the observations is as follows:

1. The electric field acts to strengthen the diffusive flux for negative ions and weaken for positive ions.

2. The primary effect of the electric field on the system was to increase the mass burning rate and shift the flame position without effecting the thermodynamics of the flame, since the maximum flame temperature stayed approximately constant.

3. These major effects were caused through the two body force terms in energy equation. The net effect of these Ohmic Heating terms was that of a net heat source which made the fuel burn faster. Contrary to the literature, ignoring this body force term limited the effect of the field on charge redistribution and removed its impact on the flame position or the mass burning rate.

4. The trend of the increasing mass burning rate stayed almost the same under both the weak and strong field limits. The main reason proposed for this was that with increase in the external field, both the
heat source and heat sink terms in the Ohmic Heating increased proportionately making the relative effect on the system to be the same.

The work done in this study represents the effect of the electric field on a very simplified system. It was established that for droplet diffusion flames, Ohmic Heating is crucial for the observed effects. There have been very few studies on droplet diffusion flames documenting the effect on the mass burning rate. Ueda et.al [14] and Yamashita et.al. [17] experimentally observed an increase in the burning rate constant with increasing positive voltage in a microgravity environment. The authors used the concept of an induced velocity due to the electric field to explain these effects. Anderson et.al. [18] also conducted experiments on droplets under a normal gravity environment and observed an increase in the burning rate constant for negative voltages and a decrease for positive voltages. Yamashita et.al. [17] performed a simulation for the droplet diffusion flame based on their experiments and again observed an increase in the burning rate constant. However, the authors only considered the effects of the Ionic Wind in their calculation and ignored any Ohmic Heating. Though there may be a general trend of observing an increase in the burning rate with applied potential in literature (reversed for [18]), the large variation in the experimental conditions and problem formulation makes it difficult to compare these observations directly with the work done here. Therefore, before further investigations are carried out with a more detailed kinetic mechanism, it may be useful to look at some of the following suggestions to further our understanding of this system :-

1. It would be interesting to get an analytical answer for the system at least in some distinguished limit to understand how the external field affects the flame.

2. Since unity Lewis numbers, ionic mobilities and molecular ratios were assumed, therefore the present system behaved symmetrically with regards to the polarity of the field. The next step may be to assume electrons as the major negative charge carriers at least for moderate fields and then see how the polarity of the field now affects the flame.

3. So far the pressure field only played a passive role in the system, therefore it was not possible to actively study flame stabilization due to the Ionic Wind as has been observed in literature. So, the next step maybe to perturb the flame thereby removing the constraint of the spherically symmetric system and investigate how the electric field stabilizes or destabilizes it. It will also be curious to see whether the Ionic Wind counteracts or strengthens the effect of Ohmic Heating in such a condition.

4. It is also seen that the effects of the external field are significantly affected if the presence of soot is considered [14], with the soot behaving like a cloud of charged particles. Therefore, it will be of interest
to artificially introduce soot or additional charged particles in the flame zone and see how the flame might behave in such a situation.
References


