Investigations of the Effects of Flame Configuration on the Combustion of Laminar Diffusion Flame

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INVESTIGATIONS OF THE EFFECTS OF FLAME CONFIGURATION ON
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LIST OF SYMBOLS AND ACRONYMS

\( r \) \quad \text{Radial coordinate}

\( z \) \quad \text{Axial coordinate}

\( a \) \quad \text{Oxygen reaction order}

\( \rho \) \quad \text{Density (kg/m}\(^3\))

\( \mu \) \quad \text{Viscosity}

\( \lambda \) \quad \text{Thermal conductivity}

\( \epsilon \) \quad \text{Emissivity}

\( T \) \quad \text{Temperature (K)}

\( M \) \quad \text{Molecular weight}

\( S \) \quad \text{Source term}

\( T_d \) \quad \text{Adiabatic flame temperature (K)}

\( R_u \) \quad \text{Universal gas constant}

\( H \) \quad \text{Flame height (m)}

\( W \) \quad \text{Flame width (m)}

\( R \) \quad \text{Radius (m)}

\( D \) \quad \text{Diameter (m)}

\( P \) \quad \text{Pressure (Pa)}

\( R_e \) \quad \text{Reynolds number}

\( v_r \) \quad \text{Radial velocity component}

\( v_x \) \quad \text{Axial velocity component}

\( C_p \) \quad \text{Heat capacity}

\([x_i]\) \quad \text{Molar concentration of specie i}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_i$</td>
<td>Mole fraction of species i</td>
</tr>
<tr>
<td>$h_i$</td>
<td>Specific enthalpy of species i</td>
</tr>
<tr>
<td>$Y_i$</td>
<td>Mole fraction of species i</td>
</tr>
<tr>
<td>$\omega_i$</td>
<td>Rate of appearance or disappearance of species due to reaction</td>
</tr>
<tr>
<td>$k_f$</td>
<td>Forward reaction coefficient</td>
</tr>
<tr>
<td>$k_r$</td>
<td>Reverse reaction coefficient</td>
</tr>
<tr>
<td>$k_{pr}$</td>
<td>Reaction constant</td>
</tr>
<tr>
<td>$k_G$</td>
<td>Global rate coefficient</td>
</tr>
<tr>
<td>$E_a$</td>
<td>Activation energy</td>
</tr>
<tr>
<td>$f_v$</td>
<td>Soot volume fraction</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal conductivity</td>
</tr>
<tr>
<td>$N$</td>
<td>Soot particle number density</td>
</tr>
<tr>
<td>sccm</td>
<td>Standard cubic center per minute</td>
</tr>
<tr>
<td>DIDF</td>
<td>Double inverse diffusion flame</td>
</tr>
<tr>
<td>DNDF</td>
<td>Double normal diffusion flame</td>
</tr>
<tr>
<td>NDF</td>
<td>Normal diffusion flame</td>
</tr>
<tr>
<td>IDF</td>
<td>Inverse diffusion flame</td>
</tr>
<tr>
<td>NO</td>
<td>Nitric oxide</td>
</tr>
<tr>
<td>PAH</td>
<td>Polycyclic aromatic hydrocarbons.</td>
</tr>
<tr>
<td>PO</td>
<td>Primary oxygen</td>
</tr>
<tr>
<td>SO</td>
<td>Secondary oxygen</td>
</tr>
<tr>
<td>SIMPLE</td>
<td>Semi-implicit method for pressure-linked equations</td>
</tr>
</tbody>
</table>
ABSTRACT

Motivation and objective to study double inverse diffusion flame is introduced, followed by the literature survey on soot formation in inverse diffusion flame (IDF), application of the unique structure of double inverse diffusion flame (DIDF), radiation effects on DIDF, factors that affect the formation of nitric oxide and effects of elevated pressure on diffusion flames.

Numerical method is validated by the result of flame height for IDF, which is consistent with result from previous research. In present work, two DIDF burner configurations with different size are used to conduct the simulation. Ethylene is used as the fuel. For each of the burner, three different flow rates of fuel are applied. By comparing the simulation result from DIDF burner with that from normal diffusion flame (NDF) burner, it is found that with the same flow rate of fuel, DIDF always produces less soot and nitric oxide (NO) than NDF does. The conclusion is drawn that DIDF burner configuration leads to less pollution than NDF burner configuration does. And this result is independent on the size of the burner.

Factors that affect DIDF flame are also investigated. Flame radiation, including soot radiation and gas radiation, leads to decreased flame temperature, decreased soot and NO formation. Preheating of primary air in DIDF results in more NO formation because flame temperature becomes higher. Elevated operating pressure has great effect on DIDF too. When the operation pressure is elevated, narrower flame is formed; more soot and more NO are produced. Diluted fuel by nitrogen can result in less soot and NO formation, which can help to reduce pollution.

As for NO formation in DIDF, there are two mechanisms in present work: thermal mechanism and prompt mechanism. It is found that thermal NO and prompt NO forms at different positions in DIDF and thermal NO is dominated compared with prompt NO.
CHAPTER 1. INTRODUCTION

1.1 Study Motivation

Flames are widely used in daily life, commercial and industrial instruments, such as ovens, candles, heaters and different type of burners for energy conversion application as well as flame reactors for material synthesis. Most of the time, it is impossible for the combustion to be complete. Besides the main reaction products during the process of combustion, there is always side product. Some of these side products, for example, nitric oxide and soot are considered as pollutant. The formation of the pollutant can lower the efficiency of the combustion, which is the reason to decrease the amount of pollutant. Another problem is that both nitric oxide and soot are harmful to human’s health and can damage the environment.

To decrease the pollution, a lot of research has been done to study the formation mechanisms of the pollutant and to find methods to decrease its formation. However, more effective method to decrease pollutant in the flame is required. The motivation to do this research is to find effective way to increase the combustion efficiency and decrease pollution in a flame. Until now, most research focus on normal diffusion flame. In present work, different burner configuration is studied: double inverse diffusion flame. The advantage of this kind of burner configuration is investigated by comparing with normal diffusion flame.

1.2 Research Objective

Numerical simulations are conducted to study laminar double inverse diffusion flame. The objective of present research is to find method to reduce the formation of pollutant, such as soot and nitric oxide, by studying the properties of laminar double inverse diffusion flame, including flame structure, flame temperature, flame shape, soot formation and nitric oxide formation mechanisms. Finite volume method is used. To verify the advantage of the burner configuration
of double inverse diffusion flame, simulation result for double inverse diffusion flame will be compared with that for normal diffusion flame with the same mass flow rate of fuel. Fuel in this research is ethylene.

Mass flow rate effect on double inverse diffusion flame will be studied too. Effect of burner scale on double inverse diffusion flame is also investigated to study the dimension dependence of the burner configuration.

Formation mechanism of nitric oxide in double inverse diffusion flame is also one of the objectives. Present research mainly focuses on thermal mechanism and prompt mechanism. Present research result will compare the formation position and relative importance of these two mechanisms.

Objective of this research also includes the investigation of the factors that affect the double inverse diffusion flame: flame radiation effect on temperature, soot and nitric oxide formation; elevated operation pressure effect on flame shape and pollutant formation; effect of preheating of the primary air and the dilution of the fuel on the flames.

1.3 Laminar Diffusion Flame

According to the Reynolds number, flame can be divided into laminar flame and turbulent flame. Although most flames in practical applications are turbulent, laminar flame is of importance by providing basic and necessary prerequisite to study turbulent flame. Investigation of laminar flame structure, flame height, luminosity, species distribution, stability and soot formation pave the way to study turbulent flames.

Flames are classified as premixed flames and diffusion flames. In premixed flame, fuel and oxidizer are premixed before ignition. As for diffusion flame, reaction occurs at the interface where oxygen and fuel meets. Both premixed flame and diffusion flame have their own
advantages respectively. A comparison is summarized in Table 1.1 by previous research [3].

Table 1.1 Main differences between premixed flames and diffusion flames [3]

<table>
<thead>
<tr>
<th>Premixed flames</th>
<th>Diffusion flames</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Premixed nature of the fuel and air promotes rapid combustion, with a short, easily controlled flame for laboratory purposes facilitating use of wide variety of fuels.</td>
<td>As the flame length is inversely proportional to the stoichiometric fuel mass fraction, i.e. only fuels, which requires less air for complete combustion, produce shorter flames, hence limiting the use of fuels.</td>
</tr>
<tr>
<td>2. Easily adjustable stoichiometry of the reacting gases and hence the flame chemical compositions.</td>
<td>Chemistry of diffusion flames cannot be described by a single equivalence ratio.</td>
</tr>
<tr>
<td>3. Dilution of the premixed gases with an inert gas is not required, as the soot produced in premixed flames is less when compared to diffusion flames.</td>
<td>Dilution of fuel stream with inert gas is critical to nanotube synthesis as absence of inert gas resulted in soot formation and the complete encapsulation of the metal nanoparticles with no nanotubes [8].</td>
</tr>
<tr>
<td>4. They are not diffusion limited hence the reactive gas profile can be made uniform by the burner system [7].</td>
<td>Mixing of gases is limited to diffusion.</td>
</tr>
<tr>
<td>5. Less safe as there is scope for detonation.</td>
<td>No such problem.</td>
</tr>
<tr>
<td>6. Premixed flames sustain the growth of particles under a wide range of conditions (fuel, stoichiometry, temperature) producing a wide variety of particles.</td>
<td>Diffusion flames are less flexible, but allow a faster growth and a better control on the final product as the particles can be removed from the fuel side of the flame, thus preventing undesired oxidation with air [9].</td>
</tr>
</tbody>
</table>

In diffusion flames, fuel and oxidizer are not premixed well and it is possible that there is not sufficient oxidizer for the combustion process to be complete, which makes it much easier for the diffusion flame to produce more soot than premixed flame. Soot is the product of incomplete reaction and one kind of pollution to the environment, resulting in low energy
efficiency and high pollutants emission. Thus, there exists a need to study soot formation in the diffusion flame and develop effective means to increase the energy efficiency and decrease pollutants emission. The present study focuses on different types of laminar diffusion flame in order to investigate the flame temperature distribution, flame height, luminosity, species distribution and soot formation.

In particular, the following configurations of laminar diffusion flames are studied: (a) normal diffusion flame, (b) inverse diffusion flame, (c) double inverse diffusion flame.

1.4 Coflow Diffusion Flame

In this section the formation of soot in coflow diffusion flame is investigated. According to the relative position of fuel and oxidizer, diffusion flame can be classified as normal diffusion flame and inverse diffusion flame. This is displayed in the figures below.

A probe is usually placed into the center of the flame while collecting soot particles in NDF, which is very likely to disturb the flame. Another method is to collect samples after the soot has passed through the oxidation zone. It is easy to collect soot samples in IDF, since soot forms on the outside of the IDF, avoiding passing through the high temperature reaction zone. IDF provides a more convenient way to study soot inception and growth and the formation of soot precursors [4].

Figure 1.1 Schematic diagrams of (a) normal diffusion flame and (b) inverse diffusion flame
In Figure 1.1, the position of fuel and air is opposite for normal diffusion flame and inverse diffusion flame. Inverse diffusion flame burning in atmospheric environment, as shown in Figure 1.2, will lead to the formation of DIDF: one inner flame and one outer flame.

Different selections of shroud gas in IDF can achieve different aims. Shroud air helps to display and study the interaction of inner flame and outer flame. While nitrogen environment can prevent the formation of double flame and help to study the soot formation as mentioned above. Nitrogen is not the only choice, but nitrogen is of low cost and not harmful when compared with other inert gas such as argon [4].

Present research focuses on flame structure, soot and NO formation in laminar double inverse diffusion flame.

1.5 NO Formation Mechanism

Nitric oxide is one kind of pollution produced in the burning process. Since NO would cause acid rain and ozone depletion, it is important to understand the formation mechanism of NO in improving current burner configuration and designing new kind of burner configuration. There are mainly four processes to produce NO: Thermal NO formation, Prompt NO formation, Fuel NO formation and NO formation by reburning.

Thermal mechanism is also named Zeldovich mechanism. Thermal NO is formed when nitrogen of air is oxidized. Thermal NO is highly dependent on temperature. The amount of
thermal NO will increase when flame temperature increases [11] [53].

The thermal mechanism consists of two chain reactions:

\[ O + N_2 \leftrightarrow NO + N \]  \hspace{1cm} (1.1)

\[ N + O_2 \leftrightarrow NO + O \]  \hspace{1cm} (1.2)

Which can be extended by adding the following reaction:

\[ N + OH \leftrightarrow NO + H \]  \hspace{1cm} (1.3)

Reaction rate for these three equations are evaluated by Hanson and Salimian [1] and will not be listed here in detail. Equations 1.1 to 1.10 are from Fluent tutorial [53]. More details can be found in this tutorial.

Thermal mechanism with the Quasi-Steady Assumption for [N].

\[
\frac{d[NO]}{dt} = 2k_{f,1}[O][N_2]^{1/2} \frac{1 - k_{r,1}k_{r,2}[NO]^2}{k_{f,1}[N_2]k_{f,2}[O_2]^{1/2}} \frac{\text{g/mol}}{m^3.s} \]  \hspace{1cm} (1.4)

Use equilibrium method to determine [O],

\[ [O] = 3.97 \times 10^5 T^{-1}[O_2]^{1/2} e^{-31090/T} \frac{\text{g/mol}}{m^3} \]  \hspace{1cm} (1.5)

The following equation is used to determine [OH],

\[ [OH] = 2.219 \times 10^2 T^{-0.57} e^{-4595/T} [O]^{1/2} [H_2O]^{1/2} \frac{\text{g/mol}}{m^3} \]  \hspace{1cm} (1.6)

To summary:

\[ S_{thermal,NO} = M_{W,NO} \frac{d[NO]}{dt} \]  \hspace{1cm} (1.7)

Prompt mechanism, which is also named Fenimore mechanism [63], is related to the combustion chemistry of hydrocarbons. Prompt NO always forms under the conditions of low temperature and fuel rich place. Prompt NOx (flame generated NOx) forms at the flame front due to high speed reactions [53].
Prompt mechanism:

\[
\frac{d[NO]}{dt} = k_{pr}[O_2]^a[N_2][FUEL]e^{\frac{E_a}{R_u T}}(kmol/m^3\cdot s) \tag{1.8}
\]

For C\(_2\)H\(_4\) (ethylene)-air flames,

\[
k_{pr} = 1.2 \times 10^7 (R_u T/P)^{a+1} \tag{1.9}
\]

\[
E_a = 251151 J/gmol \tag{1.10}
\]

In these equation,

\(d[NO]/dt\) is the rate of formation of NO

\([NO], [O], [N_2], [OH], [O_2], [H_2O], [FUEL]\) signifies concentration of NO, O, N\(_2\), OH, O\(_2\), H\(_2\)O and fuel respectively. All concentrations have units of gmol/m\(^3\).

\(k_{f,1}, k_{f,2}, k_{f,3}\), are the forward rate constants

\(k_{r,1}, k_{r,2}, k_{r,3}\), are the reverse rate constants

\(M_{w,NO}\) is the molecular weight of NO(kg/gmol)

\(S_{\text{thermal,NO}}\) is the source term of NO

\(a\) is the oxygen reaction order

\(E_a\) is the activation energy

\(k_{pr}\) is reaction constant

\(R_u\) is universal gas constant

\(T\) is temperature

\(P\) is pressure

In present work, for double inverse diffusion flame, only thermal mechanism and prompt mechanism for NO formation will be studied.

Flame radiation is also important in investigation the combustion process. This subject will be discussed in next section.
1.6 Flame Radiation

In burning flame, there is heat transfer, including heat conduction, convective heat transfer and heat loss by flame radiation. Radiation is one way of heat transfer modes and is transmitted in the form of electromagnetic waves.

As for flame radiation, two parts need to be considered: soot radiation and radiation from gases.

a. Emission of the soot particles. Although all materials at any temperature can emit radiation energy, when the temperature is relatively low, such as 300K, the radiation energy can be ignored. However, burning flames are often of high temperature, soot particles in the flame can significantly influence the flame structure because of the radiation heat loss.

b. Emission of the gases

Different molecules can absorb energy in certain frequencies because of their ability to change shape and move to different energy states. Due to different molecular structures, the emission of gases must be considered separately.

Of the gases commonly present in a fire, only carbon dioxide (CO\textsubscript{2}) and water vapor (H\textsubscript{2}O), which have three atoms in one molecule, contribute to the emissivity. Oxygen and nitrogen (O\textsubscript{2} and N\textsubscript{2}) consisting of symmetrical molecules have negligible radiation power, emitting and absorbing radiation only at much higher temperatures.

Furthermore, solid black bodies and gray bodies radiate in all wavelength, while gases only radiate in select narrow bands. For black body emission, when the temperature increases, the total radiation energy emitted will increase, whereas when the temperature of the emitter decreases the total emitted energy will decrease. For gas radiation, such as CO\textsubscript{2} and H\textsubscript{2}O, shown
in the following figure, gas only emits energy in certain bands.

Figure 1.3 Example of CO$_2$ and H$_2$O absorption spectrum [6]

In this chapter, burner configuration of double inverse diffusion flame is introduced. Formation mechanism of nitric oxide and flame radiation is also explained briefly. Literature survey will be done in the following chapter.
CHAPTER 2. LITERATURE SURVEY

2.1 Soot Formation on Inverse Diffusion Flame

A significant number of investigations have been carried out on normal diffusion flame [59, 60, 61]. Thus in this work the focus is the inverse diffusion flame, especially as pertains to soot formation in such flames. Several studies have been performed in this type of flames [14, 17, 18]. Representative results are briefly introduced here.

The structure of laminar inverse diffusion flames of methane and ethylene was studied by Mikofski [14]. In this investigation, several flames of the same fuel flow-rate with various air flow-rates were examined. It is found that increased air flow rates resulted in longer flames while flame heights determined from visible images were overestimated; soot is present on the fuel side of the flame in the fuel rich region and located closer to the reaction zone than Polycyclic aromatic hydrocarbons (PAH).

The effects of oxygen enhancement on normal and inverse laminar jet diffusion flames was studied by Sunderland et.al. [15], concluding that oxygen-enhanced conditions can increase flame luminosity, soot formation for both normal and inverse flames. Experimental measurements of flame structure and soot characteristics for ethene inverse diffusion flames were performed by Lee et.al. [16]. They found that ethene inverse diffusion flames were more stable at small flow rates when compared with methane inverse diffusion flames; radial distribution of the PAHs and soot was similar for both inverse diffusion flames and normal diffusion flames; soot growth became weak over the primary reaction zone defined by OH radical; calculated results of the flame height and shape qualitatively agreed well with an actual flame; soot inception occurred in the lower region in the diluted inverse diffusion flame with the temperature range of 1550–1600 K. Fuel dilution and temperature difference because of dilution
had a weak influence on soot inception; soot growth was influenced by residence time and temperature when the fuel was diluted with nitrogen while the temperature is not an effective parameter on soot growth.

Fourier Transform-InfraRed Spectroscopy and Proton Nuclear Magnetic Resonance characterization on the product of an ethylene inverse diffusion flame by Santamaría [17] suggested that soot formation process involves several general steps in both the gaseous phase and the condensed phase by providing useful information on the molecular structure of soot precursors. This work is of potential use to develop soot evolution model by considering the contribution of the aliphatic species or decomposition reactions by the experimental results presented.

Direct numerical simulations were conducted on normal diffusion flames and inverse diffusion flames of coflowing methane–air to study the effects of the fuel-to-air velocity ratio and the relative positions of the fuel and air streams on soot formation [18]. Aim of this work is to further explore the experimental phenomena to understand the effects of temperature and stoichiometry history on soot formation rates by numerically tracking the soot parcels along the path line that goes through the maximum sooting region. For normal diffusion flames, soot production increases when the fuel to oxidizer ratio increases because of the increase of residence time which allowed enhanced soot particle surface growth. If the fuel to oxidizer ratio is small, the particles are more quickly oxidized after reaching their peak soot volume fraction, which leads to lower soot production.

Figure 2.1 shows the significant differences in soot formation between normal and inverse diffusion flames while keeping the same fuel and air velocities, indicating that inverse flames produce much less soot than normal flames with the same fuel and air velocity. For example, the
peak soot volume fraction for normal diffusion flame is 6.2e-7, but it is only 3.6e-9 for inverse diffusion flame. That is the peak soot volume fraction is 172 times higher than in normal diffusion flames [18]. In the following Table, Normal 10/10 and Inverse 10/10 means that fuel and air has the same velocities: 10cm/s.

<table>
<thead>
<tr>
<th>Differences in Sooting Characteristics Between Normal and Inverse Diffusion Flames With Same Fuel and Air Velocities</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Normal 10/10</strong></td>
</tr>
<tr>
<td>Peak soot volume fraction</td>
</tr>
<tr>
<td>Peak soot number density (cm⁻³)</td>
</tr>
<tr>
<td>Total soot mass (g)</td>
</tr>
<tr>
<td>Peak mean particle diameter (nm)</td>
</tr>
<tr>
<td>Location of sooting region</td>
</tr>
<tr>
<td>Peak nucleation rate (g/cm³s)</td>
</tr>
<tr>
<td>Peak surface growth rate (g/cm³s)</td>
</tr>
<tr>
<td>Peak OH oxidation rate (g/cm³s)</td>
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<tr>
<td>Peak O₂ oxidation rate (g/cm³s)</td>
</tr>
<tr>
<td>Particle pathlines show that:</td>
</tr>
<tr>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Figure 2.1 Differences in sooting characteristics between normal and inverse diffusion flames with same fuel and air velocities. [18]

Dynamics of an inverse diffusion flame and its role in PAH and soot formation is studied by Katta et.al. [19]. This work is aimed to understand the chemical and physical structure of the soot which is proved to be partially carbonized.

Early soot from inverse diffusion flame is also studied by Linda G. Blevins et.al. [20], stating that soot particles collected in an IDF tip are large, stacked, plate-like particles which have clumped together and appear to be surrounded by liquid-like material when reaching the exhaust. It is also pointed out that a few ordered soot structures are present under the liquid like material. Results of this work provide information to study the soot inception and growth in
diffusion flames [20].

According to previous research mentioned above, although with different fuel types, the same conclusion was drawn about the advantage of inverse diffusion flame on soot formation. That is, soot is produced on the outside of the inverse diffusion flame without passing through the high temperature reaction zone. Such result provides a better platform to study soot formation in reverse diffusion flame than in normal diffusion flame.

The next section focuses on soot formation in inverse diffusion flame; however it is still necessary to study flame properties of double inverse diffusion flame, such as NO and soot formation, pressure effect, radiation effect, and flame shape.

2.2 Double Inverse Diffusion Flame

Schematic diagram of double inverse diffusion flame has been displayed in Figure 1.2 (a). One of the applications of the double inverse diffusion flame is the gasification of municipal solid waste (MSW), studied by Kwak et.al [21] using the double inverse diffusion flame (DIDF) burner and the double normal diffusion flame (DNDF) burner. These two burners and the inlets for fuel and air configurations are displayed in Figure 2.2 (a) and Figure 2.2 (b).

![Figure 2.2 Double inverse diffusion flame (DIDF) burner and the double normal diffusion flame (DNDF) burner [21]](image-url)
In this reference, gasification with the DIDF burner was determined to be more effective than that with the DNDF burner: The radiation heat and slag recovery rate of the DIDF burner are greater than that for the DNDF burner, while the generation of fly ash was less (0.76kg/h) in the DIDF burner than in the DNDF burner (1.36kg/h). That is, gasification with the DIDF burner which consumed less energy and with the production of a better-quality synthesis gas was more energy efficient than that with the DNDF burner.

Sobiesiaka and Wenzellb [22] studied this type of DIDF with natural gas by keeping the centerline fuel laminar and air jet in the turbulent flow regime and reported the following results: partial premixing exists in this non-premixed discharge configuration of reactants which developed into a well-mixed reaction zone on the flame centerline surrounded by an outer normal diffusion flame, resulting in the unique double-flame structure; the normalized length of the inverse flame are significantly influenced by the velocity ratio of the inner air jet and outer fuel; inverse flame stability is affected by the anchor laminar diffusion flame at the nozzle.

Since the research with respect to double inverse diffusion flame is rather limited because of its significant potential implications, further study is needed to better understand soot formation processes, temperature and species distribution, flame shape and flame stability.

In the following section, flame stability will be introduced.

2.3 Investigation on Flame Stability

Flame stability is of great importance in studying both normal diffusion flame and inverse diffusion flame. Prevent lifting, blowing off, flashback and explosion is necessary for safety reason and the pursuit of high efficiency of the flames. Some methods, such as pilot flames, oxygen-rich coflows, bluff bodies, and swirling flows have already been employed in flame stabilization. For example, Muñiz and Mungal [26] use pilot flames to stabilize laboratory scale
non-premixed flame, and Prakash et.al [27] use pilot flames to stabilize premixed flames.

Lift-off stability of hydrocarbon jet diffusion flames in coflowing air at earth gravity has been investigated by Takahashi and Katta [29]. In this work, the lifting limits of methane jet diffusion flames in coflowing air are measured, and then numerical simulations with a C3-chemistry model were performed, suggesting that the reaction kernel (reaction peak spot) keeps stationary combustion in the incoming flow by realizing the balance between the overall reaction time and the residence time. Reaction kernel was pushed inwardly and downstream when increasing the velocity of the coflowing air. When the standoff distance is increased, the reaction kernel broadened while the slopes of reaction kernel correlations decreased toward liftoff.

The following figure shows the measured stability limits, the critical mean jet velocity at the stability limit ($U_{jc}$) decreased as the mean co-flowing air velocity was increased.

![Figure 2.3 Stability limits of co-flowing jet diffusion flames [29]](image-url)
Quenching limits for inversed diffusion flame were measured by Yi and Peters [51]. In this reference, different burner diameters were used. The fuels are propane, ethylene and methane. It is found that the quenching limits of inverse flames scaled with the mole fraction of O$_2$ according to the relation $(X_{O2})^{-1.4}$. Another conclusion was that the quenching limit is independent of burner diameter and proportional to the fuel’s quenching distance in premixed tests.

Stability for inverse diffusion flame was also studied by M. A. Mikofski [42]. The figure below showed selected visible images of methane inverse diffusion flames with varied air flow. Low and high points in the flickering cycle were shown to demonstrate the degree of unsteadiness. It was observed that smaller flames appeared stable, and flickering was more evident in the larger flames.

![Figure 2.4 Visible images of selected methane inverse diffusion flame [42]](image)

Stability limits and behaviors of the inverse diffusion flame have been studied by Yoshimoto et. al [28]. It is found that the flame length of the laminar flame for the small diameter is determined by the air flow rate in the case of IDF as well as that of NDF. The air average velocity at the transition from the attached flame to the blow-off or lifting is much lower
than that of the normal diffusion flame. This is attributed to the fact that the upstream end of the diffusion flame is located at the air side. Consequently, the air velocity is sensitive to the flame stability.

Although jet diffusion flame has been studied extensively so far, flame stability mechanisms have not been fully explored and therefore more work is needed in this respect. Now, most of these studies about flame stability are done on normal diffusion flame with only very few are done on inverse diffusion flame.

NOx formation, as one kind of flame pollutants, needs to be investigated. In the next section factors that affect NOx formation in flames will be discussed.

2.4 Factors that Affect NOx Formation

Many factors can affect NOx formation in a flame. The effect of flame type, equivalence ratio, gas fuel type, preheating air, additives in the flame, and soot interaction on NOx formation are explained in detail.

2.4.1 Effect of Flame Type on NOx Formation: Premixed Flame and Diffusion Flame

In the following figure, NOx formation in premixed flame and diffusion flame is compared.

![Figure 2.5 NOx emissions measured for operation in diffusion and premixed mode [45]](image)

Figure 2.5 NOx emissions measured for operation in diffusion and premixed mode [45]
Work conducted by Petter E. Røkke and Johan E. Hustad [45] on a gas turbine combustor with the aim to investigate how different factors can influence the formation of NOx reported the results displayed in Figure 2.5. It is evident that diffusion flame is more likely to produce NOx than premixed flame. The reason for this conclusion is that there is always a flame surface with a stoichiometric fuel-air composition for diffusion flame. As such, the temperature at the flame surface is significantly higher than temperature in a premixed flame where the overall equivalence ratio is leaner than stoichiometry, i.e. less than one.

2.4.2 Effect of Equivalence Ratio on the Formation of NOx

As may be seen from Figure 2.5, for both premixed flame and diffusion flame, NOx formation increases when the equivalence ratio approaches. Because a more fuel rich flame is formed with increased equivalence ratio, this more fuel rich flame also leads to higher flame temperature and then more thermal NOx forms. (Zel’dovich et.al, 1947) [45].

2.4.3 Gas Fuel Type Effect on NOx Formation

From the figure below, it is evident that fuel type affects the formation of NOx.

![Figure 2.6 Effect of fuel type on NOx emission with air as an oxidizer](image-url)

Figure 2.6 Effect of fuel type on NOx emission with air as an oxidizer [46]
The possible reason is that different fuel has different element composition, different molecular weight, and different enthalpy. Flame temperature depends on the enthalpy of reactants and products. That is, different fuel will lead to different flame temperature, and then the temperature difference will affect the formation of NOx accordingly [46].

2.4.4 Effect of Preheating Air on the Formation of NOx

Juy and Niiokaz [47] studied NOx emission in a two-dimensional laminar jet methane–air diffusion flame. From this work, it was concluded that preheating of air increases the formation of NO in the flame.

![Figure 2.7 Distribution of mole fractions of NO for temperatures of (a) 500K and (b) 1300K [47]](image)

From the figure above, it is evident that when preheating air temperature was increased from 500K to 1300K, mole fraction of NO increased from 1.0e-04 to 1.0e-03. The possible reason for this is higher temperature leads to more thermal NOx formation.

2.4.5 Additives in the Flame can Affect Formation of NOx

Rokke and Hustad [45] studied the effect of additives in the flame on the formation of NOx. Figure 2.8 shows how different additives affect the NOx formation in diffusion flame. It is evident that additive affects NOx formation more than that with air. For example, additive oxygen injected into fuel leads to more NOx emission than that injected into air. Another
conclusion is that additive oxygen can lead to more NOx formation both when injected into fuel stream and air stream [45].

![Figure 2.8 Additives effect on NOx emission in diffusion operation [45]](image1)

Figure 2.8 Additives effect on NOx emission in diffusion operation [45]

Figure 2.9 shows how different additives affect the NOx formation in premixed flame. The result is different with that for diffusion flame.

![Figure 2.9 Additives effect on NOx emissions in premixed operation [45]](image2)

Figure 2.9 Additives effect on NOx emissions in premixed operation [45]

Additive oxygen leads to less NOx formation in premixed flame while it leads to more NOx formation in diffusion flame. The possible reason for the decreasing of NOx formation is that for
premixed flame, the mixture is diluted by additives and then fuel has a lower concentration in the mixture, which will lead to lower flame temperature and less NOx formation [45].

2.4.6 Soot and NOx Interaction

The following figure shows the NOx formation under two different conditions: with soot and without soot in the flame.

![Figure 2.10 NOx volume fraction with soot and without soot](image)

Figure 2.10 NOx volume fraction with soot and without soot [48]

Most of time, soot and NOx is studied separately, however, the interactions between soot and NOx formation in the flame is also important. Smooke and Long studied laminar methane-air diffusion flame and showed how the pressure of soot affected the formation of NOx [48].

It is indicated by Figure 2.10 that in the flame, NOx formation was increased from 1.4-e04 to 1.6-e04 when soot formation was not included. The reason is that, when there is no soot, the flame radiative heat loss is decreased and then flame temperature is increased. This is explained in the flame radiation part that soot contributes to great heat loss. Without soot radiation, higher flame temperature leads to more NOx formation [48].

In the next chapter, numerical simulation for present work will be introduced in detail.
CHAPTER 3. MATHEMATICAL MODEL

3.1 Burner Configuration

In present study, double inverse diffusion flame will be investigated. Figure 3.1 shows the schematic diagram of the model used.

![Schematic diagram of the model](image)

Inlets for primary air, fuel and secondary air are already shown in the above figure. Inner radius of the burner (Ra) is 0.564cm, the thickness for the inner pipe (t₁) is 0.0355cm; outer radius (Rb) is 0.80cm, the thickness for the outer pipe (t₂) is 0.07625cm. Radius of the inlet for secondary air (Rc) is 10cm.

In order to do the simulation, the schematic diagram in Figure 3.1 is simplified into a two dimensional mathematic model, as shown in Figure 3.2. Since the burner is co-axial cylindrical, two dimensional axisymmetrical model is applied. The centerline is the axis.
In present study, computational fluid dynamics software Fluent is employed to carry out the simulation by solving the conservation, momentum and energy equations. The calculation is based on finite volume method. Width of the domain is 10cm at each side along the axis. Height of the domain is 20cm. First, the calculation domain is meshed into small control volumes. Unstructured mesh is used here.

After meshing, the governing equations and boundary conditions can be applied to the control volumes. The governing equations are listed in the following section.

3.2 Governing Equations

Mass continuity equation:

\[ \frac{\partial}{\partial z} (\rho v_r) + \frac{1}{r} \frac{\partial}{\partial r} (\rho v_r r) = 0 \]  

(3.1)

\( v_r \) is radial velocity component
\( v_z \) is axial velocity component

Momentum equation:

Momentum in radial direction:

\[
\left( r \rho v_r \frac{\partial v_r}{\partial r} + r \rho v_z \frac{\partial v_r}{\partial z} \right) - 2 \frac{\partial}{\partial r} \left( r \mu \frac{\partial v_r}{\partial r} \right) - \frac{\partial}{\partial z} \left( r \mu \frac{\partial v_r}{\partial z} \right) - \frac{2}{3} \frac{\partial}{\partial r} \left( \mu \frac{\partial (rv_r)}{\partial r} \right) + \frac{2}{3} \frac{\partial}{\partial z} \left( r \mu \frac{\partial v_z}{\partial z} \right) - \frac{\partial}{\partial z} \left( r \mu \frac{\partial v_z}{\partial z} \right) + 2 \mu \frac{v_r}{r} + \frac{2}{3} \frac{\partial}{\partial r} \left( rv_r \right) - \frac{2}{3} \mu \frac{\partial v_z}{\partial z} + r \frac{\partial p}{\partial z} = 0
\]

(3.2)

Momentum in axial direction:

\[
\left( r \rho v_r \frac{\partial v_z}{\partial r} + r \rho v_z \frac{\partial v_z}{\partial z} \right) - \frac{\partial}{\partial r} \left( r \mu \frac{\partial v_z}{\partial r} \right) - 2 \frac{\partial}{\partial z} \left( r \mu \frac{\partial v_z}{\partial z} \right) + \frac{2}{3} \frac{\partial}{\partial r} \left( \mu \frac{\partial (rv_z)}{\partial r} \right) + \frac{2}{3} \frac{\partial}{\partial z} \left( r \mu \frac{\partial v_z}{\partial z} \right) - \frac{\partial}{\partial r} \left( r \mu \frac{\partial v_z}{\partial z} \right) + r \frac{\partial p}{\partial z} - r \rho g = 0
\]

(3.3)

Energy equation:

\[
C_p \left( r \rho v_r \frac{\partial T}{\partial r} + r \rho v_z \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial r} \left( r \lambda \frac{\partial T}{\partial r} \right) - \frac{\partial}{\partial z} \left( r \lambda \frac{\partial T}{\partial z} \right) + r \left[ C_p Y_i \left( v_{ir} \frac{\partial T}{\partial r} + v_{iz} \frac{\partial T}{\partial z} \right) \right] + r \sum h_i w_i = 0
\]

(3.4)

\( h_i \) is specific enthalpy of species \( i \)

\( w_i \) is rate of appearance or disappearance of species \( i \) due to reaction

\[
v_{ir} = - \frac{D_i}{Y_i} \frac{\partial Y_i}{\partial r}
\]

(3.5)

\[
v_{iz} = - \frac{D_i}{Y_i} \frac{\partial Y_i}{\partial z}
\]

(3.6)

Conservation of chemical species:

\[
\left( r \rho v_r \frac{\partial Y_i}{\partial r} + r \rho v_z \frac{\partial Y_i}{\partial z} \right) - \frac{\partial}{\partial r} \left( r \rho D_i \frac{\partial Y_i}{\partial r} \right) - \frac{\partial}{\partial z} \left( r \rho D_i \frac{\partial Y_i}{\partial z} \right) - r w_i = 0, \quad i = 1, 2, ..., N
\]

(3.7)

Ideal gas equation:

\[
P = \rho R_u T
\]

(3.8)
\( R_u \) is ideal gas constant

Soot formation is calculated with the following two equations, which are listed in Fluent tutorial.

\[
\frac{\partial}{\partial t} (\rho Y_{soot}) + \nabla \cdot (\rho \vec{v} Y_{soot}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_{soot}} \nabla Y_{soot} \right) + \frac{dM}{dt} \quad (3.9)
\]

\[
\frac{\partial}{\partial t} (\rho b_{nuc}^*) + \nabla \cdot (\rho \vec{v} b_{nuc}^*) = \nabla \cdot \left( \frac{\mu_t}{\sigma_{nuc}} \nabla b_{nuc}^* \right) + \frac{1}{N_{norm}} \frac{dN}{dt} \quad (3.10)
\]

Where,

\( Y_{soot} \) is soot mass fraction

\( M \) is soot mass concentration (kg/m\(^3\))

\( N_{norm} \) is \(10^{15}\) particles

\( b_{nuc}^* \) is normalized radial nuclei concentration (particles \(\times 10^{-15}\))

\( N \) is soot particle number density (particles/m\(^3\))

Before applying these equations to the control volumes, discretization of these equations have to be done. Details about equation discretization can be found in the reference [53].

### 3.3 Simulation Method

After setting up the model, parameters to do the simulation need to be set. Procedures to do the simulation are as follows.

1. **Model.** Pressure based solver is selected, solving all equations sequentially. Gravity is taken into consideration. In the axial direction along the centerline of the burner, the gravitational acceleration is -9.8m/s\(^2\). Operation pressure is 101325Pa. Temperature for the unburned fuel and air is 300K.

2. **Material.** Mixture of ethylene-air is selected in present research. Gas mixture is assumed to be ideal gas. Material properties of all the gases, such as specific heat capacities, are functions of temperature and calculated with piecewise-polynomial instead of constants.
Detail to calculate material properties dependence on temperature is in Appendix.

3. Reaction model. Laminar Finite Rate model, which computes the chemical source terms using Arrhenius expressions and ignores the effects of turbulent fluctuations, is applied. Reaction rates are also determined by Arrhenius expressions. Radiation is included.

To make the solution converge smoothly, stiff chemistry solver is applied.

4. Boundary conditions. The flame is open boundary, so free boundary conditions are applied at the right side and left side, as shown in Figure 3.2. As for the top, pressure outlet boundary is applied. That is, the outlet pressure is 101325Pa. At the bottom, velocity inlet boundary conditions are applied. Flow rate of fuel is 252sccm at the fuel inlet. Temperature of the inlet fuel and air is set to be 300K.

5. Initial condition. Initial pressure is 101325Pa. In order to ignite the flame, the simulation zone needs to be patched at the beginning of the simulation. Patch temperature is 2000K in present research.

6. Solution. As for the pressure based segregated algorithm, SIMPLE (Semi-implicit method for pressure-linked equations) is selected. Second order discretization for the equations is applied.

Residual is monitored and plotted. The default under-relaxation parameters for all variables are one. To make the result converge better, the under relaxation parameters are decreased to be 0.5.

3.4 Validation

Before conducting numerical simulation to study properties of laminar double inverse diffusion flame, it is necessary to validate present numerical model. To validate present model, simulation on a laminar diffusion flame is done. By comparing present simulation result with
previous result, it is found that present simulation result is consistent with previous result in the reference. This consistence indicates that present simulation method is reliable.

3.4.1 Simulation Method

In this study, two dimensional axisymmetrical model is selected. Figure 3.3 shows the schematic diagram of the model used. It is for inverse diffusion flame.

Operation temperature is 298K, combined with 1atm as operation pressure. Laminar finite rate model is applied.

![Schematic diagram of the normal diffusion flame burner](image)

Figure 3.3 Schematic diagram of the normal diffusion flame burner

Unburned ethylene and air are at temperature of 298K and under the pressure of 1atm. Normal gravity is included. Inner radius of the burner (Ra) is 0.5cm; outer radius (Rb) is 1.5cm. Inlet velocity for air is 0.212m/s, inlet velocity for ethylene is 0.07m/s.

3.4.2 Simulation Result

Flame height is one important property to study flame structure. Commonly, flame height is defined as the height from the top of the burner to the position of the peak temperature along the centerline.

Temperature along the centerline in axial direction is plotted in Figure 3.4.
In the literature [32], flame height $H$ is 10mm. and in present result, from Figure 3.4, $H$ is also 10mm. That is, current result agrees well with their experiment result. In this way, the numerical model is validated.

In this chapter, the model has been validated. And in the next chapter, the simulation result will be discussed.
CHAPTER 4. RESULTS AND DISCUSSION

4.1 Comparison of Double Inverse Diffusion Flame and Normal Diffusion Flame

In this part, double inverse diffusion flame and normal diffusion flames are compared, in terms of temperature distribution, soot and NO formation. Ethylene is used. The burner configuration is shown previously in Figure 3.1. Flow rate of fuel is 252sccm for both NDF and DIDF. By plotting the temperature contour, soot volume fraction contour and NO formation contour, difference between these two configurations with the same mass flow rate is clear.

4.1.1 Comparison of the Temperature Distribution for DIDF and NDF

To study the flame structure difference between DIDF and NDF, contour of temperature distribution for DIDF and NDF is displayed below.

Figure 4.1 Temperature distribution for DIDF Figure 4.2 Temperature distribution for NDF

By comparing the two figures above, it is evident that there is an inner flame and an outer flame in double inverse diffusion flame, while there is only one flame in normal diffusion flame configuration.

To compare the temperature more clearly, temperature along the centerline in the axial direction is plotted for both DIDF and NDF.
It can be seen from the figures above that there are two flame peaks for DIDF, while there is only one flame peak for NDF. This is consistent with the temperature contour in Figure 4.1 and Figure 4.2.
Temperature at different height in the radial direction is also plotted for both DIDF and NDF.

In Figure 4.5 shown below, for double inverse diffusion flame, at height $z=0.02\text{m}$, $z=0.05\text{m}$ and $z=0.09\text{m}$, there is only one peak; while at height $z=0.01\text{m}$, where is near the exit of the burner, there are two peaks. The first peak forms in the inner flame, the second peak forms in the outer flame.

Plotting of the temperature in radial direction at different height is consistent with the flame temperature contour in Figure 4.1.

![Figure 4.5 Flame temperature in radial direction for DIDF](image)

In the following figure, for normal diffusion flame, there is only one peak at all heights, no matter the height is near the exit of the burner or far away the exit of the burner. This peak is formed by the only one flame.

This plotting is also consistent with the flame temperature contour in Figure 4.2.
4.1.2 Soot Volume Fraction for DIDF and NDF

Distribution of soot volume fraction for DIDF and NDF are compared in the following two figures.

Figure 4.6 Flame temperature in radial direction for NDF

Figure 4.7 Soot volume fraction for DIDF

Figure 4.8 Soot volume fraction for NDF
Soot volume fraction at different height in radial direction is plotted for DIDF and NDF respectively.

Figure 4.9 (a) Soot volume fraction for DIDF at different height

Figure 4.9 (b) Soot volume fraction for DIDF at height: z=0.005m
For both DIDF and NDF, the peak value of soot volume fraction is not located on the centerline.

Peak soot volume fraction is compared in the following figure.

---

Figure 4.10 Soot volume fraction for NDF at different height

Figure 4.11 Comparison of peak soot volume fraction for DIDF and NDF
The position of the peak soot volume fraction is indicated in the three figures above.

Peak soot volume fraction for DIDF is located at the position of \( z=0.018 \text{m}, r=0.0041 \text{m} \) and \( r=-0.0041 \text{m} \) on both sides of the centerline.

Peak soot volume fraction for NDF is located at the position of: \( z=0.04 \text{m}, r=0.03 \) and \( r=-0.03 \text{m} \) on both sides of the centerline.

Discussion and conclusion:

As shown in Figure 4.11, for the same mass flow rate of ethylene, peak soot volume fraction for DIDF is 42% lower than that for NDF. The possible reason is that in DIDF, fuel can react with both primary air and secondary air. More complete combustion in DIDF leads to less soot pollution.

The difference of soot volume fraction between DIDF and NDF can be seen from Figure 4.9 and Figure 4.10. In Figure 4.9, there are two layers near the exit of the burner and then merge to one layer. In Figure 4.10, there is only one layer even near the exit of the burner, because for DIDF, both the inner flame and outer flame contributes to one layer of soot volume fraction near the exit of the burner.

For DIDF, when plotting the soot volume fraction at the height of \( z=0.018 \text{m}, z=0.03 \text{m} \) and \( z=0.06 \text{m} \), there is only one peak, which is indicated in Figure 4.9 (a). But there are two peaks when plotting at the height of \( z=0.005 \text{m} \) in Figure 4.9 (b). This height is near the exit of the burner.

For NDF, when plotting at the height of \( z=0.01 \text{m}, z=0.02 \text{m} \) and \( z=0.04 \text{m} \), there is only one peak. While when plotting at the height of \( z=0.0055 \text{m} \), there is still only one peak. This is indicated in Figure 4.10. The plotting for these two flames is consistent with the contour of the two flames.
4.1.3 NO Formation for DIDF and NDF

4.1.3.1 Comparison of mole fraction of NO for DIDF and NDF

The simulation result for mole fraction of NO is plotted in Figure 4.12 and Figure 4.13.

Mole fraction of NO at different height in radial direction is also plotted.

Figure 4.12 Mole fraction of NO in DIDF  Figure 4.13 Mole fraction of NO in NDF

Figure 4.14 (a) Mole fraction of NO for DIDF at different height
Peak mole fraction of NO for DIDF and NDF is indicated in Figure 4.12 and Figure 4.13 and compared in the following figure.
Discussion and conclusion:

As shown in Figure 4.16, with the same mass flow rate, peak mole fraction of NO for DIDF is lower by 24% than that for NDF, which is indicated in. The reason for this result will be discussed in the following part.

The same as contour of soot volume fraction, there is difference between the contour of mole fraction of NO for DIDF and NDF, especially near the exit of the burner.

For DIDF, when plotting at the height of $z=0.03m, z=0.04m$ and $z=0.08m$, there is only one peak, which is indicated in Figure 4.14 (a). But there are two peaks when plotting at the height of $z=0.01m$ in Figure 4.14 (b).

For NDF, when plotting at the height of $z=0.12m, z=0.04m$ and $z=0.08m$, there is only one peak. While when plotting at the height of $z=0.01m$, there is still only one peak. This is indicated in Figure 4.15.

In this section, mole fraction of NO is discussed. In next section, the formation of NO will be discussed. Thermal mechanism and prompt mechanism will be investigated separately.
4.1.3.2 Formation mechanism of NO: thermal mechanism

Total NO formation is formed by both thermal mechanism and prompt mechanism. Thermal mechanism is studied first. Equations to form thermal NO have been discussed in Part 1.5.

Contour of rate of thermal NO formation for DIDF and NDF is displayed in Figure 4.17 and Figure 4.18. Temperature distribution for DIDF and NDF is displayed below for comparing.
By comparing the contour of rate of thermal NO formation with the contour of temperature distribution for both DIDF and NDF, it is shown that rate of thermal NO formation is consistent with the temperature distribution in the flame: where the temperature is high, rate of thermal NO formation is high. The reason for this result is that thermal NO formation mechanism is temperature dependent.

The way how temperature affects thermal NO formation can be explained in detail by the following example with Equation 4.1 - 4.5 [11].

\[
\frac{d[NO]}{dt} = k_{G}[N_2][O_2]^{1/2} (kmol/m^3.s) \quad (4.1)
\]

While concentration of nitrogen and concentration of oxygen is related to temperature,

\[
[N_2] = x_{N_2} \frac{P}{R_uT} \quad (4.2)
\]

\[
[O_2] = x_{O_2} \frac{P}{R_uT} \quad (4.3)
\]

\(x_{N_2}\) is mole fraction of nitrogen

\(x_{O_2}\) is mole fraction of oxygen

Equation 4.1 is derived into Equation 4.4:

\[
\frac{d[NO]}{dt} = k \cdot x_{N_2} \cdot x_{O_2}^{1/2} \quad (4.4)
\]

\[
k = k_{G} \cdot \left(\frac{P}{R_uT}\right)^{3/2} \quad (4.5)
\]

Assume that the mole fraction of nitrogen and mole fraction of oxygen, which is not related to temperature, is fixed. Temperature \(T\) is set as the variable, while keeping all other parameters constants. Global rate coefficient \(k_{G}\) and coefficient \(k\) varies with temperature.

Pressure \(P\) is 101325Pa. Equilibrium constant also varies with temperature. The result is shown in Table 4.1.
Table 4.1 Temperature dependence of the formation rate of thermal NO

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>( k_G )</th>
<th>( k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1500</td>
<td>1.03e-03</td>
<td>7.51e-07</td>
</tr>
<tr>
<td>1600</td>
<td>1.76e-02</td>
<td>1.17e-05</td>
</tr>
<tr>
<td>1800</td>
<td>2.00e+00</td>
<td>1.11e-03</td>
</tr>
<tr>
<td>2000</td>
<td>8.77e+01</td>
<td>4.17e-02</td>
</tr>
<tr>
<td>2100</td>
<td>4.44e+02</td>
<td>1.96e-01</td>
</tr>
<tr>
<td>2200</td>
<td>1.93e+03</td>
<td>7.79e-01</td>
</tr>
</tbody>
</table>

From Table 4.1, it can be seen that when mole fraction of nitrogen and oxygen is fixed, \( k_G \) increases significantly with increased temperature, \( k \) also increases greatly. This verifies that the formation rate of thermal NO is sensitive to temperature and thermal NO forms mainly at the position where temperature is high. Present simulation result is consistent with this theory prediction.

4.1.3.3 Formation mechanisms of NO: prompt mechanism

Prompt mechanism for NO formation is studied in this section. Like thermal mechanism discussed in previous section, contour of rate of prompt NO formation for DIDF and NDF is displayed in Figure 4.19 and Figure 4.20.

As shown in these two figures below, it is evident that prompt NO forms at different positions compared with thermal NO. Prompt NO mainly forms nearly the fuel exit of the burner, while thermal NO forms at the place where temperature is high. Different formation positions are determined by different formation mechanisms. This can also be explained by the equations.
As for prompt NO, rate of formation is related to the concentration of fuel. With the following equation that is previously listed in Part 1.5,

$$\frac{d[NO]}{dt} = k_{pr}[O_2]^a[N_2][FUEL]e^{-\frac{E_a}{RT}}(kmol/m^3.s) \tag{1.8}$$

Equation 1.8 can be simplified into Equation 4.6 and Equation 4.7,

$$\frac{d[NO]}{dt} = k \cdot x_{N_2} \cdot x_{O_2}^a \cdot x_{FUEL} \tag{4.6}$$

$$k = k_{pr} \cdot \left(\frac{P}{RT}\right)^{(2+a)}e^{-\frac{E_a}{RT}} \tag{4.7}$$

It can be seen that when all other parameter are fixed, the formation rate of prompt NO is proportional to the concentration of fuel. This is why prompt NO formed at the place where fuel is rich. In a flame, fuel is rich at the exit of the burner, and prompt NO should form near the exit of the burner. Present result of the contour of rate of prompt NO is consistent with this theory prediction.

4.1.3.4 Compare of the relative importance of two NO formation mechanisms

Although there are two formation mechanisms, it doesn’t mean that both of these mechanisms make the same contributions to NO formation in a flame. To investigate the relative
importance of these two mechanisms, both peak formation rate and total formation rate of NO from these two mechanisms are compared.

Peak formation rate of NO from these two mechanisms for both DIDF and NDF are already indicated in the contour from Figure 4.17 to Figure 4.20.

Total rate of NO formation by each mechanism is the result of integration. For example, in Figure 4.17, formation rate of thermal NO at each point is indicated by color map. By integrating the formation rate over the volume, total formation rate can be calculated.

The comparison for DIDF and NDF will be investigated separately. NDF will be studied first.

For NDF:

Peak rates of NO formation by the two formation mechanisms for normal diffusion flame, which are indicated in Figure 4.18 and Figure 4.20, are compared in Figure 4.21. Total rate of NO formation by the two formation mechanisms are compared in Figure 4.22.

![Peak rate of NO](image)

Figure 4.21 Comparison of peak formation rate of thermal NO and prompt NO (kgmol/m³-s)
Figure 4.22 Comparison of total thermal NO and prompt NO (kgmol/s)

The ratio of peak rate of NO formation by thermal and prompt mechanism is 1:0.19. And the ratio of total rate of NO formation by thermal and prompt mechanism is 1:0.03. NO formed by thermal mechanism is much more than that from prompt mechanism. From Figure 4.18 and Figure 4.20, it can also be seen that thermal NO forms in large area in the flame while prompt NO only forms near the exit of the burner. To conclude, thermal mechanism is dominated for NO formation in normal diffusion flame.

After comparing thermal and prompt mechanism in normal diffusion flame, comparison of these two mechanisms in double inverse diffusion flame will be done.

For DIDF:

Like for NDF, the same comparison for DIDF is done. Peak rates of NO formation by the two formation mechanisms for DIDF, which are indicated in Figure 4.17 and Figure 4.19, are compared in Figure 4.23. Total rate of NO formation by the two formation mechanisms are compared in Figure 4.24.
Figure 4.23 Comparison of peak formation rate of thermal NO and prompt NO (kgmol/m³·s)

Figure 4.24 Comparison of total thermal NO and prompt NO (kgmol/s)

For DIDF, ratio of peak rate of NO formation by thermal and prompt mechanism is 1:0.84. Ratio of total rate of NO formation by thermal and prompt mechanism is 1:0.13. Thermal mechanism for NO formation is dominated in double inverse diffusion flame, too.
4.1.3.5 Comparison of the total NO formation in DIDF and NDF

In this section, total NO formation in DIDF and NDF will be compared. While total rate of NO is the sum of rate of NO by both thermal mechanism and prompt mechanism. Contour of total rate of NO formation for DIDF and NDF are displayed in Figure 4.25 and Figure 4.26. The peak rates indicated in these two figures are compared in Figure 4.27.

Figure 4.25 Rate of NO in DIDF (kgmol/m³-s)

Figure 4.26 Rate of NO in NDF (kgmol/m³-s)

Figure 4.27 Comparison of peak rate of NO formation for DIDF and NDF (kgmol/m³-s)
Total NO formation in DIDF and NDF are compared in Figure 4.28.

Figure 4.28 Comparison of total amount of NO formation for DIDF and NDF (kgmol/s)

Form Figure 4.27, it can be seen that with the same mass flow rate of fuel, peak rate of NO formation for DIDF is higher than that for NDF. However, as shown in Figure 4.28, total amount of NO formation for DIDF is lower than that for NDF, which means that DIDF produces less NO than NDF by 18%. This is one advantage of DIDF compared with NDF.

In this section, from the simulation result, it is clear that DIDF flame produces less soot and NO pollution compared with NDF with the same flow rate of fuel. However, only one flow rate of fuel is applied. To make this conclusion more convincible, more simulations are worked out with flow rate of 84sccm and 168sccm.

4.2 Effect of Flow Rate of Fuel on Double Inverse Diffusion Flame and Normal Diffusion Flame

In this section, the advantages of DIDF are further verified by applying the same flow rate of ethylene to both DIDF and NDF. Like in the section above, the burner shown in Figure 3.1 is used. Three cases were conducted with flow rate: 84sccm, 168sccm and 252sccm. The simulation results are shown below.
Table 4.2 Simulation result for DIDF and NDF with different flow rate of fuel

<table>
<thead>
<tr>
<th>Flow rate of fuel (sccm)</th>
<th>Peak soot volume fraction</th>
<th>Peak mole fraction of NO</th>
<th>Total NO formation (kgmol/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DIDF</td>
<td>NDF</td>
<td>DIDF</td>
</tr>
<tr>
<td>84</td>
<td>8.49E-06</td>
<td>1.67E-05</td>
<td>1.69E-05</td>
</tr>
<tr>
<td>168</td>
<td>9.10E-06</td>
<td>1.77E-05</td>
<td>1.54E-05</td>
</tr>
<tr>
<td>252</td>
<td>1.13E-05</td>
<td>1.98E-05</td>
<td>1.61E-05</td>
</tr>
</tbody>
</table>

In order to demonstrate the differences more clearly the results are also shown graphically from Figure 4.29 to Figure 4.31.

4.2.2 Comparison of Peak Soot Volume Fraction

![Graph showing peak soot volume fraction of DIDF and NDF](image_url)

Figure 4.29 Peak soot volume fraction of DIDF and NDF

Peak soot volume fraction for both DIDF and NDF will slightly increase as the mass flow rate of fuel increases, and peak soot volume fraction for NDF is always higher than that for DIDF. This result indicates that DIDF produces less soot than NDF does.

The possible reason is that in DIDF, fuel can react with both primary air and secondary air. More complete combustion in DIDF leads to less soot pollution.
4.2.3 Comparison of NO Formation

![Comparison of NO Formation](image)

In Figure 4.30, for NDF, peak NO mole fraction increases first and then decreases when flow rate of ethylene increases. However, total NO formation keeps on increasing, which is indicated in Figure 4.31.
The same thing happens to DIDF, peak NO mole fraction decreases first and then increases when mass flow rate of ethylene increases. However, total NO formation keeps on increasing, which is indicated in Figure 4.31.

To conclude, total NO formation always increases when flow rate of ethylene increases, although peak NO mole fraction will slightly fluctuate.

And no matter how NO mole fraction fluctuates, both peak mole fraction and total NO formation in DIDF is always lower than that in NDF, which means that with the same flow rate of ethylene, DIDF produces less NO pollution than NDF. The reason can be attributed to the fact that in double inverse diffusion flame, fuel can interact with both the primary air and the secondary air, which means more complete combustion results in less pollution.

By conducting simulations on three different flow rates of ethylene fuel, the same conclusion is drawn that DIDF flame leads to less pollution compared with NDF flame configuration under the same flow rate of ethylene fuel.

In the next section, the scale of the burner will be increased to continue to verify the advantage of DIDF.

### 4.3 Simulation Result with Increased Burner Scale

In previous sections, burner shown in Figure 3.1 is used to display the unique double flame structure and show the advantages of DIDF by comparing with NDF. In this section, the dimension of the burner configuration is increased by 50%. The aim is to verify the conclusion that DIDF leads to less pollution than NDF flame burner configuration is independent on the scale of the burner.

Three cases were conducted with flow rate: 192sccm, 384sccm, and 576sccm. The simulation results are shown below.
Table 4.3 Simulation result for DIDF and NDF with scale increased burner

<table>
<thead>
<tr>
<th>Flow rate of fuel (sccm)</th>
<th>Peak soot volume fraction</th>
<th>Peak mole fraction of NO</th>
<th>Total rate of NO formation (kgmol/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DIDF</td>
<td>NDF</td>
<td>DIDF</td>
</tr>
<tr>
<td>192</td>
<td>1.90E-05</td>
<td>2.28E-05</td>
<td>1.58E-05</td>
</tr>
<tr>
<td>384</td>
<td>2.11E-05</td>
<td>2.50E-05</td>
<td>1.48E-05</td>
</tr>
<tr>
<td>576</td>
<td>2.52E-05</td>
<td>2.78E-05</td>
<td>1.46E-05</td>
</tr>
</tbody>
</table>

To show the result clearly, these results were shown graphically. First, peak soot volume fraction is plotted in the following figure.

![Graph of peak soot volume fraction for DIDF and NDF](image)

Figure 4.32 Peak soot volume fraction of DIDF and NDF

From the figure above, it can be seen that peak soot volume fraction for DIDF flame is less than that for NDF with the same flow rate of fuel.

NO formation for DIDF and NDF is compared in the following two figures. It is clear from the figures above, that DIDF flame leads to less NO formation compared with NDF flame configuration under the same flow rate of ethylene fuel.
Conclusion: it has been displayed in previous three sections that DIDF burner configuration leads to less pollution compared with NDF. And this conclusion is independent on the scale of the burner.
Like normal diffusion flame, double inverse diffusion flame will also be affected by many factors, including flame radiation, operation pressure, preheating of the oxidizer and dilution of the fuel. Effect of these four factors on double inverse diffusion flame will be studied separately.

Fuel to study is still ethylene. The burner used is the one shown in Figure 3.1.

Effect of flame radiation will be studied first.

4.4 Effect of Flame Radiation on Laminar Double Inverse Diffusion Flame

Flow rate of fuel is 252sccm. Simulation result is already shown in Part 4.1 when flame radiation is taken into account. Here, the simulation is done without considering radiation effect while keeping all other parameters the same.

4.4.1 Radiation Effect on Flame Temperature

To study the radiation effect on flame temperature, flame temperature in axial direction is plotted in the following two figures for both of these two cases in Figure 4.3 (with radiation) and Figure 4.35 (without radiation).

Figure 4.3 (as seen on page 30) Flame temperature in axial direction for DIDF
Figure 4.35 Flame temperature in axial direction for DIDF: without radiation

In Figure 4.3, there are two peaks and the two peaks are evident. But in Figure 4.35, there is only one peak, because the temperature continues to increase after the first peak and then only the second peak still exists.

Maximum temperature for these two cases is compared in Table 4.4.

<table>
<thead>
<tr>
<th></th>
<th>With radiation</th>
<th>No radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum temperature (K)</td>
<td>1945</td>
<td>2270</td>
</tr>
</tbody>
</table>

It can be seen from the table above that the maximum temperature along the centerline is lower when flame radiation is taken into account because of the radiative heat loss by both soot and gas radiation. Soot radiation and gas radiation has been discussed in Part 1.6 and will not be discussed in detail here.
Flame temperature at different height in radial direction is also plotted in the Figure 4.5 (with radiation) and Figure 4.36 (without radiation) for these two cases respectively.

Figure 4.5 (as seen on page 31) Flame temperature in radial direction for DIDF

Figure 4.36 Flame temperature in radial direction for DIDF: without radiation
It can be seen from the two figures above, that at the same height, flame temperature is lower when flame radiation is taken into account. Peak flame temperature is indicated in the two figures above and compared in Table 4.5.

<table>
<thead>
<tr>
<th></th>
<th>With radiation</th>
<th>No radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak flame temperature (K)</td>
<td>2123</td>
<td>2294</td>
</tr>
</tbody>
</table>

It can be seen that the peak flame temperatures is lower by 7% because of the radiative heat loss by both soot and gas radiation when flame radiation is taken into account.

4.4.2 Radiation Effect on Soot Formation

Flame radiation can also affect soot formation in DIDF. In present study, soot volume fraction at different height is plotted in Figure 4.37 (with radiation) and Figure 4.38 (without radiation). Figure 4.37 is the combination of Figure 4.9 (a) and Figure 4.9 (b).
Figure 4.38 Soot volume fraction for DIDF: without radiation

Peak soot volume fraction is compared in Figure 4.39 for these two cases.

Figure 4.39 Comparison of peak soot volume fraction

It can be seen that for double inverse diffusion flame, when flame radiation effect is considered, peak soot volume fraction decreases by 12%.

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Previous research has been done to study the effect of flame radiation on normal diffusion flame, and the conclusion is that flame radiation will lead to lower flame temperature and less soot formation. Flame radiation has the same effect on both normal diffusion flame and double inverse diffusion flame.

The reason for the lower temperature and less soot formation is attributed to the heat loss by flame radiation, including soot radiation and gas radiation.

4.4.3 Radiation Effect on NO Formation

Radiation has certain effect on NO formation because flame radiation can affect the temperature of the flame.

In present study, to study the effect of radiation on NO formation in DIDF, mole fraction of NO at different height is plotted in Figure 4.40 and Figure 4.41, for flame with radiation and without radiation respectively. Peak mole fraction of NO is compared in Figure 4.42. Figure 4.40 is the combination of Figure 4.14 (a) and Figure 4.14 (b).

Figure 4.40 Mole fraction of NO in radial direction
It can be seen that when flame radiation is taken into account, peak mole fraction of NO decreases by 90%. It has been discussed previously that thermal NO formation is dominated and sensitive to flame temperature. So more thermal NO forms when higher flame temperature exists.
by not considering the radiation heat loss.

Rate of NO formation is also compared in Figure 4.43, which indicates the conclusion more directly.

![Rate of NO formation](chart.png)

Figure 4.43 Comparison of rate of NO formation (kgmol/s)

Conclusion:

When there is flame radiation, rate of NO formation decreases by 5% in present work. Flame radiation is very important to study double inverse diffusion flame. It can affect flame temperature, soot formation and NO formation. Flame radiation has the same effect on double inverse diffusion flame as on normal diffusion flame.

In the next section, the effect of preheating on double inverse diffusion flame will be discussed.

4.5 Effect of Preheating on Laminar Double Inverse Diffusion Flame

Effect of preheating on normal diffusion flame has been studied by previous research. In this section, effect of preheating of the primary air on laminar double inverse diffusion flame is
studied by increasing the temperature of the primary air. The burner shown in Figure 3.1 is used. Flow rate of fuel is 252sccm. Simulation result is already shown in Part 4.1 when primary air is at the temperature of 300K. Here, temperature of primary air is preheated from 300K to 400K, while temperature for fuel and secondary air is still at 300K.

Simulation results are compared for these two cases. First, the effect of preheating on flame temperature is investigated.

4.5.1 Effect of Preheating Air on Flame Temperature

To study the effect of preheating on flame temperature, temperature along the centerline in axial direction is plotted in Figure 4.1 (primary air temperature at 300K) and Figure 4.44 ((primary air temperature at 400K). From Figure 4.44, it is clear that there are still two flame peaks when primary air is heated from 300K to 400K, peak temperature is higher when primary air is at 400K. The peak temperature is compared in Table 4.6 and plotted in Figure 4.45.

Figure 4.1 (as seen on page 29) Temperature distribution for DIDF
Figure 4.44 Temperature in the axial direction: primary air at 400K

Table 4.6 Comparison of the temperature of the two peaks

<table>
<thead>
<tr>
<th></th>
<th>Peak1 temperature</th>
<th>Peak2 temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary air at 300K</td>
<td>1856K</td>
<td>1945K</td>
</tr>
<tr>
<td>Primary air at 400K</td>
<td>1955K</td>
<td>1950K</td>
</tr>
</tbody>
</table>

Figure 4.45 Effect of preheating the primary air on flame temperature
From Table 4.6 and Figure 4.45, it can be seen that temperature of the first peak increases by 5.4%, the temperature of the second peak increases only by 0.26%. Preheating of the primary air enhances the inner diffusion flame, but doesn’t have significant effect on the outer flame.

Flame temperature at different height in radial direction is plotted in Figure 4.5 (primary air at 300K) and Figure 4.46 (primary air at 400K) for these two cases. Peak flame temperature is compared in Figure 4.47.

![Flame temperature at different height for DIDF](image1.png)

Figure 4.5 (as seen on page 31) Flame temperature at different height for DIDF

![Flame temperature at different height for DIDF: primary air at 400K](image2.png)

Figure 4.46 Flame temperature at different height for DIDF: primary air at 400K
When the primary air is preheated from 300K to 400K, peak flame temperature increases by 4.5%.

The reason can be explained by the equation of adiabatic flame temperature: $T_d$. There are two adiabatic flame temperatures: constant-pressure adiabatic flame temperature and constant-volume adiabatic flame temperature. $T_d$ here is the constant-pressure adiabatic flame temperature. According to Equation 4.7 to Equation 4.9 [11], $T_d$ is calculated when there is no heat loss.

\[ H_{\text{react}} = H_{\text{prod}} \]  \hspace{1cm} (4.7)

While

\[ H_{\text{react}} = \sum_{\text{react}} N_i \bar{h}_i \]  \hspace{1cm} (4.8)

\[ H_{\text{prod}} = \sum_{\text{prod}} N_i \bar{h}_i \]  \hspace{1cm} (4.9)

To study the effect of preheating of the air on the flame temperature, $T_d$ is calculated for the following two different cases: air at 298K and air at 400K, while temperature for fuel is at 298K without changing.
The reaction is:

$$C_2H_4 + 3*(O_2 + 3.76N_2) = 2CO_2 + 2H_2O$$

At 298K,

$$H_{react} = 52283 + 0(N_2) + 0(O_2) = 52283 \text{ (kJ)}$$

$$H_{prod} = 2[-393547 + 57.677*(T-298)] + 2[-241845 + 46.102*(T-298)]
+ 3*3.76*[0 + 34.477*(T-298)] \text{ (kJ)}$$

$$T = 2369K$$

At 400K,

$$H_{react} = 52283 + 3*3031 + 3*3.76*2978 = 94911 \text{ (kJ)}$$

$$H_{prod} = 2[-393547 + 57.677*(T-298)] + 2[-241845 + 46.102*(T-298)]
+ 3*3.76*[0 + 34.477*(T-298)] \text{ (kJ)}$$

$$T = 2580K$$

All the values used in the equation above are from reference [11].

By calculation it is clear that adiabatic flame temperature will increase when air is preheating from 298K to 400K, while fuel is not preheated. $H_{react}$ is increased because the temperature is increased. One thing to mention is that, in this calculation, $Cp$, specific heat capacity, is dependent on temperature, but here, $Cp$ is considered as constant at the average flame temperature. The calculation result is not the exact value because the estimated value of $Cp$. However, the result for the temperature shows the trend that preheating air leads to higher flame temperature.

In present result, the peak flame temperature is not the adiabatic temperature because of heat loss by radiation. But the peak temperature still increases for the same reason when air is preheated.
4.5.2 Effect of Preheating Air on NO Formation

It has been shown that preheating the primary air will lead to higher flame temperature and then affect NO formation. Mole fraction of NO at different height in radial direction is shown in Figure 4.40 (primay air at 300K) and Figure 4.48 (primay air at 400K).

Figure 4.40 (as seen on page 58) Mole fraction of NO in radial direction

Figure 4.48 Mole fraction of NO in radial direction: primary air at 400K
Peak value of the mole fraction of NO is 2.98e-05 and located at the position of \(z=0.004\text{m}, \ r=0.005\text{m}\) and \(r=-0.005\text{m}\). At height of \(z=0.004\text{m}\), the first peak is much higher than the second peak. This is because of the preheating of the primary air. It is more evident when comparing the contour of mole fraction of NO when primary air is at the temperature of 300K and 400K. This is shown in Figure 4.12 (primary air at 300K) and Figure 4.49 (primary air at 400K).

![Figure 4.12](as seen on page 36)
Mole fraction of NO in DIDF

![Figure 4.49](Mole fraction of NO in DIDF (400K))

After preheating the primary air, the double flame structure is more evident. When the primary air is at the temperature of 300K, the two layers of mole fraction of NO near the exit of the burner are not so obvious, but when primary air is preheating to 400K, the inner layer becomes more evident. The reason for this result is that higher inner flame temperature caused by preheating leads to more NO formation in the inner diffusion flame. The reason that thermal NO is dominated and sensitive to temperature has been discussed previously.

Mole fraction of NO at different height has been plotted in Figure 4.40 and Figure 4.48. Here, peak mole fraction of NO and rate of NO formation will be compared in the following two figures.
Discussion:

From the figures above, it may be seen that when primary air is preheated from 300K to 400K, the peak flame temperature increased and more soot and NO formed in the double inverse diffusion flame.
In the reference [47], preheating air leads to more NO formation in laminar diffusion flame. The reason that leads to more NO formation can be attribution to the higher temperature. By comparing the reference [47] result to present work, it seemed that preheating the air has the same effect on normal diffusion flame as that on double inverse diffusion flame.

### 4.6 Effect of Elevated Pressure on Laminar Double Inverse Diffusion Flame

The objective in this section is to study the effect of elevated pressure on laminar double inverse diffusion flame. Three operation pressures are applied: 1atm, 2atm to 4atm. Effect of elevated pressure on flame width, soot and NO formation is studied.

The burner used is shown in Figure 3.1. Flow rate of fuel is 126sccm. Ethylene is applied.

#### 4.6.1 Effect of Elevated Pressures on Flame Temperature

Elevated pressure will affect flame temperature. Temperature distribution in axial direction is plotted for these three cases: 1atm, 2atm and 4atm.

![Figure 4.52 Temperature in axial direction: 1atm](image)

Figure 4.52 Temperature in axial direction: 1atm
According to Figure 4.5 to Figure 4.54, peak temperature in axial direction is compared in Table 4.7 and plotted in Figure 4.55.
Table 4.7 Comparison of peak temperature in axial direction

<table>
<thead>
<tr>
<th></th>
<th>1atm</th>
<th>2atm</th>
<th>4atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak temperature (K)</td>
<td>1940</td>
<td>2030</td>
<td>2080</td>
</tr>
</tbody>
</table>

Figure 4.55 Peak temperature in axial direction varies with pressure

It can be seen from Figure 4.55 that peak temperature in axial direction increases with elevated pressure.

After comparing flame temperature in axial direction, flame temperature distribution in radial direction is also compared for these three cases. Flame temperature at different height in radial direction is plotted in the following three figures: from Figure 4.56 to Figure 4.58. It can be seen that flame temperature increases when operation pressure is increased. Trend of temperature variation in radial direction is the same as that in axial direction.
Figure 4.56 Temperature in radial direction: 1atm

Figure 4.57 Temperature in radial direction: 2atm
Position and value of peak flame temperature for these three cases is included in the three figures above and compared in Table 4.8 and plotted in Figure 4.59.

Table 4.8 Comparison of peak flame temperature

<table>
<thead>
<tr>
<th></th>
<th>1atm</th>
<th>2atm</th>
<th>4atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak flame temperature (K)</td>
<td>2126</td>
<td>2144</td>
<td>2165</td>
</tr>
<tr>
<td>Position in radial direction (m)</td>
<td>0.0068</td>
<td>0.00564</td>
<td>0.00414</td>
</tr>
<tr>
<td>Position in axial direction (m)</td>
<td>0.008</td>
<td>0.0016</td>
<td>0.0851</td>
</tr>
</tbody>
</table>
Figure 4.59 Peak flame temperature varies with pressure

From Figure 4.59, it can be seen that peak temperature in axial direction increases by 20K when operation pressure doubles.

4.6.2 Effect of Elevated Pressures on Flame Width (W)

For normal diffusion flame, flame width is defined in the following way: there is a peak temperature at the side. The distance from the centerline to the peak temperature at the side is half of the flame width.

While for double inverse diffusion flame, which has not been studied thoroughly, there is no standard to define what the flame width is. In this way, same method is used to determine the flame width for double inverse diffusion flame: take the distance from the peak temperature at the side to the centerline as half flame width.

In present work, position of peak flame temperature is already shown in Table 4.10. Position in radial direction is defined as half flame width.

Result from Table 4.8 is displayed in Table 4.9.
According to the result in Table 4.9, it can be seen that elevated pressure leads to narrower flame.

Discussion:

Effect of elevated pressure can lead to narrower flame for normal diffusion flame and opposed diffusion flame, which is discussed in the literature part. In present work, it is evident that elevated pressure can lead to narrower flame for double inverse diffusion flame too. Elevated pressures affect flame shape in the same way although flame burner configuration is different.

Effect of elevated operation pressure on flame temperature and flame shape has been discussed in this section. In the next section, effect of elevated pressure on soot formation in double inverse diffusion flame will be discussed.

4.6.3 Effect of Elevated Pressures on Soot Formation

Soot formation under varied pressures is investigated in this section. To study the effect of elevated pressure on the formation of soot, soot volume fraction at different flame height in radial direction is plotted in the following three figures, for the three cases respectively: 1atm, 2atm, and 4atm. It can be seen that, when pressure is increased, soot volume fraction in radial direction is increased.

Table 4.9 Flame width under varied operation pressures

<table>
<thead>
<tr>
<th></th>
<th>1atm</th>
<th>2atm</th>
<th>4atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Half flame width (m)</td>
<td>0.0068</td>
<td>0.00564</td>
<td>0.00414</td>
</tr>
</tbody>
</table>


Figure 4.60 Soot volume fraction in radial direction: 1 atm

Figure 4.61 Soot volume fraction in radial direction: 2 atm
Peak soot volume fraction is displayed in Table 4.10. When pressure is increased, soot volume fraction will increase.

Table 4.10 Peak soot volume fraction under varied operation pressures

<table>
<thead>
<tr>
<th></th>
<th>0.1Mpa</th>
<th>0.2Mpa</th>
<th>0.4Mpa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak soot volume fraction (fv)</td>
<td>8.60E-06</td>
<td>3.92E-05</td>
<td>1.64E-04</td>
</tr>
</tbody>
</table>

In the next section, effect of elevated pressures on NO formation in double inverse diffusion flame will be investigated.

4.6.4 Effect of Elevated Pressures on NO Formation.

NO formation under varied pressures is investigated. Mole fraction of NO at different heights in radial direction is plotted in the following figures.
Figure 4.63 Mole fraction of NO in radial direction: 1atm

Figure 4.64 Mole fraction of NO in radial direction: 2atm
Figure 4.65 Mole fraction of NO in radial direction: 4atm

Peak soot volume fraction is compared and displayed in Table 4.11 and plotted in Figure 4.66. It can be seen from Figure 4.66, peak mole fraction of NO almost doubles when operation pressure doubles. Elevated pressure lead to more NO formation because higher temperature leads to higher flame temperature. Present simulation result is the same as that from the reference [44] which was discussed in the literature survey part. That is, elevated operation pressure will lead to more NO formation for both normal diffusion flame and double inverse diffusion flame. Elevated pressure affects NO formation in the same way for these two burner configurations.

Table 4.11 Peak mole fraction of NO under different operation pressures

<table>
<thead>
<tr>
<th></th>
<th>1atm</th>
<th>2atm</th>
<th>4atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak mole fraction of NO</td>
<td>1.56E-05</td>
<td>2.91E-05</td>
<td>7.02E-05</td>
</tr>
</tbody>
</table>
Conclusion:

Elevated pressure has significant effect on flame width, soot and NO formation. It is very important in double inverse diffusion flame. Most practical devices are operated at higher pressure. Methods to decrease NO pollution is required. The next section will discuss one efficient method to decrease NO pollution.

4.7 Effect of Fuel Dilution on Laminar Double Inverse Diffusion Flame

In previous simulation result, the fuel is pure ethylene. In order to decrease NO pollution, pure ethylene is diluted by nitrogen. Nitrogen concentration in fuel is increased from 0% to 5% and then to 10%. That is, pure ethylene becomes the mixture of ethylene and nitrogen. The burner used is the one shown in Figure 3.1. Mole flow rate of ethylene is 252sccm. Simulation result is already displayed in Part 4.1 when nitrogen in fuel is 0%. Comparison of temperature distribution, soot formation and NO formation for these three cases are displayed below.

Effect of nitrogen dilution on flame temperature will be studied first.
4.7.1 Effect of Nitrogen Dilution on Flame Temperature

Flame temperature will be affected by the dilution of fuel. Temperature distribution in axial direction is plotted below. Figure 4.3 is the result when there is 0% nitrogen in fuel.

Figure 4.3 (as seen on page 30) Flame temperature in axial direction for DIDF

Figure 4.67 Flame temperature in axial direction for DIDF: 5% nitrogen in fuel
Figure 4.68 Flame temperature in axial direction for DIDF: 10% nitrogen in fuel

Peak flame temperature in axial direction for these three cases is displayed in Table 4.12 and plotted in Figure 4.69. It is evident that when mole concentration of nitrogen in the fuel is increased, peak temperature in axial direction decreases. The reason for the flame temperature decrease can be that when fuel is diluted, the concentration of fuel is decreased and then the chance for fuel to react with air is decreased.

Table 4.12 Comparison of peak temperature in axial direction

<table>
<thead>
<tr>
<th>Mole concentration of nitrogen in the diluted fuel</th>
<th>0%</th>
<th>5%</th>
<th>10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak temperature in axial direction (K)</td>
<td>1950</td>
<td>1930</td>
<td>1920</td>
</tr>
</tbody>
</table>
After comparing the peak temperature in the axial direction, peak flame temperature will be compared. Peak flame temperature is not located on the centerline, but on the side of the centerline. Here, peak flame temperature for these three cases is displayed in Table 4.13 and plotted in Figure 4.70. It can be seen from Figure 4.70 that when fuel is diluted by nitrogen, flame temperature decreases by 1.4K when mole fraction of nitrogen in fuel increases every one percent.

Table 4.13 Comparison of peak flame temperature

<table>
<thead>
<tr>
<th>Mole concentration of nitrogen in the diluted fuel</th>
<th>0%</th>
<th>5%</th>
<th>10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Flame Temperature (K)</td>
<td>2123</td>
<td>2117</td>
<td>2109</td>
</tr>
</tbody>
</table>
4.7.2 Effect of Nitrogen Dilution on Soot Formation

Soot formation is affected by the dilution of fuel. Soot volume fraction at different height in radial direction is plotted below. Figure 4.37 is the result when there is 0% nitrogen in fuel.
Figure 4.71 Soot volume fraction for DIDF: 5% nitrogen in fuel

Figure 4.72 Soot volume fraction for DIDF: 10% nitrogen in fuel

Peak soot volume fraction of these three cases is compared in the following table and plotted in Figure 4.73.
Table 4.14 Comparison of peak soot volume fraction

<table>
<thead>
<tr>
<th>Mole concentration of nitrogen in the diluted fuel</th>
<th>0%</th>
<th>5%</th>
<th>10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak soot volume fraction</td>
<td>1.13e-05</td>
<td>1.04e-05</td>
<td>9.26e-06</td>
</tr>
</tbody>
</table>

Figure 4.73 Variation of peak soot volume fraction

From the figure above, it is evident that when fuel is diluted by nitrogen, peak soot volume fraction decreases by 18% when mole concentration of nitrogen in fuel increases ten percent. Dilution of fuel by nitrogen leads to less soot formation in laminar double inverse diffusion flame.

After discussing effect of nitrogen dilution on soot formation in this section, effect of nitrogen dilution on NO formation will be investigated in the following section.
4.7.3 Effect of Nitrogen Dilution on NO Formation

Mole fraction of NO in radial direction is plotted when nitrogen concentration in fuel varies from 0% to 5% and 10%. Figure 4.37 is the result when there is 0% nitrogen in fuel.

Figure 4.40 (as seen on page 58) Mole fraction of NO in radial direction

Figure 4.74 Mole fraction of NO in radial direction: 5% nitrogen in fuel
Figure 4.75 Mole fraction of NO in radial direction: 10% nitrogen in fuel

Peak mole fraction of these three cases is compared Table 4.15 and plotted in Figure 4.76.

Table 4.15 Comparison of peak mole fraction of NO

<table>
<thead>
<tr>
<th>Mole concentration of nitrogen in the diluted fuel</th>
<th>0%</th>
<th>5%</th>
<th>10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak mole fraction of NO</td>
<td>1.61e-05</td>
<td>1.48e-05</td>
<td>1.32e-05</td>
</tr>
</tbody>
</table>

Figure 4.76 Variation of peak mole fraction of NO
Rate of NO formation is also compared in Table 4.16 and plotted in Figure 4.77. It can be seen that when the mole concentration of nitrogen in the diluted fuel is increased, peak mole fraction of NO and rate of NO formation will decrease. The reason is that lower temperature leads to less NO formation. Because thermal NO is dominated and sensitive on the temperature, when flame temperature decreases, NO formation will decrease.

Table 4.16 Comparison of peak mole fraction of NO

<table>
<thead>
<tr>
<th>Mole concentration of nitrogen in the diluted fuel</th>
<th>0%</th>
<th>5%</th>
<th>10%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rate of NO</td>
<td>1.79E-10</td>
<td>1.67E-10</td>
<td>1.42E-10</td>
</tr>
</tbody>
</table>

Figure 4.77 Comparison of rate of NO formation (kg/s)

According to the simulation result, it is found that diluted ethylene with nitrogen can decrease NO and soot pollution effectively.
5. SUMMARY AND CONCLUSION

The advantages of double inverse diffusion flame are verified by comparing with normal diffusion flame. Two DIDF burners with different burner configuration are applied, each with three different flow rate of fuel. Double inverse diffusion flame leads to less soot and NO formation than normal diffusion flame does with the same flow rate of ethylene fuel.

Factors that affect double inverse diffusion flame are investigated. Flame radiation affects double inverse flame in the same way as it does to normal diffusion flame: flame radiation leads to lower flame temperature, less soot and NO formation. Preheating of the primary air leads to higher temperature and more NO formation because flame temperature is increased. Elevated pressure leads to narrower flame and more soot and NO formation, while dilution of fuel by nitrogen can help to decrease the pollution of soot and NO.

The advantages of double inverse diffusion flame burner configuration have been studied in present research, however, more work needs to be done. Effect of the scale of DIDF burner configuration should be studied more thoroughly. The dimension of the inner diameter and outer diameter of the DIDF burner has certain effect on the application of DIDF burner configuration too. More fuel types can be studied by using DIDF burner configuration to further verify the advantage of DIDF burner.
REFERENCES


Proceedings of Combustion Institute - Canadian Section, Spring Technical Meeting, University of Toronto.


40. Graph by Robert Simmon, based on model data from the NASA GSFC Laboratory for Atmospheres.


APPENDIX DEFINING MATERIAL PROPERTIES USING TEMPERATURE DEPENDENT FUNCTIONS [53]

Material properties, such as specific heat capacity and density, are not constants. While conducting calculations, these material properties can be defined as functions of temperature. There are basically three ways to define the temperature dependent property for a material: polynomial, piecewise-linear and piecewise-polynomial. Each of these three will be introduced briefly.

For polynomial:

\[ \phi(T) = A_1 + A_2 T + A_3 T^2 + \cdots \]

For piecewise-linear:

\[ \phi(T) = \phi_n + \frac{\phi_{n+1} - \phi_n}{T_{n+1} - T_n} (T - T_n) \]

where \( 1 \leq n \leq N \) and \( N \) is the number of segments.

For piecewise-polynomial:

\[ \begin{align*}
&\text{for } T_{\text{min},1} \leq T \leq T_{\text{max},1}: \phi(T) = A_1 + A_2 T + A_3 T^2 + \cdots \\
&\text{for } T_{\text{min},2} \leq T \leq T_{\text{max},2}: \phi(T) = B_1 + B_2 T + B_3 T^2 + \cdots
\end{align*} \]

In the equation above, \( \phi \) is the material property and \( T \) is the temperature (K).
VITA

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