EFFECT OF CHANGES IN FLOW GEOMETRY, ROTATION AND HIGH HEAT FLUX ON FLUID DYNAMICS, HEAT TRANSFER AND OXIDATION/DEPOSITION OF JET FUELS

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EFFECT OF CHANGES IN FLOW GEOMETRY, ROTATION AND HIGH HEAT FLUX ON FLUID DYNAMICS, HEAT TRANSFER AND OXIDATION/DEPOSITION OF JET FUELS

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ABSTRACT

EFFECT OF CHANGES IN FLOW GEOMETRY, ROTATION AND HIGH HEAT FLUX ON FLUID DYNAMICS, HEAT TRANSFER AND OXIDATION/DEPOSITION OF JET FUELS

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Jet fuel is used in high-performance military flight vehicles for cooling purposes before combustion. It is desirable to investigate the influence of the flow and heating conditions on fuel heat transfer and thermal stability to develop viable mitigation strategies. Computational fluid dynamics (CFD) simulations and experiments can provide the understanding of the fuel physical phenomena which involves the fluid dynamics, heat transfer and chemical reactions. Three distinct topics are studied:

The first topic considers the effect of flow geometry on fuel oxidation and deposition. Experiments and CFD modeling were performed for fuels flowing through heated tubes which have either a sudden expansion or contraction. It was found that the peak deposition occurs near the maximum oxidation rate and excess deposition is formed near the step. This study provides information for the fuel system designer which can help minimize surface deposition due to fuel thermal oxidation.
In the second area of study, the fuel passed heated rotational test articles to investigate the effect of rotation on fuel heat transfer. The coupled effects of centrifugal forces and turbulent flow result in fuel temperatures that increase with rotational speed. This indicates that the convective heat transfer is enhanced as rotational speed increases. This work can assist the understanding of using jet fuel to cool the turbine engine.

In the third segment of research, the fuel was exposed to “rocket-like” conditions. This investigation is to explore the effect of high heat flux and high flow velocity on fuel heat transfer and oxidation/deposition. Simulations show a temperature difference over several hundred degrees in the radial direction within the very thin thermal boundary layer under rapid heating. The fuel contacting the interior wall is locally heated to a supercritical state. As a result, the heat transfer is deteriorated in the supercritical boundary layer. Both simulated and measured deposit profiles show a peak deposit near the end of the heated section. These observations may eventually have an application to the design of high speed supersonic vehicles with improved cooling capabilities.
I would like to give my sincere appreciation to my dissertation advisor, Dr. Jamie Ervin, for his support, guidance and patience. I wish also to thank Dr. Steven Zabarnick for his efforts on the course of my study, and the members of my doctoral committee, Dr. Tim Edwards and Dr. Kevin Hallinan, for reviewing this dissertation. I am grateful to Mr. Ted Williams, Mr. Richard Wills, Mr. Zachary West, Dr. Matthew Dewitt, Dr. Scott Stouffer and Mr. Joseph Mantz for their assistance in my research and the laboratory.

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LIST OF SYMBOLS/ABBREVIATIONS

Symbols:

A = pre-exponential factor in Arrhenius rate expression (mole, L, s)

Cp = specific heat (J/kg-K)

Ea = activation energy (kcal/mole)

en = enhanced wall function

Er = relative internal energy (kJ)

\( \vec{F} \) = force (N)

g = gravitational acceleration (m/s\(^2\))

G = mass flow rate flux (kg/m\(^2\)-s)

h = specific enthalpy (kJ/kg)

\( r \) = relative total enthalpy (kJ)

I = turbulent intensity (%)

K = thermal conductivity (W/m-K)

k = turbulent kinetic energy (kJ/kg)
\( m \) = mass (kg)

\( \dot{m} \) = mass flow rate (kg/s)

\( \text{Nu} \) = Nusselt number

\( P \) = pressure (MPa)

\( \bar{p} \) = mean pressure (MPa)

\( p' \) = pressure fluctuation (MPa)

\( P_c \) = critical pressure (MPa)

\( \text{Pr} \) = Prandtl number

\( \dot{q} \) = volumetric heat generation (kW/m³)

\( q'' \) = heat flux (kW/m²)

\( \dot{Q} \) = volume flow rate (mL/min)

\( \text{Ra} \) = Rayleigh number

\( \text{Re} \) = Reynolds number

\( \text{st} \) = standard wall function

\( T \) = temperature (K)

\( \bar{T} \) = mean temperature (K)

\( T' \) = temperature fluctuation (K)

\( T_c \) = critical temperature (K)

\( \bar{u} \) = absolute velocity (m/s)
Abbreviations:

ASTM $= \text{American Society for Testing and Materials}$

BC $= \text{Boundary Condition}$

CFD $= \text{Computational Fluid Dynamics}$

GC $= \text{Gas Chromatograph}$
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<tr>
<td>HTC</td>
<td>Heat Transfer Coefficient</td>
</tr>
<tr>
<td>HTD</td>
<td>Heat Transfer Deterioration</td>
</tr>
<tr>
<td>ID</td>
<td>Inner Diameter of a tube (m)</td>
</tr>
<tr>
<td>NIFTR</td>
<td>Near-Isothermal Flowing Test Rig</td>
</tr>
<tr>
<td>NIST</td>
<td>National Institute of Standards</td>
</tr>
<tr>
<td>OD</td>
<td>Outer Diameter of a tube (m)</td>
</tr>
<tr>
<td>RNG</td>
<td>Re-Normalization Group</td>
</tr>
<tr>
<td>rpm</td>
<td>revolutions per minute</td>
</tr>
<tr>
<td>SEM</td>
<td>Scanning Electron Microscope</td>
</tr>
<tr>
<td>SIMPLEC</td>
<td>Semi-Implicit Method for Pressure-Linked Equations Consistent</td>
</tr>
<tr>
<td>SKE</td>
<td>Standard $k$-$\varepsilon$ model</td>
</tr>
<tr>
<td>SRF</td>
<td>Single Rotating Reference Frame</td>
</tr>
<tr>
<td>SS</td>
<td>Stainless Steel</td>
</tr>
<tr>
<td>SST</td>
<td>Shear Stress Transport</td>
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<tr>
<td>Temp</td>
<td>Temperature (°C or K)</td>
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CHAPTER I

INTRODUCTION

Future high performance aircraft will face significant thermal management challenges due to engines that operate at higher temperature and airframes that are exposed to higher aerodynamic temperatures. Early aircraft used ambient air to remove waste heat; the air was simply taken onboard and dumped overboard. As aircraft became capable of greater speeds, the heat loads increased dramatically.\(^1\) Therefore, alternative methods, other than ambient air, are necessary for modern aircraft.

In addition to serving as the combustion propellant, jet fuel often serves as a convenient, zero weight penalty cooling media for the lubrication system, environmental control system, and other engine components of military aircraft.\(^2,3,4\) Fuels provide heat absorption by convection heat transfer and through a potential chemical reactions. When fuel is pumped from the tank to the engines, a series of heat exchangers can be integrated into the fuel lines.\(^1\) The heat exchangers interface with coolant loops that carry waste heat from various subsystems. Figure 1.1 shows that fuel is the ultimate heat sink for all major heat sources on the aircraft.
Unfortunately, as hydrocarbon fuels exposed to higher temperatures, a series of chemical reactions occur within fuels to form undesirable products. Some of these chemical products become surface deposits in the fuel flow passages. Figure 1.2 shows that temperature strongly influences the fuel thermal stability. In the temperature range of ~ 300 - 750 F (150 - 400°C), autoxidation reactions occur in the fuel to form thermal-oxidative deposits. When the temperature reaches ~ 900 F (~ 480°C), pyrolysis reactions start with the productions of the pyrolytic deposits, and pyrolytic deposits increase rapidly with the fuel temperature. Because the dimensions of the fuel passages are small (for example, the order of ~0.01 inches for a fuel nozzle), the deposition could cause distorted spray patterns. Moreover, the fouling of the components in the engine fuel system can obstruct the fuel flow path, resulting in loss of engine thrust or even catastrophic failure of the engine system.
Designers of engines and fuel systems rely heavily on empirically determined rules and limits, such as nozzle fuel and surface temperature limits, to allow the fuel to be used as a coolant while limiting fuel degradation. However, as these empirical rules need to be conservative, they can greatly limit the efficiency of using fuel as a coolant, which in turn limits engine and aircraft capabilities. This dissertation considers three research areas related to the use of hydrocarbon fuel as coolants. The first investigation considers the effects of changes in flow geometry on surface deposition when fuels pass through a sudden expansion or contraction cylindrical tube. The second study involves fuel heat transfer when fuel is heated in rotating passages. The third topic is to explore the fuel behavior under conditions of large heat fluxes and large flow velocities.
1.1 Background

Thermal Oxidation/Deposition along Heated Flow Path

Hydrocarbon fuel is comprised of thousands of chemical species and, thus, hundreds of chemical reactions can occur as fuels are exposed to the heated flow path.\textsuperscript{10} Zabarnick developed a pseudo-detailed chemical kinetic mechanism\textsuperscript{11} to describe fuel thermal-oxidation chain mechanism as shown in Figure 1.3. In this chemical kinetics mechanism, jet fuel is assumed to be a single compound (RH). A free radical (R\textsuperscript{-}) reacts rapidly with dissolved O\textsubscript{2} to form a peroxy radical (RO\textsubscript{2}^\textbullet), which extracts a hydrogen atom from RH to form a hydroperoxide (ROOH). ROOH is decomposed and regenerates free radicals (R\textsuperscript{-}). Figure 1.3 shows that peroxy radical inhibitor (AH) acts as an antioxidant by intercepting RO\textsubscript{2}^\textbullet which can decrease the oxidation rate. The hydroperoxide decomposer (SH) can remove ROOH from the system without increasing the free radical population. Thus, the presence of AH and SH species within the fuel can slow oxidative reactions.\textsuperscript{12}

![Figure 1.3 Representation of hydrocarbon thermal-oxidation mechanism\textsuperscript{11}](#)
In recent years, the thermal oxidations chemical kinetic mechanism has been combined with a computational fluid dynamics (CFD) model to simulate and predict fuel autoxidation and deposition in flowing through cylindrical tubes.\textsuperscript{13} The work has shown that fuel-to-fuel variability in oxidation and deposition rates can be understood and predicted based upon quantitative chemical analysis measurements of key species classes (e.g., phenols, reactive sulfur, and metals) in combination with the CFD/chemical kinetic mechanism.\textsuperscript{13,14} In addition, the model works well over a range of temperatures and flow regimes (i.e., both laminar and turbulent flow) and should extrapolate well to unstudied conditions.\textsuperscript{16}

These previous model development efforts concentrated on fuel degradation and flow within straight cylindrical tubes.\textsuperscript{12,15,16,17} In aircraft fuels systems, fuel flows through an extremely complex series of flow passageways from the fuel tank to the combustor. Figure 1.4 shows an example of this complexity through a cross section of a fuel nozzle which contains two fuel flow pathways, primary and secondary. The primary circuit is used during combustor ignition and engine idle operation, while the secondary circuit is actuated during cruise and high power operation.\textsuperscript{18} Partial or complete blockage of either circuit would negatively impact engine operation, inhibiting ignition with primary blockage and creating spray imbalance and engine hot streaks if either circuit is blocked. It is important to better understand the role of complex flow passageways on the heat transfer, flow, and oxidation/deposition chemistry which occurs in aircraft fuel systems to prevent catastrophic failures, minimize maintenance, and to more efficiently utilize the fuel heat sink.
The empirical design analysis method used currently by designers is exemplified by a report of a fuel nozzle thermal analysis that provides the temperature distribution in the primary and secondary fuel circuits.\textsuperscript{18} The analysis implies that deposition is a strong function of the wetted-wall temperature and shows that the amount of the deposits roughly doubles for every 20°F increase in wall temperature. One previous study used computational fluid dynamics with a global chemistry model to calculate the temperature and deposition rates in a flow nozzle simulation geometry that consisted of two flow channels with a “bridge” shape, including air gaps and the metal nozzle wall.\textsuperscript{19} An unsteady turbulent flow model was performed to calculate the heat transfer, which included the effect of the changing thickness of the surface deposits on the flow and heat transfer in the flow path. However, this study did not report the influence of flow geometry on the fuel fluid dynamics and heat transfer and utilized an empirically-derived global chemical mechanism.
Unfortunately, the effects of changes in the heated flow passage geometry on fuel heat transfer, flow, oxidation, and deposition are not well understood. The flow regime (e.g., laminar vs turbulent) has an obvious effect on heat transfer but the coupling of flow regime changes with chemistry has not been well studied. The simplest flow geometry changes occur when the fuel encounters a sudden expansion or contraction in cylindrical tube flow. Such sudden geometry changes are encountered in numerous locations in the feed fuel line between the fuel tank and the engine, especially for the contraction case. As fuel flows through a sudden expansion in flow path, a recirculation flow is created which should increase the local fuel residence time. We can hypothesize that this will result in greater dissolved oxygen consumption with a resulting increase in deposition near the expansion. For the contraction case, the fuel will encounter a stagnation zone at the contraction, which will also increase the local fuel residence time. We can also hypothesize a possible increase in surface deposition near the contraction. Increased local deposition rates can have important implications for the design of fuel systems and nozzles. For example, a fuel system designer would want to avoid close tolerance passageways and high surface temperatures in locations with increased local fuel residence times. No studies have been performed previously to quantify the effect of these flow changes (i.e., determination of the amount of deposition increase and its location) on fuel deposition for aircraft fuel system conditions.

**Turbine Blade Cooling Studies**

Cooling of gas turbine blades and other rotating flow passages have been studied by several researchers but remain an area of scientific inquiry. Since the 1940s, there has
been interest in the internal cooling of gas turbines by liquids rather than air due to the relatively higher convective heat transfer rates available with liquids.\textsuperscript{20} Thus, liquid-cooling of rotating equipment could potentially allow higher flight velocities or longer engine life. However, early experimental studies were hindered by sealing problems, severe vibrations, flow control difficulties, and the lack of measurements.\textsuperscript{21,22} There has been much recent technological progress in these limiting areas, and the use of the liquid-cooled blades may yet offer potential.

Due to cost and safety concerns, few previous studies have used hydrocarbon fuels as water was commonly selected as the cooling fluid. Experimental turbine blades that used water for cooling were subject to corrosion and fouling.\textsuperscript{21} There is relatively little available in the literature concerning the study of heated hydrocarbon fuels within a rotating passage. However, the flow of a fluid through rotating passage has important the practical applications in the cooling of rotating machinery.

The numerical simulation of the involved rotation and heat transfer is a research challenge. The turbulent flow of heated fuel in rotating passages has complex flow fields, which arise due to imposed centrifugal and Coriolis forces. For example, Nobari et al. have shown that the centrifugal and Coriolis forces strongly influence the heat transfer in a rotating U-shaped duct.\textsuperscript{23} Liu et al. indicated that the Coriolis force contributes to the flow vorticity and wall-normal turbulent heat flux in a complex way for spanwise rotating channel flow.\textsuperscript{24} It was shown that large-scale rotation cells have a significant influence on temperature fluctuations and the turbulent heat flux.\textsuperscript{24} In early studies with heated liquids, the detailed fluid dynamics simulations of rotating blades were simply unavailable.
High Heat Flux Studies

Much of the previous research involving the thermal degradation of hydrocarbon fuels has been for the flow and thermal conditions employed in conventional military aircraft. In recent years, there has been renewed interest in the regenerative cooling designs of rockets and hypersonic vehicles, which involve the flow of hydrocarbons through combustion wall passages. However, the conditions within the cooling passageways of thrust chamber walls of rockets are very different from those within the fuel systems of conventional military aircraft engines. The heat fluxes imposed on cooling-passage surfaces within a rocket thrust chamber are large relative to those found in aircraft. As a consequence, high fuel flow velocities in a rocket are necessary within regenerative cooling passages to produce large convective heat transfer rates to avoid thrust chamber material failure.

High fuel flow velocities necessarily mean shorter residence times for chemical reactions within the fuel, which is desirable for limiting deposit production. On the other hand for rockets and missiles, the maximum surface temperature contacting the fuel is greater than that within jet aircraft. Higher temperatures translate to faster reaction rates and reaction pathways that are likely different from those present in jet aircraft. At temperatures above the critical temperature of a hydrocarbon fuel, the major species react to form smaller hydrocarbons through a series of pyrolysis reactions. As with thermal-oxidation, the accumulation of surface deposits during pyrolytic degradation is a critical concern for rockets as deposition is the limiting issue for using hydrocarbon fuels in regenerative cooling. Surface deposits have a low thermal conductivity and, in effect,
are thermal insulators. Thus, their accumulation can lead to chamber-wall material failure.\textsuperscript{3}

From a fuel system designer’s perspective, unusual behavior has been observed in connection with hydrocarbon fuels in the presence of rocket-like conditions. Removal of the dissolved oxygen from the fuel would normally be expected to result in less deposition. However under rocket flow and thermal conditions, deoxygenation has shown little effect in reducing the deposition rate on non-copper surfaces (on copper surfaces the primary deposition mechanism is sulfur-enhanced corrosion).\textsuperscript{27} In a past study under conditions of high velocity/short residence time, JP-8, JP-8+100, JP-7, JP-10, and RP-1 fuels all showed similar deposition rates on stainless-steel surfaces despite their very different deposition tendencies at lower heat flux levels.\textsuperscript{28} The work described above shows that the influences of fuel chemistry, heat transfer, and fluid dynamics on deposition at high heat flux conditions are not understood.

In nearly all thermal stability flowing experiments, circular tubes are used. Under conditions of well-mixed turbulent flow, the temperature distribution in the radial direction is nearly uniform across most of the tube diameter. However, under conditions of high heat flux and large flow rate, there may be large temperature gradients in the radial directions. NASA has performed experiments to simulate the thermal and flow conditions in regenerative cooled rockets.\textsuperscript{28} At an average heat flux of 3,600 kW/m\textsuperscript{2} and a pressure of 1000 psi (above the critical pressure for JP-8), unusual heat transfer behavior was observed (i.e. the wall temperature sharply increased above the critical temperature and, then rapidly decreased to form a peak in the wall temperature). Also, Roback et al. observed a peak in the interior wall temperature near the inlet when kerosene fuel flowing
under the relative higher heat fluxes condition. These unusual temperature profiles may be related to the formation of a supercritical thermal boundary layer near the wall. Fuel properties change dramatically as a fuel is heated from the liquid to the supercritical phase. In addition, the fuel temperature strongly influences fuel thermal reactions, the resulting reaction pathways and reaction rates can be very different for supercritical and subcritical thermodynamic regimes. The behavior of flowing supercritical fluids under conditions of high heat flux is not well understood and remains an area of active research.

The majority of past heat transfer studies involving supercritical fluids concerned water and to a lesser extent CO₂ and H₂. However, few past studies consider heat transfer involving hydrocarbons in the supercritical phase under conditions of high heat fluxes. Previous studies involving large heat fluxes combined with high flow velocities (i.e., rocket conditions) have not provided detailed measurements of temperature, dissolved oxygen concentration, and surface deposition rates along the heated flow path. Thus, there is a need for detailed, well-controlled experiments and numerical simulations to better understand the observed effects.

1.2 Research Objectives

This dissertation seeks to investigate jet fuel behavior via experiments and computational fluid dynamic simulations incorporating chemical reactions. The purpose is to understand the fuel physical phenomena which involves complex interactions between the fluid dynamics, heat transfer and fuel chemistry. Chapter 2 studies the formation of deposits due to changing in inner diameter of a cylindrical tube. The goal is to understand the effect of the changes in flow geometry on the fuel flow, oxidation, and
surface deposition along the heated flow path. Chapter 3 examines the influence of rotation on the resulting flow and heat transfer for a heated, rotating fuel. CFD model is used to simulate the flow velocities and fuel temperatures under different rotational speeds and flow geometries. Chapter 4 is to explore the heating of the fuel by large heat fluxes in order to understand the fuel heat transfer and thermal stability which involves the supercritical regime.
CHAPTER II

EFFECT OF A STEP CHANGE IN FLOW GEOMETRY ON JET FUEL SURFACE DEPOSITION IN A TUBE

2.1 Introduction

In this chapter, an effort is made on investigating the influence of a sudden change in inner diameter in cylindrical flow geometry on fuel oxidation and surface deposition rates under isothermal laminar flow conditions using both measurements and CFD model with chemistry simulations. The isothermal flow conditions are employed to concentrate on the effect of the flow geometry changes on the fluid dynamics and oxidation/deposition rates through the tube without the complication of varying temperatures. Both contraction and expansion tube geometries were employed under conditions of complete oxygen consumption with the goal of having the maximum deposit rate occur near the tube geometry change. The use of the Near-Isothermal Flowing Test Rig (NIFTR) and isothermal conditions limits the experiments to laminar flow conditions. The experimental measurements are used to determine the deposition rate along the tube length. Computational fluid dynamics combined with a pseudo-detailed chemical kinetic mechanism and deposit sub-mechanism are used to simulate the dissolved oxygen consumption and the deposit formation as a function of flow rate. The calculations are used to allow extrapolation to other conditions that are not amenable to experiments. The primary goals of this work are to increase our understanding of the role
of flow geometry changes on fuel deposition and to improve the ability of fuel system and nozzle designers to efficiently utilize the fuel heat sink while preventing the negative impact of fuel degradation associated with high temperature fuel autoxidation.

2.2 Experimental Section

The experimental tests were performed in the Near-Isothermal Flowing Test Rig (NIFTR) (Figure 2.1). A syringe pump was used to pump the fuel through a 40-inch length of SS316 tubing, with a 32-inch tube section tightly clamped in a copper block heater. A back pressure regulator maintained the system pressure (2.3 MPa) to ensure a single liquid-fuel phase during the test duration. Temperature controllers were used to maintain a constant wall temperature of the heated section. A thermocouple was installed in the fuel line exiting the heated tubing and these temperature measurements were used to ensure that the flow was at a steady-state temperature by monitoring the temperature change with time.

![Figure 2.1 Schematic diagram of the Near-Isothermal Flowing Test Rig](image)
Two types of tubing step changes (expansion & contraction) and two fuel samples (F4177 & F3084) were utilized in the experimental arrangement. The conditions are summarized in Table 2.1. The experimental parameters were chosen to obtain complete oxygen consumption within the heated section and to have the oxygen consumption rate and deposit location be a maximum near the tube step. Requiring the O₂ to be fully consumed within the test tube allows comparison of the total deposit mass for different flow conditions. The fuel reaction time in each experiment was controlled by varying the fuel flow rate. We performed preliminary experimental measurements and CFD calculations which confirmed that the volume of fuel employed here (990 mL) exposed at 478K was sufficient to produce a measurable level of deposits. In Table 2.1, “primary tube” refers to the inlet tube, and “secondary tube” refers to the downstream tube after the step change.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Expansion tube</th>
<th>Contraction tube</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tube ID (mm)</td>
<td>Primary 0.6858</td>
<td>2.159</td>
</tr>
<tr>
<td></td>
<td>Secondary 2.159</td>
<td>0.6858</td>
</tr>
<tr>
<td>Flow rate (mL/min)</td>
<td>0.1 - 1.0</td>
<td>0.25-0.8</td>
</tr>
<tr>
<td>Residence time (s)</td>
<td>1,384 - 138</td>
<td>233 - 73</td>
</tr>
<tr>
<td>Test duration (hour)</td>
<td>165 - 16.5</td>
<td>66 - 20.6</td>
</tr>
<tr>
<td>Length of primary (mm)</td>
<td>203.2</td>
<td></td>
</tr>
<tr>
<td>Length of secondary (mm)</td>
<td>609.6</td>
<td></td>
</tr>
<tr>
<td>Tube OD (mm)</td>
<td>3.175</td>
<td></td>
</tr>
<tr>
<td>Fuel sample</td>
<td>F4177 &amp; F3084</td>
<td></td>
</tr>
<tr>
<td>Inlet temperature (K)</td>
<td>300</td>
<td></td>
</tr>
<tr>
<td>Wall temperature (K)</td>
<td>478</td>
<td></td>
</tr>
<tr>
<td>Operating pressure (MPa)</td>
<td>2.3</td>
<td></td>
</tr>
<tr>
<td>Fuel flowing volume (mL)</td>
<td>990</td>
<td></td>
</tr>
<tr>
<td>Tube material</td>
<td>stainless steel 316</td>
<td></td>
</tr>
</tbody>
</table>
At the completion of the test run, the heated tube was cut into fourteen segments for carbon deposit quantification. Since the area around the step change is of primary interest, a tube segment was cut 0.5-inches on either side of the weld seam, then two segments for each 1.3-inch from the remaining tubes. Eleven segments of 2-inches were removed from the rest of the heated test pieces. Bulk insoluble deposits were collected at the tube exit by 0.2 and 0.45 µm filters. The tube segments and filters were rinsed with heptane and dried in a vacuum oven at 100°C. The tube segments and filters were analyzed for total surface carbon using a LECO RC-412 surface-carbon analyzer. The carbon quantities obtained represent an average of the deposits over the tube segment and the entire test period. The actual surface deposit quantity, expressed in units of micrograms of carbon, are an amount of measured carbon obtained from each test segment subtracted from the carbon background obtained for a clean tube segment of the same length, ID, and OD.

The experimental setup subjected the fuel to a sudden enlargement or compression in flow path depending on flow direction. Figure 2.2a depicts how two tubes with the same OD but different IDs were machined and joined to form the tube step. At the junction of the two pieces, the diameter of the small tube (surface A) was machined to match the large tube ID allowing a light press-fit of the two sections. Surface B was machined flat to assure that it was perpendicular to the tube axis. Surfaces A and B are perpendicular to each other within less than ±1° tolerance. Figure 2.2b shows the cross section of the tubes after they were fitted together for welding. The 4.8-mm of engagement assured that the small and large ID tubes remained concentric. A Swagelok
welder (SWS-M100-MS-13-202) was employed to weld the tubes along the joining seam.\textsuperscript{39}

![Figure 2.2 Schematic of the overlapping weld (a) components and (b) section CC-CC](image)

**2.3 Numerical Section**

**2.3.1 Computational Fluid Dynamics Method**

Numerical simulations were performed to explore the effect of a sudden expansion or contraction in the flow path on the fuel motion, chemistry, and surface deposition. A commercially available computational fluid dynamics code—Fluent,\textsuperscript{40} was used to solve the Navier-Stokes, energy, and species equations for the velocity, pressure, temperature, and species mass fractions. The flow was assumed to be steady, two-dimensional, and axisymmetric. Since the Reynolds number was always below 200 in the simulations, the flow was assumed to be laminar. The enthalpy of reaction was not included in the energy equation because the thermal-oxidative reactions involve trace
species. In addition, heating by viscous dissipation was neglected. The transport properties were assumed to be temperature-dependent.

With regard to the boundary conditions, the wall boundary was held at a constant temperature of 205°C. For simplicity, uniform velocity and temperature profiles (25°C) were assumed at the inlet, and the exit plane velocity and temperature profiles were calculated by extrapolation from interior cell values. The length of the thermal entrance region is relatively small, and the fuel becomes isothermal after ~1 cm (L/L₀ = 0.013) at all flow rates. Since the flow is essentially isothermal and horizontal, the gravitational body force in the momentum equation was neglected. Because the tube wall was thin (<1.5 mm), the radial temperature variation within the tube wall was neglected. Thus, the inner wall temperature was assumed to be the same as that of the copper block. The effect of the deposits on the heat transfer was also neglected as the deposits were assumed to be thin.¹⁶,²⁹

The computational grids which represent the two geometries in the experiments are shown in Figure 2.3. The governing equations in finite volume form were solved iteratively using a second-order accurate upwind scheme. In addition, the SIMPLEC (Semi-Implicit Method for Pressure-Linked Equations Consistent) pressure-velocity coupling scheme was used in the solution of the momentum equations. When the normalized error residuals for all of calculated variables were reduced by six orders of magnitude below their maxima, the solution was considered to be converged.⁴⁰
Figure 2.3 Axisymmetrical computational grid structure (not to scale) for (a) the expansion tube with 14,040 cells and (b) the contraction tube with 8,640 cells.
Grids that were uniform in the radial direction were used since the temperature, velocity, and species varied slowly in the radial direction relative to their greater variation along the tube axis. As the length of the tube (0.81 m) is significantly greater than the tube inner diameter (2.16 mm), the grid in the axial direction was non-uniformly spaced to reduce computational time. The axial grid size was altered by taking 95% of the previous grid size for each new grid as the step was approached. After the step, the axial grid size was altered by 102% of each previous axial grid size towards the outlet. The computational cells were clustered near the step region to better capture the larger flow and temperature gradients there.

A grid density study was performed to ensure the grid independence of the solutions. Table 2.2 shows the number of the cells for three meshes involving the expansion tube: a coarse mesh (scheme A), a radially fine mesh (scheme B) and an axially and radially fine mesh (scheme C). Comparing scheme A with scheme B, the maximum difference in the deposition rate was 1.7%. However, the different cell spacing in the axial direction between schemes B and C results in a 17% difference in the deposition rate. The simulation results appear to be more sensitive to the axial grid density than to the radial grid density. Further mesh refinement was performed using the adaption approach of the gradient in standard normalization of the O₂ mass fraction and deposition rate, and the total cells of 37,900 were obtained. The computational results show a negligible increase in accuracy compared with scheme C. Therefore, scheme C with the total cells of 14,040 were used in the simulation for the expansion tube. Greater cell densities are also needed for the contraction case in the area adjacent to the step.
change. A similar analysis was performed for the contraction tube and the grid structure shown in Figure 2.3b was used to provide an accurate solution.

<table>
<thead>
<tr>
<th>Direction</th>
<th>Coarse (A)</th>
<th>Radial fine (B)</th>
<th>Axial &amp; radial fine (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radial</td>
<td>26</td>
<td>42</td>
<td>42</td>
</tr>
<tr>
<td>Axial</td>
<td>200</td>
<td>200</td>
<td>420</td>
</tr>
</tbody>
</table>

2.3.2 Chemical Reaction Mechanism

Jet fuel is a complex mixture of hydrocarbons comprised of hundreds of chemical species that vary with the petroleum source and processing conditions. The large number of species precludes the detailed kinetic modeling of jet fuel thermal oxidation. Treating the fuel components as classes of species in a kinetic mechanism, which has been referred to as pseudo-detailed chemical kinetic modeling, has been used successfully in simulating the thermal oxidation of jet fuel.\(^\text{12,16}\) Pseudo-detailed kinetic mechanisms are comprised of realistic chemical reactions with rate parameters that are based on literature and theoretical values. Jet fuel is a complex mixture which includes trace concentrations of heteroatomic species. It is known that heteroatomic species are responsible for differences in the oxidation and deposition behavior among fuel samples. Knowledge of the detailed behavior of trace heteroatom species remains incomplete due to the difficulties in measuring trace species concentrations and their variation among fuel samples. Table 2.3 lists the reactions used to simulate thermal oxidation and deposit formation.\(^\text{11,16}\) Reactions 1-5 represent the main autoxidation chain. Reactions 6-9
represent antioxidant reactions that interfere with the chain and create precursors for deposition. Reactions 10-18 represent the chemistry which occurs when hydroperoxides decompose at higher temperatures. Reactions 19-21 are a set of global reactions that produce soluble and insoluble products, as well as deposits. This mechanism also includes the effect of dissolved metals on hydroperoxide decomposition.

In the experimental measurements two jet fuel samples, a JP-8 fuel (F4177) and a Jet A fuel (F3084), were used to study the thermal oxidation and deposits formed on the heated surface. This particular JP-8 sample tended to exhibit relatively low amounts of deposit upon thermal exposure, while the Jet A sample tended to exhibit higher levels. Previous work has shown that the oxidation and deposition behavior of fuel samples can be differentiated by experimental measurements of a few species classes that play important roles in the autoxidation chemical kinetic mechanism. Table 2.4 lists the concentrations of these species used as initial concentrations for the two fuel samples. These values were obtained from experimental measurements performed previously on these fuels. The initial inlet concentrations of the other nineteen species (Table 2.3) were assumed to be zero.
Table 2. 3 Pseudo-Detailed Chemical Kinetic and Global Deposition Mechanism\textsuperscript{11,16}

<table>
<thead>
<tr>
<th>Rxn</th>
<th>Reactants</th>
<th>Products</th>
<th>Arrhenius “A” Factor (mol, L, s)</th>
<th>Activation Energy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>I -</td>
<td>R·</td>
<td>1.00E-03</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>R· O₂ →</td>
<td>RO₂⁻</td>
<td>3.00E+09</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>RO₂⁻ RH →</td>
<td>ROOH</td>
<td>R·</td>
<td>3.00E+09 12</td>
</tr>
<tr>
<td>4</td>
<td>RO₂⁻ RO₂⁻ →</td>
<td>TERMRO₂RO₂</td>
<td>3.00E+09</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>R· R· →</td>
<td>R₂</td>
<td>3.00E+09</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>RO₂⁻ AH →</td>
<td>ROOH</td>
<td>A</td>
<td>3.00E+09 5</td>
</tr>
<tr>
<td>7</td>
<td>A RH →</td>
<td>AH</td>
<td>R·</td>
<td>1.00E+05 12</td>
</tr>
<tr>
<td>8</td>
<td>A RO₂⁻ →</td>
<td>PRODAH</td>
<td>-</td>
<td>3.00E+09 0</td>
</tr>
<tr>
<td>9</td>
<td>ROOH SH →</td>
<td>PRODSH</td>
<td>-</td>
<td>3.00E+09 18</td>
</tr>
<tr>
<td>10</td>
<td>ROOH -</td>
<td>RO· ·OH</td>
<td>1.00E+15</td>
<td>39</td>
</tr>
<tr>
<td>11</td>
<td>RO· RH →</td>
<td>ROH</td>
<td>R·</td>
<td>3.00E+09 10</td>
</tr>
<tr>
<td>12</td>
<td>RO· - →</td>
<td>RPRIME</td>
<td>CARBONYL</td>
<td>1.00E+16 15</td>
</tr>
<tr>
<td>13</td>
<td>·OH RH →</td>
<td>H₂O</td>
<td>R·</td>
<td>3.00E+09 10</td>
</tr>
<tr>
<td>14</td>
<td>RO· RO· →</td>
<td>TERMRO</td>
<td>R·</td>
<td>3.00E+09 0</td>
</tr>
<tr>
<td>15</td>
<td>RPRIME RH →</td>
<td>ALKANE</td>
<td>R·</td>
<td>3.00E+09 10</td>
</tr>
<tr>
<td>16</td>
<td>RO₂⁻ →</td>
<td>R· O₂</td>
<td>1.00E+16</td>
<td>19</td>
</tr>
<tr>
<td>17</td>
<td>RO₂⁻ R· →</td>
<td>TERMRO₂R</td>
<td>R·</td>
<td>3.00E+09 0</td>
</tr>
<tr>
<td>18</td>
<td>ROOH M →</td>
<td>RO· ·OH +M</td>
<td>3.00E+10</td>
<td>15</td>
</tr>
<tr>
<td>19</td>
<td>PRODAH - →</td>
<td>SOLUBLES</td>
<td>-</td>
<td>1.00E+09 0</td>
</tr>
<tr>
<td>20</td>
<td>PRODAH - →</td>
<td>INSOLUBLES</td>
<td>-</td>
<td>3.80E+10 6.5</td>
</tr>
<tr>
<td>21</td>
<td>INSOLUBLES - → DEPOSITS</td>
<td>-</td>
<td>3.00E+03 16.3</td>
<td></td>
</tr>
</tbody>
</table>

Symbol Expression: I, initiator species; R·, hydrocarbon radical; RO₂⁻, peroxy radical; RH, hydrocarbon; ROOH, hydroperoxide; AH, phenol; SH, sulfur hydroperoxide decomposing species (e.g., sulfide); M, dissolved metal species
Table 2.4 Initial Concentrations of Species Used in the Chemical Kinetic Mechanism\textsuperscript{16}

<table>
<thead>
<tr>
<th>Species</th>
<th>Initial mass fraction (kg/kg)</th>
<th>F4177</th>
<th>F3084</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$2.08 \times 10^{-9}$</td>
<td>$2.08 \times 10^{-9}$</td>
<td></td>
</tr>
<tr>
<td>O$_2$</td>
<td>$7.08 \times 10^{-5}$</td>
<td>$7.12 \times 10^{-5}$</td>
<td></td>
</tr>
<tr>
<td>ROOH</td>
<td>$3.24 \times 10^{-6}$</td>
<td>$3.29 \times 10^{-6}$</td>
<td></td>
</tr>
<tr>
<td>AH</td>
<td>$5.91 \times 10^{-5}$</td>
<td>$5.67 \times 10^{-5}$</td>
<td></td>
</tr>
<tr>
<td>SH</td>
<td>$2.35 \times 10^{-3}$</td>
<td>$9.40 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>M</td>
<td>$1.41 \times 10^{-6}$</td>
<td>$3.17 \times 10^{-8}$</td>
<td></td>
</tr>
<tr>
<td>RH</td>
<td>$0.999939486$</td>
<td>$0.999943268$</td>
<td></td>
</tr>
</tbody>
</table>

Normal dodecane has a critical temperature and pressure similar to the pseudo-critical temperature and pressure of the jet fuel samples. Thus, for simplicity the temperature dependent thermal properties (density, thermal conductivity, dynamic viscosity, and specific heat) of the liquid phase fuel were assumed to be the same as that of n-dodecane, and these were obtained from SUPERTRAPP software.\textsuperscript{41} The pressure (2.3 MPa) measured in the experiments was used for property determination. Since the mass diffusivities of the individual species in jet fuel are unknown, a constant mass diffusivity ($8 \times 10^{-8} \text{ (m}^2\text{s})$) was assumed for all species. Mass transfer diffusivities of this order has been shown to sufficiently represent the mass transfer in similar flows.\textsuperscript{16}
2.4 Results and Discussion

Experiments and fluid dynamics with chemistry calculations were performed on fuel flow in two cylindrical heated tubes, the first with a sudden expansion and the second with a sudden contraction in flow geometry. The experiments and numerical modeling computations were performed at a single wall temperature using two fuels which differed in their propensity to form surface deposits. A comparison of the deposit peak locations, deposit width, and deposit quantity of the experimental and the computational surface deposits was employed to elucidate the flow physics at the step and its effect on the reaction chemistry. In all cases studied, the flow was laminar for the flow rates used. All experiments and modeling were performed for wall temperatures of 205°C and a range of fuel flow rates so that oxygen consumption was complete at the end of the heated tube. The experimental conditions (wall temperature, flow rate, test period, etc.) were designed so that the deposition peak and maximum oxidation rate occur at or near the geometry step change to maximize the effect of the step change fluid dynamics on the reaction chemistry. Prior to performing the work, it was hypothesized that flow recirculation zones and/or areas of low flow created by the expansion and contraction geometries would cause increased oxygen consumption near the step with a concomitant increase in surface deposition.
2.4.1 Expansion Tube

2.4.1.1 Measured and Simulated Deposits for Two Fuels at Varying Flow Rates

Figures 2.4a and 2.4b show measured and simulated deposits from the two fuel samples (F4177 and F3084) along the heated primary and secondary tubes. Three different flow rates were used for each fuel to study the effect of reaction time and oxidation extent on the surface deposit distribution near the expansion step. Previous NIFTR experiments at 185°C showed that F4177 oxidized more rapidly than F3084. As a result of these differing oxidation rates two different flow rate ranges, as shown in Figure 2.4, were used for the two fuels to keep the deposit near the step and maintain complete oxygen consumption.

Figure 2.4 compares the measured carbon deposit with the total simulated deposit (carbon and other species) masses along the tube length for the two fuels. The experimental data points are measured carbon deposit masses averaged over the internal surface of the tube segment. As shown in the figure, at the lowest flow rate the deposit peak occurs just downstream of the tube step for both fuels. Increasing the flow rate results in the deposit profile widening and the peak occurs further downstream. All tests were conducted using 990 mL of fuel so that deposit masses could be compared between runs, which require that the total test time be varied for the various flow rates. Significantly lower flow rates would be required to move the deposit peak prior to the step location, which would result in impractically long test durations (many days or weeks) under these conditions.
Figure 2.4 Measured and computed deposits masses along the expansion tube at different flow rates for (a) JP-8 (F4177) and (b) Jet-A (F3084) fuel.
The simulated deposition rates (kg/m\(^2\)-s) were converted to an equivalent mass (micrograms) by multiplying the deposition rate by the internal surface area of the tube and by the experimental test period for each flow condition. To best compare the measured data, which are single values representing the deposit mass over a tube segment, the simulated deposits were calculated based upon these tube segments. Each point is the sum of the deposit mass of each grid cell over a tube segment length and is located on the plot at the midpoint of the segment as in the case of the carbon burn off measurements. The simulation curves shown in Figure 2.4 are fitted to these calculated tube segment data points.

The predicted locations of the deposit peak for both fuels agree well with the experimental peak locations under the lower flow conditions, and are slightly offset when compared to the measured peaks at the higher flow rates. This good agreement occurs without any modification of the chemical kinetic mechanism developed previously.\(^{16}\) Because the deposition rate is a function of the fuel oxidation and the wall deposition reaction rates, fuels that oxidize slowly move the peak location downstream and have broader deposit peaks for a given flow rate.

Figure 2.4 shows that the measured deposit masses are significantly lower than the model for the F4177 fuel sample, but better matched for the F3084 sample. This is due to the fact that the kinetic mechanism was developed to represent the behavior over a range of jet fuel samples.\(^{16}\) The previous work also showed that the model under predicts the deposition of the F4177 fuel but exhibits improved agreement for the F3084 fuel sample.
2.4.1.2 Simulated Dissolved O$_2$ and Deposition Rates of F3084 Fuel along the Expansion Tube

Ideally the experimental studies would be performed under conditions where the deposit peak straddles the step location to maximize the ability to observe the effects of the step, but experimental limitations do not allow this. With the low level of deposition observed at the step, the data do not show a sudden large increase in the deposition rate at the tube step. However, the good agreement between the simulated and experimental results for fuel F3084 provides confidence in our ability to perform simulations to extrapolate the results to other conditions that are beyond the present experimental capability. Thus, two additional slower flow rates (0.03 and 0.06 mL/min) were simulated in an effort to explore the deposition behavior very near the step using fuel F3084. In addition, a faster flow rate of 0.6 mL/min was simulated to study how the deposition rate changes around the step under the condition of very low oxygen consumption within the primary tube.

Figure 2.5 shows the simulated dissolved O$_2$ concentrations and deposition rates along the flow direction for fuel F3084 fuel for the expansion tube case. Six flow rates were simulated including the three experimentally measured conditions. For the lowest flow rate of 0.03 mL/min, the peak deposition occurs near the step with ~75% oxygen consumption in the primary tube. In contrast, for the highest flow rate of 0.6 mL/min, <1% of the dissolved oxygen is consumed in the primary tube, which results in nearly all of the deposition occurring downstream of the step. The figures show that the dissolved oxygen consumption rates depend on the fuel flow rate and tube radial dimensions under these isothermal flow conditions. The oxidation rate increases greatly upon transition
from the primary to secondary tube, due to the cross sectional area increasing by a factor of ten between these tube segments, with a corresponding increase in residence time for oxidation to proceed.

Figure 2.5b shows that the deposition rates increase gradually on the primary inner wall, and rapidly on the secondary inner wall where the deposit peak occurs. The peak locations of the deposition rate move downstream along the flow direction as the flow rate increases since the deposition rate peak normally occurs near the maximum oxidation rate. The figure demonstrates a close coupling between the dissolved oxygen consumption and surface deposition rate, as expected.
Figure 2. 5 Simulated profiles along the flow direction of F3084 fuel flowing in the expansion tube at different flow rates (a) dissolved O₂ concentrations and (b) deposition rates
While Figure 2.5 does show the effect of flow rate on the oxygen consumption and deposition rate, the step change occurs at different fuel residence times for each flow rate, which makes it difficult to ascertain the influence of the step on deposition when the data is plotted versus tube length. In Figure 2.6 we show the same deposition data as in Figure 2.5b, but have converted the tube length abscissa to an average residence time for the fuel. The residence times are calculated using the mean velocities of the primary and secondary flows along with the tube cross sectional areas, as the experiments were conducted with a constant mass flow rate and with a near constant temperature. In a tube without a step change, conversion of various flow rate experiments to residence time ordinarily causes the deposition profiles at various residence times to collapse upon a single curve, as the oxidation and deposition rates are primarily a function of chemical reaction time. Thus, any effect of the tube step change should be more easily observed with the data plotted versus residence time. Figure 2.6 shows that for five of the six flow rates the deposition profiles are very similar except for the residence times which correspond to the area near the step for each flow rate. In fact, for each flow rate the deposition rates increase nearly identically in the primary tube until the fuel approaches the expansion plane. This step occurs at various residence times based on the flow rate. As an example, it takes only 6.2 s for the fuel to reach the step for the fastest flow of 0.6 mL/min, while 62 s is required for the flow rate of 0.06 mL/min.
Figure 2.6 shows that for all flow rates there is a sudden increase in the deposition rate at the location of the step. This deposition rate increases, with some variations near the step location, until the deposition peak location, at a residence time of 110 s, for five of the six fuels, after which the deposition rate declines due to oxygen consumption. As observed previously,\textsuperscript{12} the deposition peak normally occurs near the same residence time as the maximum oxidation rate. However, the sudden expansion in the flow path changes
the deposition profile and increases the local deposition rate near the step, as will be discussed in more detail later.

Figure 2.6 shows that the deposition rate behavior for the lowest flow rate modeled (0.03 mL/min) is different from the other flow rates. The maximum deposition rate occurs at a longer residence time (134 s) than for the other five flow rates. But, careful study of the plot shows that if there was no step change along the flow path, the peak deposition rate would occur at the same residence as the other flow rates (near 110 s). In fact there is a peak in the deposition rate at this residence time prior to the step change at this flow rate. It is important to note that this peak at 110 s occurs in the primary tube for this flow rate, while the deposit peak occurs in the secondary tube for the higher flow rates. Thus, the peak height of the 0.03 mL/min flow rate simulation is lower than the other flow rates due to the lower deposition rates observed in the primary tube. The peak observed near 134 s for this flow rate is due to the increase in deposition rate upon transition to the secondary tube, which greatly increases the deposition rate due to the increased residence time in the wider tube, combined with nearing the complete consumption of dissolved oxygen which reduces the deposition rate after the peak at 134 s. In the next section we more closely examine the importance of the step change in influencing the fuel fluid dynamics and the effect this has on fuel deposition.

2.4.1.3 Fuel Behavior near the Flow Path Expansion

It is important to understand how fluid dynamics/chemistry interactions influence the surface deposition rate near the step change. Figure 2.7 illustrates the simulated velocity vectors, the dissolved O$_2$ concentrations and the deposition rates for F3084 fuel
passing through the expansion tube at a flow rate of 0.03 mL/min. Rather than showing the entire tube length, the area near the step change is expanded in the figure for clarity. Via 2-D velocity vectors, Figure 2.7a shows that a recirculation zone occurs after the expansion plane with P representing the axial location of the recirculation zone center, Q representing the axial location at the secondary inner wall where the recirculation flow ends, and F representing where the flow becomes fully developed.

Figure 2.7b shows the simulated dissolved O$_2$ concentrations at three different radial locations: the tube center (R$_0$), the primary inner wall radius (R$_e$), and the secondary inner wall (R$_w$). A continuous decrease in the O$_2$ concentration along the tube center (R$_0$) is due to the relatively constant velocity there. Except for small differences near the transition region after the expansion plane, the O$_2$ profile in the radial direction is essentially uniform. Thus, the O$_2$ profile along the primary radius (R$_e$) has the same concentration as the tube center (R$_0$). The small, sudden drop in O$_2$ concentration near the inner expansion corner (r$_a$) results from the sudden velocity decrease as the fuel enters the secondary tube. The lowest O$_2$ concentration is observed along the secondary inner wall (R$_w$) within the transitional regime. This is due to an increase in the local residence time due to the recirculation flow, and therefore increased reaction time. The largest O$_2$ radial concentration gradient occurs after the expansion, which results in the advection of dissolved O$_2$ from the tube center to the secondary inner wall until the fuel flow becomes fully developed, where the radial gradient of the O$_2$ concentration tends to zero.
Figure 2.7 Fuel behavior near the expansion step for the 0.03 mL/min flow case (a) 2-D velocity vector, (b) Dissolved O₂ concentration and (c) deposition rate. (Please note that the axis scale is different for the velocity vector plot (8a) than for the other two plots (8b and 8c). The expansion plane occurs at 203.2 mm for all three plots)
Figure 2.7c shows the simulated deposition rate along the primary tube inner wall (Re) and secondary tube inner wall (Rw). The simulation predicts that the deposition rate increases gradually after the step plane up to the 205 mm axial location in the tube, at which point the deposition peaks and decreases thereafter. In the absence of a recirculation zone, one would expect the deposition to continue decreasing as oxygen consumption is near 75% complete in this section of the tube. This is illustrated in Figure 2.7c by the dashed line, which is a qualitative estimation of the expected reduction in deposition in the absence of fuel recirculation. The figure also shows the excess deposition due to the recirculation zone predicted by the simulation, as indicated by the striped region, above that expected without the presence of the recirculation zone. As described above, this excess deposition is likely due to the increased oxygen consumption in this region caused by the increased residence time in the larger tube and also an additional increase in the fuel residence time due to fuel recirculation (Figure 2.7a) near the corner (rb) created by the transition to the large tube.

The excess deposition is difficult to observe experimentally due to its narrow axial width compared with the length of the sectioned tube segments. This increased deposition due to the step is difficult to observe at the faster flow rates simulated. But, a careful examination of Figure 2.6 shows a very narrow spur-like deposition increase near the step location for each of the other faster flow rates. For a closer examination, Figure 2.8 shows the simulated flow and chemistry profiles near the expansion step regime for fuel F3084 at 0.3 mL/min.

By comparison of Figure 2.8a with Figure 2.7a, one sees that the length of the recirculation zone increases with flow rate, with distances of 0.55 and 3.8 mm for the
flow rates of 0.03 and 0.3 mL/min, respectively. In addition, the center of the recirculation zone moves downstream as the flow rate increases, with distances from the expansion plane to the recirculation center (P) of 0.2 mm for 0.03 mL/min and 1.1 mm for 0.3 mL/min. The figures show that the flow velocity magnitude in the recirculation flow is higher in the 0.3 mL/min flow than in the 0.03 mL/min flow. The larger recirculation zone and the higher velocity at higher flow, result in different characteristics for the dissolved O₂ profiles and the resulting deposition profiles for the two flow rates.

Figure 2.8b shows the simulated dissolved O₂ concentration at three radial locations (R₀, Rₑ, Rₓ). Along the tube center (R₀), oxygen is gradually consumed, as is the case for the 0.03 mL/min flow. Along the primary radius (Rₑ), the oxygen concentration is the same as the center (R₀) within the primary tube; however, there is a sharp drop in the oxygen concentration after the step change, followed by an increase in oxygen concentration as the flow approaches the end of the recirculation zone at axial location Q. Along the secondary tube wall (Rₓ), the oxygen concentration starts off relatively low, gradually rises until the end of the recirculation zone, and then begins to decrease. There are two possible causes for the O₂ concentration drop along the primary radius Rₑ, first is the velocity decreasing after the sudden expansion, which increases the residence time of the fuel. But this oxygen concentration decrease is much faster than that observed further downstream, after the flow becomes fully developed (point F). More likely, the oxygen concentration decrease is due to the flow of low oxygen fuel from near the secondary tube wall towards the tube center. This flow is accentuated by the recirculation zone created by the step. The oxygen concentration then begins to increase along Rₑ, after the
center of the recirculation zone, as oxygen rich fuel flows from the center of the tube on the opposite side of the recirculation zone center.

The velocity vector color scale of Figure 2.8a indicates the lowest velocity is near the outer expansion corner \( (r_b) \), which corresponds to a long fuel residence time. Thus, the lowest \( O_2 \) concentration is at this location, which explains the low oxygen concentration near the secondary tube wall \( (R_w) \). The increase in oxygen concentration along \( R_e \) after the recirculation center \( P \) is due to convective flow of high oxygen fuel from the tube center. Diffusion is not likely to play a significant role in this region as the oxygen concentration gradient is minimal.
Figure 2.8 Fuel behavior near the expansion step for the 0.3 mL/min flow case (a) 2-D velocity vector, (b) dissolved O₂ concentration, (c) ROOH concentration and (d) deposition rates
Figure 2.8c shows color contour plots of the fuel hydroperoxide species (ROOH). The highest concentration of ROOH is near the outer expansion corner ($r_b$) as a result of the large amount of $O_2$ consumption caused by the increased residence in the corner. Figure 2.8d shows that the deposition rate peaks near this corner of the secondary wall. Increased hydroperoxide levels and increased oxygen consumption indicate enhanced autoxidative reactivity, and as a result the deposition rate is greatest in this location. The deposition rate along the secondary wall ($r_b$) decreases after the center of the recirculation zone (P) due to increased fuel velocities which cause decreased fuel residence times. When the flow becomes fully developed (near location F), the deposition rate once again begins to increase as the oxygen consumption rates become similar through the tube radius.

The same phenomenon of a minimum in the oxygen level and a peak in the deposition rate near the recirculation zone at the step location is also seen at other flow rates. The width and magnitudes of these oxygen minima and deposition rate peaks are functions of the flow rate, but these effects are relatively small compared with the oxygen consumption and deposition rate changes occurring throughout the tube. But, as this deposition rate peak occurs in a single narrow area of the tube, the concern is that this increased deposition could cause fuel system problems in narrow fuel passageways with diameter changes. In Figure 2.8d is drawn a dashed line that qualitatively indicates the expected deposition rate which would occur in the absence of increased residence time due to fuel recirculation at the step. The deposition rate would be expected to increase due to the increased residence time in the wider secondary tube, approaching the simulated deposition rate after the fully developed flow location (F). The figure also
shows the excess deposition due to the recirculation at the step as a striped region. While the absolute magnitude of the deposition rate in this region is not large compared with the deposition rate further downstream in the secondary tube (see Figure 2.5), the deposition rate does increase by a factor of 2.5 above that expected without recirculation, with this excess deposition occurring in a very narrow tube area.

To this point the surface deposition studied has been on the horizontal wall surfaces only. We now briefly consider the vertical wall plane surface at the step (the wall from point $r_a$ to $r_b$ in Figure 2.8a, which is shown in a 3-D view in Figure 2.9a, and a 2-D view of the vertical plane looking down from the tube exit is shown in Figure 2.9b. Figure 2.9c shows the simulated deposition rates on the vertical expansion plane at six different flow rates. The figure shows that the deposition rates on the vertical wall are larger at the lower flow rates in agreement with the deposition rates on the adjoining horizontal walls, as shown in Figure 2.5b. The $y$-axis in Figure 2.9c represents the distance from the tube center to the secondary inner wall along the expansion plane, and the $x$-axis represents the deposition rate formed on the expansion plane. The parabolic-like shapes of the deposition rate profiles in Figure 2.9c result from the recirculation flow pattern. The simulations indicate that the recirculation center moves towards the tube center in the radial direction as the flow rate decreases, resulting in the deposition peak skewing toward the tube center.
Figure 2.9 Deposition rates around the expansion corner (a) 3-D image of the expansion section, (b) 2-D image of expansion plane and (c) deposition rates along the expansion plane at different flow rates
2.4.2 Contraction Tube

2.4.2.1 Measurement and Simulation along the Contraction Tube

Now we begin study of the contraction case, where the primary tube has a relatively wide ID and the secondary tube is narrow bore. Figure 2.10 compares measured and simulated deposits for the JP-8 and Jet A fuel samples. The results for this contraction flow show that the predicted peak deposit axial locations agree reasonably well with the measured deposit peak, as also observed in the expansion tube. As in the expansion tube, the agreement in deposit magnitude is significantly better for the Jet A fuel (F3084) than for the JP-8 fuel (F4177). Figure 2.10 shows that for both fuels the bulk of the deposits accumulate on the primary inner wall at all flow rates. As in the expansion tube case, it is difficult to observe evidence of excess deposition near the step using the experimental measurements.

It is essential to examine the dissolved $O_2$ consumption to better understand the deposit formation under different flow conditions. Figure 2.11 shows the simulated $O_2$ concentrations and deposition rates along the heated contraction tube for the Jet A fuel at four different flow rates. Figure 2.11a illustrates that most of the oxygen is consumed before the step change due to the large inner diameter and relatively long residence time in the primary tube. When the flow enters the secondary tube, the oxidation rates decrease due to higher velocities and shorter residence times. Figure 2.11b shows the distribution of the simulated deposition rate as a function tube length which can be compared with the dissolved oxygen concentrations in Figure 2.11a. The deposition rates quickly grow from the inlet until the maximum oxidation rate is reached, and then rapidly
decrease until the contraction plane is approached. The peak deposition rates for all the flow rates are located on the primary inner wall.

**Figure 2. 10** Measured and simulated deposits masses along the contraction tube at different flow rates for (a) F4177 (JP-8) and (b) F3084 (Jet A) fuel
A goal of this study was to perform the experiments at conditions where the deposit peak occurs near the step change. Unfortunately, it was not possible to increase the flow rate to move the deposit peak further downstream due to the self-imposed requirement of having complete oxygen consumption within the tube. Figure 2.11 shows that even at the 0.31 mL/min flow rate oxygen consumption is no longer complete within the tube. As in the expansion tube case, the figure demonstrates a tight coupling between flow rate and O₂ consumption, and as well as a strong correlation between the oxygen
consumption rate and the location of the deposit maximum. Unfortunately, the requirements of complete oxygen consumption in the tube limit the range of flow rates that can be employed for the contraction tube case. As a result the dissolved O₂ profiles vary only slightly for the different flow rates, and the deposition rate maxima are all in the primary tube and within 7 cm of each other. Figure 2.11b shows interesting behavior in the deposition rate near the step location, particularly for the highest flow rate (0.31 mL/min). At this flow, where the deposition peak is closest to the step, a sharp increase in deposition occurs near the step. The secondary tube also shows interesting behavior in the deposition rate, with a rapid drop in deposition rate after the step followed by a much slower decrease in deposition rate further downstream.

2.4.2.2 Fuel Behavior near the Step for the Contraction Case

To better understand the flow and chemistry behavior near the step region for the contraction case, Figure 2.12 shows velocity profiles, species concentration contours, and deposition rates for a flow rate of 0.28 mL/min. Figure 2.12a shows the simulated 2-D velocity vectors around the step change. The fully developed flow in the primary tube becomes disrupted by the step in the narrow axial region 1 mm upstream to 2 mm downstream of the contraction plane. In contrast with the expansion case, there is no recirculation flow near the step corner (rₙ), but instead the fuel flows downward near the step corner to the tube center. Also, the velocity rapidly increases as the fuel enters the throat of the narrow secondary tube and continues to increase until becoming fully developed in the secondary tube. This flow pattern indicates that the flow velocity decreases as the rₙ-rₙ plane is approached and the velocity tends to zero near the rₙ corner.
As this corner is a stagnant flow area, fuel resides at this location for a relatively long time which results in increased oxygen consumption, with only ~1.4% oxygen remaining there as shown in Figure 2.12b. The flow pattern forces the lower O₂ concentration fuel from the r_b corner to pass the inner contraction corner (r_a), mixing with the higher dissolved oxygen of the main flow. As a result, the dissolved oxygen concentration near the wall at the beginning of the secondary tube is relatively low. Further downstream in the secondary tube, the dissolved O₂ is slowly consumed due to the fast flow rate and short residence time in this tube as the flow becomes fully developed again.
Figure 2.12 Fuel flow and chemistry behavior near the contraction step for the 0.28 mL/min flow rate using F3084 Jet A fuel (a) Velocity vector, (b) O₂ mass fraction color contour, (c) insoluble mass fraction color contour and (d) deposition rate
Figure 2.12c shows a color contour plot of the simulated mass fraction of the insoluble species, which are the products of autooxidative reactions and are direct precursors of surface deposition (see Reaction 21 in Table 2.3). Figure 2.12c shows that significant quantities of insolubles are produced within primary tube due to the long residence time, with lower levels near the wall due to reaction at the wall to produce surface deposits. In the fully developed flow region (downstream) of the secondary tube, the faster flow rate and resulting lower oxidation rate results in fewer insolubles being produced there.

Figure 2.12d shows the simulated deposition rate along the primary and the secondary inner walls. The deposition rate on the primary tube wall slowly increases due to oxygen consumption, but suddenly drops at the outer contraction corner (r_b) as a result of the low dissolved O_2 concentration at that location. The highest deposition rate occurs in the secondary tube near the inner contraction corner (r_a). This high deposition rate on the wall of the secondary tube near the step occurs despite the fast flow rate and low oxidation rate in this tube. The deposition rate decreases rapidly over a distance of ~0.1 m after the contraction plane, and then decreases more slowly until the end of the heated tube as shown in Figure 2.12d. The higher deposition rate early in the secondary tube is caused by insolubles, produced in the primary tube, being forced into the secondary tube by the high flow rate at the throat. These high levels of insolubles react at the secondary inner wall to form surface deposits. If there were no additional insolubles injected from the primary tube, the deposition rate in the secondary tube would be significantly lower at the tube entrance. This excess deposition is shown in Figure 2.12d as a region above a line drawn qualitatively which estimates the deposition rate expected without injected
insolubles. The narrow tube ID, high velocity, and resulting short fuel residence time results in a low deposition rate expected there in the absence of the insolubles injected from the primary tube. This excess deposition occurs in a narrow flow passageway, greatly increasing the opportunity for fuel flow disruption, but fortunately it occurs over a fairly wide 10 cm axial distance.

The phenomenon of excess deposition at the secondary tube wall near the step is also observed for the other flow rates as shown in Figure 2.11b. The deposition rate in the secondary tube exhibits a rapid decrease near the step with a more gradual decrease further downstream for each flow condition. In Figure 2.13, the simulated deposition rate is plotted versus residence time with the axial distance converted to residence time at each flow rate as explained previously. Figure 2.13a shows that when plotted versus residence time the deposition rate profiles in the primary tube are identical until the contraction plane is reached. At the step location the deposition rate changes rapidly for each flow rate case, but the deposition rates again converge at long residence times after the flows become fully developed. Near the contraction plane, the magnitudes of the decrease in deposition near \( r_b \) and the increase in deposition near \( r_a \) both appear to be related to how close the step plane is to the peak in the deposition rate. For example, a large decrease in deposition rate near \( r_b \) and large increase near \( r_a \) is noted for the 0.31 mL/min flow rate which occurs closest to the maximum deposition rate. In contrast, at 0.21 mL/min the changes in deposition rate at these locations are significantly smaller. Thus, to minimize the excess deposition in the narrow tube it is important to avoid having the maximum deposition rate (and maximum oxidation rate) occurs near sudden flow geometry contractions.
Figure 2. 13 Simulated deposition rates vs. residence time for (a) 0-250 s and (b) 115-185 s for F3084 fuel flowing in the contraction tube at different flow rates.
Figure 2.14 shows the simulated deposition rates for the vertical surface at the contraction plane for four different flow rates. In contrast to the peaked deposition behavior observed for the vertical surface in the expansion case, the deposition profile is nearly linear from the outer corner ($r_b$) to the inner step corner ($r_a$) with the deposition increasing towards the tube center axis. The lower deposition rate in the outer corner ($r_b$) is likely due to the lower oxygen level at this location. In addition, the figure shows that the deposition rate increases with increasing flow rate, which agrees with the adjoining deposition on the primary and secondary tube horizontal surfaces (Figure 2.11b). The deposition rate for the 0.21 mL/min flow rate is quite low due to the very low oxygen level (~1.5%) adjacent to the wall at this flow rate. For the expansion case, higher flow rates caused decreased deposition on this vertical surface while for the contraction case the reverse is true.

![Figure 2.14 Simulated deposition rates along the contraction plane at different flow rates](image-url)
2.4.3 Implications for Fuel System Design and Operation

One goal of this work is to improve the ability of fuel system and nozzle designers to efficiently utilize the fuel heat sink while preventing the negative impact of fuel degradation associated with high temperature fuel autoxidation. While aircraft fuel systems and nozzles contain extremely complex flow pathways, the simple cylindrical expansion and contraction systems studied here provide interesting information that can be used to help design fuel system components that minimize excessive surface deposition from fuel autoxidative degradation.

For the expansion tube case, recirculation flow causes excess deposition at the beginning of the wider secondary. As this deposition occurs in the wider tube it is not as likely to cause problems as if it occurred in the narrower bore tubing. Although care must be taken, as at most reasonable flow rates the deposit occurs over a relatively narrow axial range. The designer needs to consider both the flow rate and the wall and fuel temperatures for this situation. Lower flow rates, such as will occur for fuel flowing through a leaky valve, along with high fuel and wall temperatures will decrease the length of the recirculation zone and shorten the axial length of the tube in which the deposits occur. This will greatly increase the deposit mass per unit area and may cause narrowing of the passageway even for relatively wide flow passages.

The contraction case is more likely to be found in aircraft systems, as fuel is transported through wide tubing in the fuel tank to narrow passageways in the nozzle. For the contraction case the excess deposition occurs at the beginning of the narrow secondary tube, which is the type of tight clearance location in which deposition needs to be avoided. Therefore, the designer should avoid sudden contractions in passageway
diameter in locations where the fuel and wall temperatures are high. Fortunately, the acceleration of flow in the narrow tube causes the surface deposition to be spread over a greater axial region than in the expansion case. The fuel flow rate will play a role in how the deposition is spread over the length of the tube, with higher flow rates being desirable to minimize deposit quantity per unit surface area in the narrow tubing after a contraction.

In both expansion and contraction situations, the designer should avoid having the peak of oxidation and deposition rates occur near these flow geometry changes. Ideally, performing the CFD with chemistry calculation shown here for the entire heated section of the fuel system would allow prediction of the location of maximum deposition as a function of the engine throttle setting and indicate engine settings and fuel system locations where deposition can be of concern. Although it may not be currently practical to simulate such a large and complex region, it may be possible to perform these calculations on the highest temperature regions of the fuel system.
CHAPTER III

NUMERICAL SIMULATIONS OF THE FLUID DYNAMICS AND HEAT TRANSFER WITHIN A ROTATING PASSAGE

3.1 Introduction

In Chapter 3, the effect of rotation and flow path geometries on fuel heat transfer in heated rotating passages is considered. In general, flow in a rotating passage is a complex phenomenon due to the centrifugal and the Coriolis forces. The facts that the fluid is fuel and that the fuel is heated in rotating tubing greatly increases the difficulty. Computational fluid dynamics (CFD) simulations can now permit visualization and analysis of the flow for behavior that is otherwise unobservable within a heated, rotating metal tube. The purpose of this work is to use a CFD model to simulate fuel flow velocities and temperatures under different rotational speeds. Two geometries were modeled to study the effect of the flow path on fuel heating time. However, for this initial work, fuel chemistry is not modeled.

3.2 Overview of the Experimental Rig

The Air Force has begun an experimental and computational research program to study the influence of rotation on the heat transfer for a heated, flowing hydrocarbon liquid. At the time of the writing of this dissertation, the experimental facility was
incomplete. However, preliminary simulations were performed to assist in the design of the test articles. This section provides a brief overview of the experimental rig.

The experiment involves the flow of a hydrocarbon fuel through a heated, rotating passage. In Figure 3.1, liquid fuel enters the horizontal shaft and flows into two opposing tubular test specimens (stainless-steel 316) with a mass flow rate of 7 g/sec. The flow of fuel through these test pieces is simulated in this work. Two test pieces are required for balancing the shaft loads during rotation, and they are heated as they rotate in front of an annular burner with maximum flame temperatures on the order of 1200°C (2192°F) provided by ethylene combustion (Figure 3.2). A variable-speed electric motor (68 HP) turns the shaft and tube assembly which is supported by high speed bearings and bearing holders (Figure 3.2). The rotating components are surrounded by a steel-plate shield that is reinforced with sand bags. The exiting fuel is cooled by means of a heat exchanger and exits to a scrap tank. Temperatures are measured along the external tube walls and at a few internal locations. In addition, we set an operating pressure of 4 MPa to keep the fuel from boiling as fuel temperature increased above the critical temperature. The system pressures increase when the test specimens rotate, which are measured along the flow passage.
Figure 3. 1 Test pieces mounted on rotating shaft for heated fuel flow

Figure 3. 2 Experimental apparatus
3.3 Numerical Section

A numerical investigation was conducted to study the flow characteristics and heat transfer in the experimental rig. Figure 3.3 shows the test specimen, which is vertical in the y-direction and rotates about the x-axis. When the tube rotates, centrifugal and Coriolis forces are imposed on the fuel. The centrifugal force is proportional to the square of the rotational speed and acts outward in the radial direction. The Coriolis force is proportional to the rotational speed and its direction is roughly perpendicular to the rotation axis and to the velocity of the body in the rotating frame. The combination of centrifugal and Coriolis forces act to influence the fuel velocity field. Also, the heated fuel flowing in rotating passages of a small diameter may potentially have relatively large velocities, resulting in turbulent flow. The temperature difference between the heated wall and the fuel results in fuel density differences which generate buoyancy forces within the flow ($F_B = \Delta \rho g \beta \Delta T$, $\Delta \rho$ and $\Delta T$ are the difference of the density and temperature, respectively. $g$ is gravity and $\beta$ is the thermal expansion coefficient). Both natural and forced convective heat transfer can occur in the fuel. Therefore, the involved heat transfer is complex.
3.3.1 Governing Equations

The unsteady, three-dimensional Navier-Stokes and energy equations were solved using a commercial software package (Fluent). A single rotating reference frame (SRF) was used to simulate the fuel flowing through a test article. The governing equations written for a relative velocity formulation are:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}_r) = 0 \tag{3.1}
\]

\[
\frac{\partial}{\partial t} (\rho \vec{v}_r) + \nabla \cdot (\rho \vec{v}_r \vec{v}_r) + \rho (\vec{\omega} \times \vec{\omega} \times \vec{r} + 2\vec{\omega} \times \vec{v}_r) = -\nabla P + \nabla \cdot \vec{\tau}_r + \vec{F} \tag{3.2}
\]

\[
\frac{\partial}{\partial t} (\rho E_r) + \nabla \cdot (\rho \vec{v}_r H_r) = \nabla \cdot (K \nabla T + \vec{\tau}_r \cdot \vec{v}_r) \tag{3.3}
\]

\[
\vec{u} = \vec{v}_r + \vec{\omega} \times \vec{r} \tag{3.4}
\]

Here \(\rho\) is the fuel density, \(\vec{v}_r\) is the relative velocity, \(\vec{\omega}\) is the angular velocity and \(\vec{r}\) is the position vector from the x-axis. \(P\) is the pressure, \(\vec{\tau}_r\) is the relative stress tensor, \(\vec{F}\)
is the gravitational body force, \( E_r \) is the relative internal energy, \( H_r \) is the relative total enthalpy, \( K \) is the thermal conductivity, \( T \) is the fuel temperature and \( \bar{u} \) is the absolute velocity.

Equations (3.1), (3.2) and (3.3) are the mass, momentum and energy equations, respectively. Equation (3.4) relates the absolute velocity to the relative velocity. In a rotating reference frame, the centrifugal \( (\bar{\omega} \times \bar{\omega} \times \bar{r}) \) and Coriolis \( (2\bar{\omega} \times \bar{v}_r) \) accelerations appear in the momentum equation (3.2). \(^{40,42}\)

### 3.3.2 Turbulent Flow Equations

Turbulent flow is irregular, random, and chaotic. The instantaneous variables may be decomposed into a mean value and a fluctuating value \( (\bar{u} = \bar{u} + u', P = \bar{P} + p' \text{ and } T = \bar{T} + T') \).\(^{43}\) Inserting the instantaneous velocities into the momentum equation, six additional unknown terms (called Reynolds stresses, \( \tau_{ij} = -\rho u_i u_j \)) are formed. The Boussinesq approximation represents the Reynolds stresses as a function of the mean velocity gradient. The Reynolds-averaged k-\( \varepsilon \) turbulence model involves two transport equations to solve for the turbulent kinetic energy \( (k) \) and the turbulent dissipation rate \( (\varepsilon) \). Thus, other turbulent variables, such as turbulence intensity and turbulent viscosity can be obtained through the turbulent kinetic energy and the turbulent dissipation rate. In the present work, the standard wall function was used to calculate the flow variables near the wall. The standard wall function permits relatively coarse grids in the wall region to reduce computational time.
3.3.3 Numerical Solver and Grids in the Calculation Domain

The SIMPLEC (Semi-Implicit Method for Pressure-Linked Equations Consistent) algorithm was employed to solve the governing equations under the pressure-velocity coupling scheme. For complicated flows involving turbulence and flow rotation, the SIMPLEC method improves convergence relative to other algorithms when solving the governing equations iteratively.$^{44}$

To numerically solve the dependent variables ($P$, $u$, $v$, $T$, etc.) in the governing equations, a finite-volume technique was used. The domain was discretized using a tetrahedral/hybrid unstructured grid (Figure 3.4). The total number of computational cells was 72,798 with 6 cells across the small diameter and 16 cells across the horizontal shaft diameter. A second-order accurate upwind scheme for momentum, energy, and turbulent transport equations was used. The transient implicit formulation was second-order accurate representation of the time derivative. The simulations required a small time step of the order 0.1 ms due to convergence difficulties. In order to gain a converged solution, 50 iterations were used for each time step. Convergence was assumed when the error residuals were reduced below four orders of magnitude from their maximum, and the mass imbalance was two orders of magnitude smaller than mass flow rate.
Figure 3.4 Illustration of the tubing size and three-dimensional unstructured grid with (a) enlarged view of the bottom junction, (b) view of the entire tube system, and (c) enlarged view of the top rectangular flow path.
3.3.4 Boundary and Initial Conditions

In the current simulations, the initial wall temperatures were selected based on maximum temperature expectations in a similar application. Figure 3.5 shows the wall temperatures imposed on the tubing. Because a flame is intended to be supplied to the exterior of the rectangular shape in the experiments, a 1100 K outer wall temperature was assumed there. Along the inlet leg, the wall temperature varied linearly from 300K (bottom junction) to 600 K (top junction). Along the outlet leg, the wall temperature was assumed to linearly vary from 1100 K (top junction) to 300 K (bottom junction) due to the flame on the outlet side. For the horizontal shaft, a 300 K wall temperature was assumed because rotating carbon seals contained the coolant that was used to cool the horizontal shaft.

In the rotating reference frame, the inlet velocity is required in terms of the relative velocity. Thus, a uniform (normal to the inlet boundary and relative to the adjacent cell zone) relative velocity was set at the inlet, and the fuel there was assumed to be 300 K. Figure 3.5 shows 0.0593 m/s as the inlet velocity, which was obtained from the fuel mass flow rate of 7 g/s. This flow rate will be used in the experiments.
Figure 3.5 Boundary conditions in simulations
The temperature-dependent properties of JP-10 fuel were used in the simulations as this fuel will be used in the experiments. The density ($\rho$), specific heat ($C_p$), thermal conductivity ($K$), and viscosity ($\nu$) were represented by piecewise linear fits with temperature. For simplicity, conduction heat transfer within the thin tube wall was neglected in the calculations.

The simulations were started with an initial rotational speed of 200 rpm, and then incrementally increased by 100 rpm until convergence for each rotational speed, up to 3000 rpm. It was difficult to obtain a converged solution for a desired rotational speed if steps greater than 100 rpm were used. Convergence was assumed when the bulk outlet temperature reached steady conditions along with the reduction in residuals and a negligible mass imbalance at a rotational speed. For example, when the rotational speed is changed from 2900 rpm to 3000 rpm, Table 3.1 shows the outlet bulk temperature gradually increased until a steady value was reached at 325 ms. When the fuel reached a steady outlet bulk temperature of 379 K, the results were considered to be converged for a rotational speed of 3000 rpm.

<table>
<thead>
<tr>
<th>Time (ms)</th>
<th>10</th>
<th>25</th>
<th>75</th>
<th>125</th>
<th>175</th>
<th>225</th>
<th>275</th>
<th>325</th>
<th>350</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet Temp (K)</td>
<td>372</td>
<td>372</td>
<td>373</td>
<td>375</td>
<td>376</td>
<td>377</td>
<td>378</td>
<td>379</td>
<td>379</td>
</tr>
</tbody>
</table>

**Table 3.1** Calculated Outlet Bulk Temperatures Varied with Computational Time at 3000 rpm
3.4 Results and Discussion

The simulated results are now described for jet fuel passing through heated rotating passages. The effect of the rotational speed on the flow character and heat transfer is studied. In order to understand how the flow path influences the heat transfer in the rotating configuration, the simulations are performed using similar geometries but with and without a bypass (the passage that joins the two angled legs) under the same boundary conditions. Initially, the fuel behavior at 3000 rpm is examined since it is the highest rotational speed for the current simulations. The velocity, temperature, and pressure of the fuel are described at 3000 rpm. Then, two rotational speeds (0 rpm and 1000 rpm) are chosen to compare the fuel characteristics with those at 3000 rpm. Lastly, the results of the fuel passing through the geometry without a bypass at 3000 rpm are presented. It is necessary to perform three-dimensional simulations under the complex flow conditions. However, it is difficult to view the fuel velocities and temperatures in three-dimensions. Thus, two-dimensional slices of a three-dimensional volume are used to view the physical phenomena in the following sections.

3.4.1 Jet Fuel Flow in Heated Tubing at a Rotational Speed of 3000 rpm

Figure 3.6 shows relative velocity vectors for a rotational speed of 3000 rpm in three viewing planes marked C-C section, B-B section, and D-D section. The C-C section shows that the fuel flows to the top of the tubing, and the B-B section shows that fuels rotate in the cross-sectional area of the two vertical passages, which indicate a potential higher heat transfer there. The D-D plane shows that the fuel rotates in the horizontal
shaft, and the velocity magnitude increases proportionally in the radial direction of the
shaft.

The velocity vectors of Figure 3.6 are obtained by modeling the entire tubing in
three-dimensional. Axisymmetric simulations involving one segment of tubing showed
that the flow in the horizontal shaft did not rotate about the axis (x-axis) of rotation.
Figure 3.7 shows the incorrect relative velocity vectors in the y-z plane forming two
rotating cells (same location as the D-D plane of Figure 3.6). The correct relative velocity
vectors should all rotate about a single axis as in Figure 3.6 (section D-D). The
axisymmetric model in Fluent does not give correct results even though the physical
situation is axisymmetric (Figure 3.5).
Figure 3.6 Relative velocity vectors in different viewing planes obtained from three dimensional simulations.

Fuel inlet: $\omega = 3000 \text{ rpm}$

B-B section

D-D section

C-C section (center plane)
Figure 3.7 Incorrect relative velocity vectors in the D-D plane obtained from an axisymmetric model

Figure 3.8a shows temperature color contour in the center plane for a rotational speed of 3000 rpm. The inlet fuel temperature is 300 K and remains 300 K along the horizontal shaft of inlet side. The fuel is heated gradually along the right leg, then, heated to a higher temperature in the top portions of the rectangular flow path due to the higher wall temperature (1100 K) and large heat transfer rates there. As the heated fuel passes through the left leg, the temperature gradually decreases because the wall temperature decreases from the top junction to the bottom junction. As the fuel flows into the shaft of
the outlet side, the wall temperature of 300 K cools the heated fuel which is adjacent to the wall. The fuel remains at bulk temperature at 379 K at outlet of the horizontal shaft.

Figure 3.8b shows color contour for the dynamic pressure in the center plane as the tubing rotates at 3000 rpm. The dynamic pressure increases in the y-direction largely due to centrifugal force. The maximum dynamic pressure is at the tip of the article. There is a slight difference in the dynamic pressure between the inlet side and the outlet side at the same radial location, resulting from the influence of the fuel temperature on the density and the relative velocity.
Figure 3.8 Simulated color contours at the center plane for a rotational speed of 3000 rpm showing the (a) fuel temperature distribution and (b) dynamic pressure distribution.
3.4.2 Effect of Rotational Speeds on the Flow and Heat Transfer

To investigate the effect of the rotational speed on the flow and fuel temperature, simulations for 0 rpm, 1000 rpm, and 3000 rpm are compared. Figure 3.9a shows relative velocity vectors at the upper portion of the center plane (a rectangular flow path). In these figures, the vector color is proportional to the velocity magnitude. For a rotational speed of 0 rpm, relatively little fuel flows through the top flow passage with an average velocity ~ 0.06 m/s. Most of the fuel flows through the bypass with an average velocity of ~ 0.31 m/s for an inlet mass flow rate of 7 g/s. At 1000 rpm, most of the fuel passes through the top flow passage, and relatively less fuel flows through the bypass, because the centrifugal force drives the fuel through the top flow passage. At 3000 rpm, it is evident in Figure 3.9a that there is recirculation flow within the rectangular flow path with the highest flow velocity relative to 0 rpm and 1000 rpm.
Figure 3. 9 Simulations for 0 rpm, 1000 rpm, and 3000 rpm showing (a) relative velocity vectors in the rectangular flow path, (b) section view of relative velocity vectors, (c) section view of fuel temperature, and (d) temperature in rectangular flow path.
Figures 3.9b and 3.9c are two dimensional slices of the top horizontal tube, which are used to describe how the rotating flow influences the heat transfer at three rotational speeds. Section A-A is located below the center of the top horizontal tube. (The location of the viewing plane relative to the axis of rotation affects the viewed diameter of the vertical tubes, and one of the tube diameters appears larger than the others).

Figure 3.9b shows the relative velocity vectors for the three rotational speeds in section A-A. At 0 rpm, the vectors show that the fuel flows from right to left without rotating. At 1000 rpm, rotating cells can be observed. As the rotational speed increases to 3000 rpm, the rotating structures become larger. The calculated average Reynolds numbers (based on the relative velocity) in the A-A section are ~1000, 2400, and 5300 for rotational speeds of 0 rpm, 1000 rpm and 3000 rpm. The increasing Reynolds number beyond 2300 suggests a transition from the laminar to turbulent flow as the rotational speed increases. In other words, the rotation promotes turbulent flow during heating. The simulations indicate that the turbulent intensities in section A-A are ~8.5% and ~35% for rotational speeds of 1000 rpm and 3000 rpm, respectively. (The turbulence intensity is the ratio of the turbulent velocity fluctuations to the mean velocity). Therefore, in a rotating system, increases in rotational speed result in greater turbulent velocity fluctuations, which increase the heat transfer within the fuel. The vectors in Figure 3.9b show that the fuel rotates from the wall towards the tube center at 1000 rpm in the A-A section. It is observed that most of the fuel rotates in one direction at 3000 rpm. Thus, the increase in rotational speed during heating not only increases the magnitude of the flow velocity, but also changes the direction of the rotating fuel.
Figure 3.9c shows the temperature color contours in section A-A. The thermal boundary layer of the fuel is observable for all three rotational speeds. The fuel temperatures in the tube center increase as the rotational speed increases. The mass-weighted average temperatures in the A-A section are 320 K, 370 K and 465 K for rotational speeds of 0 rpm, 1000 rpm and 3000 rpm, respectively. A higher fuel temperature, which means a lower fuel density, translates to a greater relative velocity due to mass conservation. Also, the gradients in fuel density and temperature influence the buoyancy force on the flow. As a result, the heat transfer is enhanced further. Previous work has also shown similar heat transfer characteristics in a rotating system.24

Figure 3.9d shows the temperature at the upper portion of the center plane (C-C section) for three rotational speeds. The fuel temperature within the rectangular flow path is higher at 3000 rpm than at 0 rpm and 1000 rpm. At 0 rpm, the lowest flow rate relatively to the other rotational speeds (Figure 3.9a) results in the lowest heat transfer rate in the flow path. The fuel is heated along the wall because the fuel is adjacent to the wall for long residence times. However, the fuel in the tubing center still remains at the inlet temperature of 300 K. At 1000 rpm, the range of the turbulence intensity in the rectangular flow path is ~ 4.8-12%. Thus, turbulent flow dominates the heat transfer and the fuel in the tube center is heated above 300 K. At 3000 rpm, the range of the turbulence intensity is ~ 20-45%, which provides the greatest heat transfer rate relative to 0 rpm and 1000 rpm. Moreover, the recirculation in the rectangular flow path (Figure 3.9a) increases residence time and contacts with the heated surfaces, which also increases the fuel temperature further at 3000 rpm.
Figure 3.9 describes the effect of rotational speed on the magnitude and direction of the flow, and, thus the heat transfer in the upper portion of the tubing. As the rotational speed increases, the large-scale fuel motion has a greater influence on the turbulent heat transfer.

3.4.3 Comparison of Fuel Temperatures in Two Geometries

In order to explore the effect of recirculation within a heated passage on the heat transfer in a rotating system, another similar geometry without a bypass is also treated. The boundary conditions are the same as those of the geometry with the bypass. We will refer to the geometry with the bypass as the “A” shape, and to the geometry without the bypass as the “Λ” shape in the following paragraphs.

Figure 3.10a shows the relative velocity vectors in the A-A section and the upper portion of the center plane for the “Λ” shape at 3000 rpm. At the same rotational speed, the magnitude of the centrifugal and Coriolis forces on the flow should be the roughly same for the “A” shape and the “Λ” shape. However, the relative velocity vectors in the A-A section show less internal rotation in the “Λ” shape (Figure 3.10a) than in the “A” shape (Figure 3.9a) at 3000 rpm. The vector color in the center plane (C-C section) shows that the magnitude of the relative velocity is smaller in the “Λ” shape than in the “A” shape. This phenomenon results from heating of the fuel. The fuel passes through the upper portion of tubing and then flows out toward the outlet in the “Λ” shape, while the fuel recirculates in the rectangular flow path of the “A” shape. The rectangular flow path allows recirculation which increases residence time for fuel heating. In contrast, the absence of the bypass for the “Λ” shape reduces the time that the fuel resides on the
heated surface. The flow accelerates in the passage due to the higher fuel temperature. Thus, the velocity is greater for the “A” shape than for the “Λ” shape at 3000 rpm, and the heat transfer in the upper portion of the “A” shape is higher than the “Λ” shape.
Figure 3.10 Simulated (a) relative velocity vectors and (b) temperature color contours with the “Λ” shape at the sections of A–A and C–C for a rotational speed of 3000 rpm.
The temperature color contours of Figure 3.10b display that the fuel in the center of section A-A is heated relatively little. The C-C section of Figure 3.10b shows that the fuel temperature is higher along the outlet side vertical tube than the inlet side vertical tube due to surface heating of the fuel in the “Λ” shape. Whereas the recirculating flow in the “A” shape causes the likely uniform temperature distribution along the rectangular flow path as shown in Figure 3.9d. The calculated average interior heat transfer coefficients for the outlet side vertical tube is 552 W/m$^2$-k and 721 W/m$^2$-k for the “Λ” shape and the “A” shape, respectively. A shorter residence time as in the case of the “Λ” shape (which has essentially no recirculation) has relatively lower heat transfer rates. Simulation results show that the mass-weighted average temperatures in the A-A section are 413 K and 465 K for the “Λ” shape and the “A” shape, respectively. In addition, the greater heat transfer is demonstrated by the greater outlet bulk temperatures (at horizontal shaft outlet) from the “A” shape (379 K) relative to the “Λ” shape (323 K).

This study analyzes the coupled effect between fluid dynamic and fuel heat transfer. CFD simulations show the fuel temperatures increase as the rotational speed increases, indicating a higher heat transfer of the fuel within the rotating passage. The flow path with bypass geometry provides a recirculation flow, which results a longer heating time for the fuel and, thus, increases the heat transfer rate.
CHAPTER IV

STUDIES OF JET FUEL HEAT TRANSFER AND THERMAL OXIDATION UNDER HIGH HEAT FLUX AND HIGH VELOCITY CONDITIONS

4.1 Introduction

This study considers how high heat fluxes and large flow velocities influence jet fuel heat transfer and thermal oxidation/deposition using both experiments and numerical simulations. CFD model assists to understand the role of the physical phenomenon of the jet fuel that may undergoing the phase change due to large heat fluxes. Three types of turbulence models (SKE $k$-$\varepsilon$, RNG $k$-$\varepsilon$ and SST $k$-$\omega$) in association with wall treatments were used to calculate the flow and the heat transfer which involved rapid heating and the large Reynolds number flow. The pseudo-detailed chemical kinetic mechanism was used to simulate fuel thermal oxidation and global deposition sub-mechanism was used to simulate the surface deposition in the heated tubes. The experiments were performed by flowing JP-8 fuel upward through the tubing and the tube was heated by resistive heating. Resistive heating was selected to achieve heat flux levels that were representative of the environment of regenerative cooling channels in the walls of rocket and missile combustion chambers. In the first series of experiments, five tests were implemented by varying flow rates and heating levels to study the coupled effects of the heat flux and flow velocity on the fuel heat transfer in the thermal boundary layer. In the second series
of experiments, two tests were implemented that fuel was passed through two different length tubes at the same inlet flow rate but different heating levels to study the effect of heat transfer on fuel thermal stability. This investigation is applicable to the regenerative cooling designs for rockets and hypersonic vehicles.

4.2 Experimental Setup

In past fuel degradation, experiments were concerned with aircraft thermal conditions that tube heating was accomplished by the use of heated copper blocks, radiant furnaces, sand baths, induction heating, or resistive heating. Relative to the other methods, resistive heating is simple and offers high heating rates, which are limited only by the maximum temperature of the tube material. Thus, resistive heating was selected for current experiments. Figure 4.1 shows the experimental setup. In this arrangement, fuel flows through a tube held vertically between two electrical clamps. The power to the resistive heater is provided by a 50 kVA DC power supply. The applied power for resistive heating depended on the desired fuel outlet bulk temperature and was limited by the maximum temperature (1375°C) allowed for the safe use of the (316) stainless-steel tubing.

Experiments were performed in which JP-8 fuel was heated as it passed upward through a stainless-steel (316) tube (OD=0.32 cm ID =0.069 cm). The exterior temperature profile in axial direction was measured by fourteen thermocouples which welded to the exterior surface of the tube. The uncertainty of the wall temperature measurement is $\pm 10^\circ$C. The fuel bulk temperature was measured at the connecting Tee beyond the actively heated section. The heated section refers to the tubing between the
electrical clamps, and the unheated section is downstream from the upper electrical clamps to the Tee (Figure 4.1).

![Figure 4.1: Phoenix Rig](image)

**Figure 4.1** Phoenix Rig

Table 4.1 summarizes the flow and heating conditions from the experiments. The use of long (25.4 cm) and short (12.7 cm) tubes provides a range of Reynolds numbers at the tube outlet for the same inlet flow rate of 300 mL/min, so that to study the fuel degradation between long and short tubes with different residence times. For the long tube, we varied the inlet flow rates and heat fluxes to explore the characteristic of the heat
transfer under rapidly heating conditions. The heat fluxes listed in Table 4.1 were calculated from the measured outlet fuel temperatures for each flow conditions, because the uncertainty of the power measurement was off over 20%. All the experiments were carried out at a pressure of 5.52 MPa (uncertainty of ± 2%). For this pressure level, the fuel remains a liquid phase for temperatures below its critical temperature. As the temperature is higher than its critical temperature, the fuel becomes supercritical phase. The duration of each experiment was limited to 25 min to avoid potential blockage by fuel deposits.

**Table 4. 1 Experimental Parameters (Phoenix Rig)**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Long tube</th>
<th>Short tube</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner diameter (cm)</td>
<td>0.069</td>
<td></td>
</tr>
<tr>
<td>Outer diameter (cm)</td>
<td>0.32</td>
<td></td>
</tr>
<tr>
<td>Heated (unheated) section (cm)</td>
<td>25.4 (15)</td>
<td>12.7 (15)</td>
</tr>
<tr>
<td>Inlet flow rate (mL/min)</td>
<td>100-460</td>
<td>300</td>
</tr>
<tr>
<td>Inlet Reynolds No.</td>
<td>1,700-7,100</td>
<td>4,700</td>
</tr>
<tr>
<td>Inlet fuel temperature (K)</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>Outlet fuel temperature (K)</td>
<td>400 - 680</td>
<td>570</td>
</tr>
<tr>
<td>Outlet Reynolds No.</td>
<td>19,900-111,000</td>
<td>85,900</td>
</tr>
<tr>
<td>Heat flux (kW/m²)</td>
<td>2,100-8,400</td>
<td>9,900</td>
</tr>
<tr>
<td>Pressure (MPa)</td>
<td></td>
<td>5.52</td>
</tr>
<tr>
<td>Duration time (min)</td>
<td></td>
<td>25</td>
</tr>
</tbody>
</table>

The dissolved O₂ was measured at both inlet and outlet of the heated tube by means of a modified on-line gas chromatograph.⁴⁵ The mass of the surface carbon deposits was measured by sectioning the tube and performing carbon-burn off measurements on the sections using a LECO RC-412 Multiphase Carbon Determiner (each section length is ~ 2.5 cm).
4.3 Computational Fluid Dynamics Simulations

4.3.1 Numerical Methodology

To understand the effects of heat flux, temperature distribution, and flow on thermal degradation, a commercially available CFD code (Fluent 12.0) was used to simulate the fluid dynamics, heat transfer and fuel chemical reactions within a heated tube. The simulations involved the finite volume solution of the Navier-Stokes, turbulent energy, thermal energy, and species equations. Convective terms were represented by a second order accurate upwind scheme, and a version of the SIMPLEC (Semi-Implicit Method for Pressure-Linked Equations Consistent) algorithm was used in the solution procedure. The upward flow inside the vertical tube was assumed to be axisymmetric and steady. For the relatively large velocities involved in this study, buoyancy forces within the fuel were assumed to have a negligible influence on the fluid dynamics. Thus, the gravity term was not included in the momentum equations. The effect of surface deposition on the flow itself (i.e., flow blockage and heat transfer resistance) was not modeled. For the very thin deposits detected in the present experiments, this is reasonable. When the continuity, velocity, turbulent kinetic energy, turbulent dissipation and species residuals were reduced below four orders of magnitude from their maximum values, the solutions were considered to be converged.

Since jet fuel is a complex mixture of hydrocarbons, a surrogate fuel was used for simplicity. N-dodecane has a critical temperature and pressure similar to the pseudo-critical temperature and pressure of the selected JP-8 sample. In previous work, n-dodecane was used to reasonably approximate the heat transfer of a JP-8 fuel for smooth property transitions between a compressed liquid and a supercritical fluid. Hence, n-
dodecane was selected as a surrogate fuel in the present simulations. Temperature-dependent properties for the fuel (density, viscosity, thermal conductivity, and specific heat), obtained from the SUPERTRAPP hydrocarbon properties program, were incorporated in the CFD database. In addition, a piecewise linear curve was used for the tube material properties (specific heat and conductivity) in the simulations.

### 4.3.2 Boundary and Initial Conditions

The velocity and temperature profiles at inlet were assumed to be uniform for simplicity. The inlet fuel velocity was calculated from the cross-sectional flow area of the tube together with the inlet volumetric flow rate. The simulations were initialized by assuming the inlet temperature and velocity values for all interior cells. The outlet conditions were extrapolated from interior cells. The tube ends were assumed to be adiabatic.

Assuming that the resistive heating occurred uniformly throughout the volume of the tube wall, the volumetric heat generation rate ($\dot{q}$, W/m$^3$) was calculated using equation (4.1). The heat flux ($q''$, W/m$^2$) on the interior wall surface of the tube was calculated using equation (4.2).

$$\dot{q} = \frac{\dot{m}(h_{\text{outlet}} - h_{\text{inlet}})}{\text{Vol}}$$

$$q'' = \frac{\dot{m}(h_{\text{outlet}} - h_{\text{inlet}})}{A_{\text{inner wall}}}$$

In equations (4.1) and (4.2), $\dot{m}$ is the mass flow rate, $h_{\text{outlet}}$ and $h_{\text{inlet}}$ are the fuel enthalpy at outlet and inlet, respectively (enthalpy was obtained from NIST based on
fuel temperature\textsuperscript{41}). \( V_{\text{ol}} \) represents the volume of the tube wall within the heated section, and \( A_{\text{inner wall}} \) represents the area of tube interior wall surface in the heated section.

The convection heat loss from the exterior wall was estimated using the correlation of equation (4.3).\textsuperscript{46} In equation (4.3), \( \text{Nu} \) is the Nusselt number, \( \text{Ra} \) is the Rayleigh number, and \( \text{Pr} \) is the Prandtl number.

\[
\frac{\text{Nu}}{\text{Pr}^{0.492}} = 0.67 \times \left( \frac{\text{Ra}}{1 + 0.492} \right)^{1/4}
\]  

(4.3)

The radiation heat loss from the exterior wall was estimated by using a tube emissivity of tube 0.8.\textsuperscript{46} The total heat losses were taken as the sum of the convective and radiative heat losses. The calculations showed the total heat losses were less than \(~3\%\) compared to the input power. Thus, the heat losses from the exterior wall were considered negligible and were not included in the CFD calculations. In some simulation of this work, the exterior wall was assumed to be insulated as an outer wall boundary condition. In other simulations, a cubic spline curve fit of the measured exterior wall temperatures were used as an outer wall thermal boundary condition. The detail of the exterior wall boundary conditions will be explained in section of 4.4.1.

Axisymmetric computational domain was used to calculate the flow, temperature and chemical reactions for both long and short tubes. Figure 4.2 shows a representative grid structure and the cell numbers used in the simulations. Cells comprising the relatively thick tube walls were included in the computational domain. The unheated section was also included in the simulations such that the measured bulk temperature at the outlet could be used as one form of validation of the simulations.
In the axial direction of Figure 4.2, there were more computational cells in the heated region than in the unheated region. However, the cells in each of those regions were spaced uniformly in the axial direction. In addition, the cells within the tube wall were spaced uniformly in the radial direction. Due to the high heating rates, relatively large radial temperature gradients were expected at the solid-liquid interface. Thus, the structured grids were clustered more densely in this region.

4.3.3 Turbulence Models and Wall Functions

The standard k-ε turbulence model has been employed in nearly all past simulations of fuel thermal degradation within heated tubes,\textsuperscript{13,48,49} This is believed to be due to its relative simplicity and fidelity with experimental measurements in a variety of flow applications. In past simulations of fuel degradation, the Reynolds numbers and heat flux levels were much lower than those considered in the present experiments.\textsuperscript{13} Since it
is known that the standard \( k-\varepsilon \) model may be inaccurate in some situations, other turbulence models are considered for the high heat flux levels and flow velocities treated here. Higher order turbulence models (e.g., Reynolds Stress models) could be used, but the increase in complexity combined with the difficulties of chemical kinetic mechanisms would result in an impractical computational time. Thus, the turbulence models of the renormalization group (RNG) \( k-\varepsilon \) model and the shear stress transport (SST) \( k-\omega \) model are selected in this study for the simulation of turbulent fuel flow.

The RNG \( k-\varepsilon \) turbulence model was developed through the Renormalization Group Theory. The turbulent kinetic energy equation in the RNG \( k-\varepsilon \) model is similar to that of the standard \( k-\varepsilon \) model, but an additional strain rate term in the equation for the dissipation rate is one significant difference between the standard and RNG \( k-\varepsilon \) models.\(^4\)\(^0\) The RNG model is suitable to the conditions involving complicated wall boundary conditions. Past work showed that the RNG \( k-\varepsilon \) model provided reasonable fidelity relative to other turbulence models.\(^5\)\(^0\)

The SST \( k-\omega \) turbulence model was developed from features of the \( k-\omega \) and \( k-\varepsilon \) eddy-viscosity models,\(^5\)\(^4\),\(^5\)\(^9\) and the blending function is used to transfer from \( k-\omega \) to \( k-\varepsilon \) zones.\(^5\)\(^2\),\(^5\)\(^4\) In addition, the SST \( k-\omega \) incorporates a diffusion derivative term in the \( \omega \)-equation to modify the turbulent viscosity (\( \mu_t \)), thus, the calculated turbulent heat fluxes also include the effect of the low Reynolds number flow reguiib.\(^5\)\(^5\) The SST \( k-\omega \) model is known to be more accurate than the \( k-\varepsilon \) model near the wall for many flows.

Unlike the SST \( k-\omega \) turbulence model, the SKE and RNG turbulence models do not provide flow values from the far field region to the wall,\(^5\)\(^6\) wall functions have to be used to determine the flow variables near the solid boundary.\(^5\)\(^7\) The standard wall
function is based on law-of-the-wall velocity distribution, and a requirement is that the
first grid point is located above the buffer sub-layer in the region where \( y^+ \) lies between
30 and 300. The benefit for use of the standard wall function is to get convergence
solutions easier for the coarse grids in the near wall region.\(^40\) However, the use of coarse
grids there may limit the accuracy of the calculations.\(^57\) The enhanced wall function
combines a blended law-of-the wall and a two-layer zonal model to describe the flow
within the inner layer of the wall.\(^40,56\) For the enhanced wall function, the first grid point
is located within the viscous sub-layer, so that \( y^+ \leq 1 \).

In this work, simulations are performed using the standard \( k-\epsilon \) model as it is
considered here to be a baseline model for purposes of comparison. Thus, the SKE \( k-\epsilon \)
models incorporates with both the standard and the enhanced wall functions, while RNG
\( k-\epsilon \) model only combine with the enhanced wall function. The RNG \( k-\epsilon \) model employed
with the enhanced wall function has been successfully used in past heat transfer studies
but for thermal and flow conditions that are very different from the present conditions.\(^50\)
In addition, SST \( k-\omega \) turbulence model have been widely used for the flow conditions
involved complex wall boundary conditions, thus, SST \( k-\omega \) model is the one of the
selected turbulence model in this work.

4.3.4 Chemical Mechanism

To improve the understanding of the chemistry involved in fuel system deposit
formation, pseudo-detailed chemical kinetic mechanisms representing thermal-oxidation
has been developed.\(^11,13\) A pseudo-detailed kinetic mechanism treats the fuel as a mixture
of compound classes and is comprised of reactions with rate parameters that are generally in agreement with those found in the literature.\textsuperscript{12,14} Based on the pseudo-detailed chemical kinetic mechanisms, a global deposition sub-mechanism was developed to simulate the deposition rate.\textsuperscript{16} The reactions of thermal oxidation and deposition with their active energy and “A” factors are the same as Table 2.3 in chapter 2. The pseudo-detailed chemical kinetics mechanism here used the concentration of species AH and SH to differentiate fuel samples. For all thermal oxidation simulations, the small initial concentration of species I is $1.0 \times 10^{-8}$ mole/L which was also used previously by Ervin and Zabarnick.\textsuperscript{13} The initial concentrations of dissolved O$_2$ is assumed to be 70 ppm ($\sim1.8 \times 10^{-3}$ mole/L), and AH and SH are assumed to be $\sim2.18 \times 10^{-4}$ mole/L and $\sim9.447 \times 10^{-3}$ mole/L, respectively.\textsuperscript{16}

As described later in this study, the fuel is heated to the supercritical regime only in thin regions adjacent to the wall and sometimes in the bulk fuel at the tube exit. Since the pyrolytic temperature regime is confined to thin regions, cracking and the effects of pyrolysis on bulk fuel properties were ignored in the simulations. Thus, the present work does not numerically simulate the pyrolytic chemistry of jet fuel.
4.4 Results and Discussion

With regard to the simulation of the heat transfer and fuel chemistry within a turbulent flow under conditions of rapid heating, it is important to first correctly calculate the temperatures within the flowing fuel because the fuel degradation reaction rates depend on the fuel temperature. In the following paragraphs, we describe the selection of a turbulence model to simulate the fuel temperatures. This is followed by a discussion of heat transfer deterioration. Lastly, fuel temperatures and thermal-oxidative reactions are simulated within the long and short tubes to study the effects of rapidly heating and short residence time on dissolved O₂ consumption and surface deposition.

4.4.1 Studies of Turbulence Models

Accurate numerical solutions can provide improved understanding of the influence of the flow conditions on heat transfer and the thermal reactions. Thus, it is essential to select an appropriate turbulence model for the conditions of high heat flux and high flow rate. The turbulence models selected for this study are the standard $k$-$\varepsilon$ with the standard wall function (SKE-st), standard $k$-$\varepsilon$ with the enhanced wall function (SKE-en), renormalization group $k$-$\varepsilon$ with the enhanced wall function (RNG-en), and the shear stress transport $k$-$\omega$ (SST).

Two different thermal representations for the heating of the tube wall were used in the calculations to validate the selected turbulence models. The simulations were first performed using the measured exterior wall temperatures as a boundary condition for the energy equation. The outlet bulk temperatures calculated by the four turbulence models
were compared with the measured outlet temperature. The simulations were performed again using volumetric heat generation for the energy equation. In addition, an adiabatic exterior wall was assumed as a thermal exterior wall boundary condition. For this second set of simulations, the measured and simulated exterior wall temperature profiles were compared. Since the wall temperatures were calculated rather than being imposed as a boundary condition in the second treatment, it is considered to be a more stringent test of the turbulence models. In both kinds of simulations an inlet flow rate of 300 mL/min and conditions which produced a heat flux of 7,638 kW/m² were used. This flow rate results in turbulent flow within the entire tube (inlet Re of 4,680 and exit Re of 111,000).

Table 4.2 and Figure 4.3 are the simulation results in the use of the measured exterior wall temperature as a thermal boundary condition through the four turbulence models (SKE-st, SKE-en, RNG-en and SST). Table 4.2 lists the detail turbulence models and wall treatments resulting in the $y^+$ values and temperatures at outlet. The $y^+$ value is an indication that the grid density near the wall satisfies the requirements for the different wall functions/models.⁴⁰ The outlet bulk temperature (mass-weighted average) was calculated for a location at the end of the unheated section where a thermocouple measured the outlet fuel temperature. The $\Delta T_{\text{outlet}}$ in Table 4.2 represents a difference between the simulated and the measured outlet fuel bulk temperature for the each selected turbulence models.
Table 4.2 Comparison of Outlet Bulk Temperatures Calculated by Various Turbulence Models with a Measured Outlet Bulk Temperature of 677 K

<table>
<thead>
<tr>
<th>turbulence model</th>
<th>wall treatment</th>
<th>$y^+$ (range)</th>
<th>simulated outlet temperature (K)</th>
<th>$\Delta T_{\text{outlet}}$ (K) $(T_{\text{simulated}} - T_{\text{measured}})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SKE-st</td>
<td>standard wall function</td>
<td>20-120</td>
<td>712</td>
<td>35</td>
</tr>
<tr>
<td>SKE-en</td>
<td>enhanced wall function</td>
<td>0.3-0.6</td>
<td>650</td>
<td>-27</td>
</tr>
<tr>
<td>RNG-en</td>
<td>enhanced wall function</td>
<td>0.2-0.8</td>
<td>667</td>
<td>-10</td>
</tr>
<tr>
<td>SST</td>
<td>standard k-$\omega$ model</td>
<td>0.3-0.6</td>
<td>662</td>
<td>-15</td>
</tr>
</tbody>
</table>

Note: SKE = Standard k-$\epsilon$, RNG = Renormalization Group, SST = Shear Stress Transport
st = standard wall function, en = enhanced wall function.

Figure 4.3 shows simulated fuel temperatures at the tube centerline calculated by the four models, and the measured outlet fuel temperature is shown for reference. The fuel temperature determined with the SKE-st model rises more rapidly than those calculated by the other models. Thus, the use of the SKE-st model here predicts a relatively high convective heat transfer to the fuel. As shown in Table 4.2, the largest $\Delta T_{\text{outlet}}$ is associated with the SKE-st model and suggests that the use of coarse grid spacing near the wall which is required by this method is inaccurate for these high heat flux flow condition. In contrast, fine grid spacing is used near the wall for the SKE-en, RNG-en and SST turbulence models such that the first grid point lies within the viscous sub-layer as the $y^+$ value is less than 1 in Table 4.2. Figure 4.3 shows the use of fine grid spacing in the vicinity of the wall yields bulk temperatures which agree with the measured outlet fuel temperature. Since the heat flux at the interior wall is high, the turbulent transport of heat would be anticipated to be sensitive to the grid distribution.
Fine grid spacing near the wall is necessary for simulations under the rapid heating condition.

*Figure 4.3* Calculated fuel temperatures at centerline using measured exterior wall temperature as BC through various turbulence models

The calculated bulk fuel temperatures of Figure 4.3 were obtained by using the measured exterior wall temperatures as a boundary condition. However, the fuel temperatures show almost identical profiles by using the SKE-en, RNG-en and SST models with fine grid spacing near the wall. It is difficult to determine which turbulence model predicts the most accurate heat transfer by using the measured exterior wall temperatures as a thermal boundary condition in the simulations. Thus, a more stringent test of the turbulence models is to use volumetric heat generation within the tube wall as heat source together with an insulated outer wall as boundary condition. Since the heat
loss was shown earlier to be relatively small, the assumption of an insulated outer wall is reasonable. This combination of an adiabatic outer wall and spatially uniform volumetric heat generation within the tube would then allow simulation of the exterior wall and fuel temperatures. Moreover, the calculated exterior wall temperatures can now be compared with the measured values. Figure 4.4 shows the measured and simulated exterior wall temperatures in both the heated and unheated tube segments. There is a peak in the measured exterior wall temperature near the inlet. The exterior wall temperature profiles simulated by using the SKE-st and SST models do not have the initial peak. In contrast, the SKE-en model predicts the initial peak in the exterior wall temperature, but it is high relative to the measurement. Figure 4.4 shows that the calculations involving the RNG-en model reproduces the initial peak in the exterior wall temperature and exterior wall temperature profile that is closest to the measurements. The slight difference between measured and RNG-en simulated exterior wall temperature may be due to the assumptions that the volumetric heat generation is uniformly distributed along the tube length and the adiabatic outer wall boundary condition.
Figure 4.3 and Figure 4.4 show that fine grid spacing of the SKE-en model near the wall provides significant improvement over the SKE-st model which has coarse grid spacing. However, the SKE-en model under-predicts the convective heat transfer in the fuel, which is reflected by the highest exterior wall temperature (Figure 4.4) and the lowest temperature at the tube centerline (Figure 4.3). Thus, the SKE-en model is inaccurate for representation of the turbulent behavior under the high heat flux condition. Deriat et al. showed the weakness of using the standard $k$-$\varepsilon$ model to solve the flow involved complex behavior near the wall region.\textsuperscript{58} The SST model is unable to produce the initial peak in the exterior wall temperature. The RNG-en model reasonably simulates...
the heat transfer to the fuel under conditions of rapid heating and large Reynolds number flow, which is reflected by the smallest value of $\Delta T_{\text{outlet}}$ in table 4.2 and initial peak of the wall temperature in Figure 4.4. As described in following paragraphs, the peak in wall temperature near the inlet is a consequence of heat transfer deterioration.

In addition, the SKE-st, SKE-en, RNG-en and SST turbulence models were used to simulate the flow and heat transfer within the short tube (experiment parameters are shown in Table 4.1). The same heat transfer characteristics that were observed in the long tube with the use of these turbulence models were also found with the short tube. In the agreement, the RNG-en model provides the most accurate simulation results comparing with measurements for the short tube.

It is important to assess the grid independence of the numerical simulations. Thus, a grid refinement study was conducted in which the number of cells was incrementally increased until changes in the resulting temperature solution were acceptably small. In this work, the grids were refined via automated grid adaption in Fluent using the fuel temperature and mass fraction of the dissolved O$_2$. Table 4.3 shows the grid refinement study involving the RNG-en model for both long and short tubes. For both tubes, the difference between refinements in the calculated outlet fuel bulk temperatures (mass-weighted average) is less than 2 K. The chemical kinetic mechanism used to represent the fuel thermal-oxidative chemistry is employed by equations which are numerically stiff. As a result, prohibitively long run times are required for very fine grids. Thus to save computational time, the original level of grid density in Table 4.3 was used in all simulations. In addition, grid refinement studies were conducted for all the turbulence models, but only the results for the RNG-en model are shown for brevity.
Table 4. Grids Independent Study by RNG-en Model

<table>
<thead>
<tr>
<th>Tube type</th>
<th>Grid</th>
<th>Total cells</th>
<th>Outlet fuel T(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Long tube</td>
<td>Original</td>
<td>9,180</td>
<td>667.1</td>
</tr>
<tr>
<td></td>
<td>1st refinement</td>
<td>18,944</td>
<td>667.7</td>
</tr>
<tr>
<td></td>
<td>2nd refinement</td>
<td>39,429</td>
<td>668.1</td>
</tr>
<tr>
<td>Short tube</td>
<td>Original</td>
<td>7,140</td>
<td>566.4</td>
</tr>
<tr>
<td></td>
<td>1st refinement</td>
<td>18,300</td>
<td>567.3</td>
</tr>
<tr>
<td></td>
<td>2nd refinement</td>
<td>37,584</td>
<td>567.6</td>
</tr>
</tbody>
</table>

4.4.2 Studies of Heat Transfer Deterioration

In the previous discussion concerning the selection of a turbulence model, Figure 4.4 was used to compare calculated and measured external wall temperatures. It shows a peak in the measured and calculated (RNG-en and SKE-en turbulence models) exterior wall temperatures near the tube inlet. This local maximum in exterior wall temperature has a corresponding local maximum interior wall temperature due to heat conduction in the radial direction through the tube wall. A peak in the interior wall temperature is important as it directly influences the fuel chemistry and thus resulting surface deposition there. Past studies involving water have observed similar behavior that the interior wall temperature sharply increased and then rapidly decreased as water is heated from liquid to supercritical phase by a large heat flux.\(^{36, 60, 61}\)

This peak in the wall temperature near the inlet of the heated section was unexpected, which indicates a reduction in the heat transfer at this location. Heat transfer deterioration (HTD) has been defined to occur under conditions when the heat transfer
coefficient (HTC) is below the “normal” heat transfer coefficient in the subcritical phase. The HTD is characterized by a sudden rise in the wall temperature. 33,36,37 In the past studies involving water, Wang et al. attributed HTD to the changes in transport properties as a fluid transitions from a compressed liquid to a supercritical gas-like fluid. 33 It was observed that low mass flow rates are associated with heat transfer deterioration. 33,37,61 Sharabi et al. found that heat transfer deterioration is dominated by the buoyancy. 34 Mokry et al. indicated that the heat transfer deterioration is influenced by pressure, bulk temperature, mass flux and heat flux. 36 The exact mechanism behind heat transfer deterioration is unknown but appears to depend on the flow conditions, heat fluxes, and fluid properties.

4.4.2.1 Effect of Heat Flux and Flow Rate on Heat Transfer Deterioration

In order to explore the flow and thermal conditions which result in a sudden peak in wall temperature, a series of experiments were performed by varying the fuel flow rate and the heat flux levels. Table 4.4 lists various parameters including the Reynolds numbers at inlet and exit, volumetric heat generation, and heat flux to mass flux ratio (q”/G) for each test. The flow entering the heated test section is turbulent for all experiments except Test 5. The Reynolds numbers at the exit are relatively high for Tests 3 and 4, on the order of 100,000. q” is derived from equation 4.2 and G comes from the product of the inlet volumetric flow rate and fuel density divided by the cross-sectional flow area of the tube at inlet. The parameter q”/G has been used in past studies to characterize the rate of applied thermal energy at the heated wall and its convective heat removal rate. 33,37
Table 4.4 Thermal and Flow Conditions Concerning Temperature Peak near Flow Inlet

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Test 1</th>
<th>Test 2</th>
<th>Test 3</th>
<th>Test 4</th>
<th>Test 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow rate (mL/min)</td>
<td>373</td>
<td>452</td>
<td>457</td>
<td>300</td>
<td>109</td>
</tr>
<tr>
<td>Inlet Reynolds No</td>
<td>5,800</td>
<td>7,050</td>
<td>7,130</td>
<td>4,680</td>
<td>1,700</td>
</tr>
<tr>
<td>Outlet Reynolds No.</td>
<td>19,900</td>
<td>52,000</td>
<td>97,000</td>
<td>111,000</td>
<td>43,000</td>
</tr>
<tr>
<td>Measured outlet temp (K)</td>
<td>402</td>
<td>502</td>
<td>598</td>
<td>677</td>
<td>683</td>
</tr>
<tr>
<td>Heat generation $\dot{q}$ ($\times 10^{-8}$ W/m$^3$)</td>
<td>6.16</td>
<td>15.9</td>
<td>24.2</td>
<td>21.1</td>
<td>7.9</td>
</tr>
<tr>
<td>Heat flux $q''$ ($\times 10^{-6}$ W/m$^2$)</td>
<td>2.15</td>
<td>5.55</td>
<td>8.4</td>
<td>7.37</td>
<td>2.75</td>
</tr>
<tr>
<td>$q''/G$ (kJ/kg)</td>
<td>0.17</td>
<td>0.37</td>
<td>0.55</td>
<td>0.74</td>
<td>0.76</td>
</tr>
</tbody>
</table>

Notes: $q'' = \text{heat flux (kW/m}^2\text{)}, \ G = \text{mass flow rate flux (kg/m}^2\text{-s)}$

For the above flow and heating conditions, the simulations were performed using the RNG turbulence model with the enhanced wall function. In addition, volumetric heat generation within the tube wall was used as heat source. An adiabatic exterior wall was used as an outer wall boundary condition. Figure 4.5a shows measured and simulated exterior wall temperatures and shows reasonable agreement between the simulations and the measurements for tests 1 to 4. The difference between the measured and simulated external wall temperature of test 5 may be due to buoyancy effects or laminar to turbulent transition. These need to be investigated further. Figure 4.5b shows simulated interior wall temperatures with peaks near the inlet for tests 3 to 5. An important observation is that the peaks in the inner wall temperatures of tests 4 to 5, are above the critical temperature (shown for reference). There is a relatively small temperature peak near the inlet for test 3 which just approaches the critical temperature. Since the pressure is above the critical pressure and the temperatures associated with the peak are near or above the critical temperature for tests 3 to 5, the fuels are in the supercritical phase. Therefore, heat transfer deterioration occurs in the supercritical regime, which has been observed by others.$^{33,35,37}$
Figure 4.5 (a) Measured (dotted lines) and simulated (solid lines) exterior wall temperatures for five flow conditions and (b) Simulated interior wall temperatures for five flow conditions (HTD = Heat Transfer Deterioration)
As described above in connection with Table 4.4, the parameter $\eta''/G$ includes the effects of heating rate and mass flux. Figure 4.5 shows that the peak in the wall temperature, associated with the degree of HTD, increases as $\eta''/G$ increases for tests 3 through 5. Test 5 has the lowest flow rate but yet has the greatest $\eta''/G$ and correspondingly the most obvious HTD as given by the measured exterior wall temperature of Figure 4.5a. These results show that the degree of HTD is related to $\eta''/G$. Most importantly, Figure 4.5b shows that as the interior wall temperature near the inlet approaches the critical temperature and $\eta''/G$ increases, the monotonic increase in fuel temperatures (test 1 & 2) from the inlet to the end of heated section gives way to a temperature peak (tests 3 to 5). In our work, it appears that there is an occurrence of HTD for the fuel in the supercritical phase and when $\eta''/G$ is greater than 0.55 (test 3) at the operating pressure of 5.5 MPa. Previous studies involving supercritical water have also shown HTD to occur for a critical $\eta''/G$ which depended on the pressure and flow path geometry.\textsuperscript{33, 34,37}

Past study implied that buoyancy governs HTD for the upward flow.\textsuperscript{34} In order to examine the effect of buoyancy on HTD, the simulations were performed with and without buoyancy in the CFD model for test 1 to 5. The same fuel temperature profiles are obtained. The simulated interior wall temperatures depicted in Figure 4.5b show the HTD occurs near the inlet for tests 3 to 5, which did not include the buoyancy in the CFD model. Therefore, there is no effect of the buoyancy on the heat transfer deterioration for fuel flowing with a large Reynolds number. Polko et al. studied the influence of buoyancy on the water heat transfer, they pointed out that the buoyancy is not the only phenomenon resulting in the HTD.\textsuperscript{60}
Heat transfer deterioration occurs within the supercritical layer, it is likely due to a combination of simultaneously occurring, coupled events. A plot of the heat transfer coefficient (HTC) in the fuel along the interior wall provides a more direct means of showing heat transfer deterioration. Figure 4.5b suggests that the heat transfer between the fuel and the wall is deteriorated for tests 4 and 5. Figure 4.6 shows the simulated inner wall temperature and heat transfer coefficient (HTC) along the heated section for the test 4. The occurrence of the maximum HTC at the inlet is characteristic of normal heat transfer near the entrance of a heated tube. Figure 4.6 shows that the HTC sharply drops after the maximum HTC which is near the location where the fuel contacting the wall transitions to the supercritical phase. Rather than monotonically decreasing or leveling, the HTC rises again after the HTC minimum near the inlet. Similar reduction in the HTC for water has been observed by Pizzarelli, Mokry and others. Figure 4.6 shows that the HTC sharply drops after the maximum HTC which is near the location where the fuel contacting the wall transitions to the supercritical phase. Rather than monotonically decreasing or leveling, the HTC rises again after the HTC minimum near the inlet. Similar reduction in the HTC for water has been observed by Pizzarelli, Mokry and others.31,33,36

**Figure 4.6** Simulated heat transfer coefficient and interior wall temperature for the conditions of test 4
When the heat transfer coefficient suddenly decreases locally below the normal HTC, the wall temperature rapidly increases above the critical temperature, and the heat transfer is deteriorated.\textsuperscript{36,37} Because HTC is a function of the flow field and fluid properties, in the next section, we are going to explore these issues to understand the physical phenomena of the HTD.

\subsection*{4.4.2.2 Characteristics of Heat Transfer Deterioration in JP-8 Fuel}

The peaks of the interior wall temperatures are located near the inlet in tests 3 to 5, suggesting that the initial peak may be related to the fuel inlet temperature. Therefore, the CFD models were built in an effort to study the influence of the inlet fuel temperature on the HTD. Simulations involved by varying the inlet fuel temperatures (300 – 600 K) using the RNG-en turbulence model with a constant exterior wall temperature of 1000 K along a short tube. The constant exterior wall temperature was used for avoiding the effect of the complex outer wall temperature profile on the simulated temperatures. A short tube was employed because the inlet section was the region of concern and short tube has small amount of cells, so that to save computational time. In addition, an inlet flow rate of 300 mL/min was used in the simulations. With this large turbulent flow (Re > 100,000), the buoyancy force didn’t include in the simulations.
Figure 4.7 shows the simulated interior wall temperatures associated with four different inlet fuel temperatures. All simulated interior wall temperatures are above the critical temperature, however, the initial peak only appears in the case that the inlet temperature at 300 K. With the increasing of the inlet temperature, the peak in the interior wall temperature vanishes and the temperature profiles tend to be more continuous. A higher inlet fuel temperature means a smaller temperature difference between the heated wall and bulk fuel under the same heating and flow conditions. The indication is that the appearance of the initial peak is related to the radial temperature gradient in a cylinder tube. For the flow with 300 K inlet temperature, the interior wall temperature rapidly rises above the critical temperature due to high heat flux imposed on the interior wall.
However, the bulk fuel stays room temperature (300 K) near the inlet. The large
difference between the wall temperature and bulk temperature increases the heat transfer
from the wall to the bulk fuel, thus, the heat transfer is enhanced locally, resulting in the
interior wall temperature decrease. Therefore, a peak in the wall temperature is formed.
Duffey et al. showed the heat transfer increased at a region of that the wall temperature
was greater than critical temperature and bulk temperature was lower than critical
temperature.\textsuperscript{37}

As the wall temperature changes with fuel transits from subcritical to supercritical, the fuel properties dramatically change due to the density ($\rho$), viscosity ($\mu$),
specific heat ($C_p$) and thermal conductivity ($K$) are the functions of the temperature.
Previous researcher studied the role of the transport properties on heat transfer
deterioration.\textsuperscript{33} It is desirable to investigate which property has the greatest effect on the
wall temperature involved a peak.

A series of simulations were performed by keeping one property constant while
allowing the others to vary with the fuel temperature. The inlet fuel temperature was at
300 K with a flow rate of 300 mL/min. The outer wall temperature was taken a constant
value of 1000 K as a boundary condition. Figure 4.8 shows the simulated interior wall
temperatures for each property held constant in turn. In the legend of Figure 4.8, “$\rho$-
constant” means that the density was held constant and $\mu$, $C_p$ and $K$ were functions of the
fuel temperature. The legend of “none held constant” means that all transport properties
simultaneously varied with fuel temperature. To better understand the fuel heat transfer
characteristics in the liquid and supercritical phases, the simulations were performed for
the properties evaluated at a temperature of 390 K (liquid phase) (Figure 4.8a) or at a
temperature of 780 K (supercritical phase) (Figure 4.8b).

The red solid lines (“$\mu$ -constant (390K)” and “$\mu$ -constant (780K)”) in Figure 4.8a and 4.8b represent the simulated interior wall temperatures as the fuel viscosity ($\mu$) was forced a constant value in the simulations. The continuous increase in both curves is observed when the viscosity ($\mu$) was held as a temperature independent. This indicates the variation in the fuel viscosity dominate the temperature peak. In addition, there is no initial peak in the interior wall temperature for the case of the “$\rho$ -constant (780K)”, implying that the temperature peak is also related to the fuel density which affects the heat transfer in the supercritical region. Figure 4.8a and 4.8b show that the $C_p$ and conductivity (K) have little influence on the formation of the initial peaks. Therefore, as fuel is heated from liquid to supercritical, the heat transfer in the fuel is very sensitive to the changes of the fuel viscosity.
Figure 4.8 Simulated interior wall temperatures with either one property held constant and the others were allowed to vary with temperatures (a) fuel temperature at 390 K (Note: “\(\mu\)-constant (390K)” represents simulated temp at \(\mu = 4.7\times10^{-4}\) (kg/m-s) and \((\rho, C_p, K) = f(T)\); and so on and (b) fuel temperature at 780 K (Note: “\(\mu\)-constant (780K)” represents simulated temp at \(\mu = 3.18\times10^{-5}\) (kg/m-s) and \((\rho, C_p, K) = f(T)\); and so on. “none held constant” represents the simulated temp with \((\rho, \mu, C_p, K) = f(T)\)
As the fuel enters the heated tube with the inlet temperature of 300 K, the magnitude of the viscosity is higher due to the fuel is in the liquid phase. The viscous boundary layer blocks the heat transfer from the wall to the bulk fuel, causing the interior wall temperature rapidly rises above the critical temperature. In consequential results, the heat transfer is enhanced in the supercritical layer and this supercritical thermal layer would be no longer insulating the heat from the wall, which reflected by a sharp decrease in the interior wall temperature. Thus, the peak in the wall temperature is formed as the liquid fuels become supercritical.

In this study, a series of experiments and simulations were conducted to investigate the heat transfer deterioration as JP-8 fuel flows in a heated tube. Some observations could be reached:

(1) RNG turbulence model combined with the enhanced wall function is a reasonable model to simulate the occurrence of the HTD within the thin supercritical layer near the wall.

(2) HTD occurs for in the flow conditions of a large heat flux \( q'' \) with a low mass flux rate \( G \). For JP-8 fuel upwards flowing in a cylinder tube at pressure of 5.5 MPa, the heat transfer is deteriorated in the supercritical layer when the parameter \( q''/G \) is greater than 0.55. The degree of the HTD increases with the parameter \( q''/G \).

(3) The buoyancy is not required for the occurrence of the HTD for the high flow velocity condition.

(4) HTD is defined by a rapid decrease in the heat transfer coefficient (HTC) below the normal HTC and is reflected by a rapid increase in the wall temperature above
the fuel critical temperature. A peak in the wall temperature is related to the large
temperature difference between the interior wall and bulk fuel, which associated
fuel phase changes from subcritical to supercritical in the thermal boundary layer.
(5) As fuel is heated from the liquid to the supercritical phase, the significant
reduction in the fuel viscosity dramatically change the heat transfer characteristic
which results an unexpected peak in the wall temperature.

4.4.3 Studies of Temperature, Dissolved O₂ and Deposition in JP-8 Fuel

The previous section discussed that the large heat flux causes unusual heat
transfer behavior near the wall regime. In this section, we investigate the effect of the
heat transfer on fuel temperature and chemical reactions alongn the long and short tubes.
Here, the long and short tubes refer to the length of the heated portions which are 25.4 cm
and 12.7 cm, respectively, with the same inner diameter of 0.069 cm. Both tubes have the
same inlet flow rate at 300 mL/min, however, the heat flux is higher in the short tube than
that in the long tube. Simulations were implemented using the measured exterior wall
temperature as the outer wall boundary condition in the RNG-en model (RNG k-ε
turbulence model with an enhanced wall function). Calculated results from the long and
short tubes are compared to better understand fuel behavior involved large heat flux and
short residence time.
4.4.3.1 Boundary Layer Temperatures along the Long and Short Tubes

Figure 4.9a shows simulated fuel temperature color contour along the short tube. As the heat imposed on the inner wall surface, the fuel temperature gradually increases from wall to the tube centerline in radial direction and from inlet to the outlet in the axial direction within the heated section and fuel temperatures become uniform distribution towards the outlet. Figure 4.9a provides overview temperature distribution in both the radial and axial directions along the heated and unheated sections of the tube. Figure 4.9b shows an enlarged portion of Figure 4.9a: temperature contour for the portion of initial 5 cm after the inlet and 12% from the wall, a very thin thermal boundary layer near the wall is observed. There is a large temperature difference between this thermal boundary layer and bulk fuel.
To further reveal the temperature distribution between thermal boundary layer and bulk fuel, Figure 4.10a and 4.10b plot the measured exterior wall temperature together with simulated fuel temperatures at four radial locations along the long and short tubes, respectively. “Inner wall” and “tube center” represent the temperatures at the tube interior wall surface and at the tube center line, respectively. “0.26% and 0.85% off wall” represent the temperatures at the locations where the percentages are the distances to the interior wall along the tube radius. These two locations are used to demonstrate the radial temperature gradient in the thermal boundary layer. The temperature at the tube centerline rises gradually from the inlet to the end of the heated section. The temperatures
at the other four locations exhibit an initial peak near the inlet and then increase until the end of the heated section. As discussed in the last section, the initial peaks are due to heat transfer deterioration there.

Figure 4.10a and 4.10b show hundreds of degrees temperatures difference at the three locations of the inner wall, 0.26% off wall and 0.85% off the wall within the heated section for both long and short tubes. The difference of the temperatures between exterior and interior wall is due to a volumetric heat generation (\( \dot{q} \)) in the tube wall of the heated section. The plots suggest that the fuel contacting the interior wall is in the supercritical regime over nearly the entire heated region for both long and short tubes.
Figure 4.10 Temperature profiles at five radial locations along (a) long tube and (b) short tube (0.26% and 0.85% are the fraction of distance to the wall along the tube radius)
For the long tube in Figure 4.10a, the temperature at the location of 0.26% is below the critical temperature from the inlet to the axial location of ~ 0.2 m, which indicates the supercritical layer is very thin. However, the thickness of the supercritical layer increases along the flow direction in the heated section. For the short tube in Figure 4.10b, the temperature at the 0.26% radial location is above the critical temperature in the heated section. Thus, the supercritical layer is thicker in the short tube than that in the long tube in the heated section. This is due to higher heat flux applied to the short tube. The radial temperature gradient is greater in the short tube than that in the long tube. Moreover, the temperature at the tube center is higher in the short tube than in the long tube at the same axial location, which implies a higher heat transfer in the short tube. Therefore, the greater heat flux in the short tube creates the greater radial temperature gradient in the thermal boundary layer, as well as the greater heat transfer in the bulk fuel. With this short tube, the heat flux on the interior wall surface reaches ~ 9,900 kW/m². The parameter $q''/G$ (heat flux/mass flow flux) achieved ~ 0.995. A higher degree of heat transfer deterioration is observed near the inlet in Figure 4.10b.

Figure 4.10a shows, for long tube, the bulk fuel temperature is above the critical temperature in unheated section, while the bulk fuel temperature in short tube shown in Figure 4.10b is below the critical temperature in heated and unheated sections. Despite the same flow rate of 300 mL/min at the inlet for both tubes, the Reynolds number at the end of the heated section is higher for the long tube (25.4 cm heated) than that for the short tube (12.7 cm heated). As the Reynolds number increase, the heat transfer is enhanced. Thus, the bulk fuel is heated to supercritical at the end of heated section in the long tube, whereas it stays subcritical in the short tube.
4.4.3.2 Dissolved O$_2$ and Insoluble along the Long and Short Tubes

The study of the dissolved O$_2$ consumption is necessary for understanding how surface deposits form as a consequence of thermal-oxidative reactions, which depend on the fuel temperature history, velocity profile, and heating conditions. A pseudo-detailed kinetic mechanism is used to simulate the thermal oxidative reactions. In previous work, this pseudo-detailed kinetic mechanism has successfully predicted fuel thermal oxidative degradation over a wide fuel temperature range. Here, the unchanged chemical kinetic model will be employed to examine the current conditions of high heat flux and large flow velocity.

Figure 4.11a plots the simulated dissolved O$_2$ along the interior wall and tube centerline of the long length tube. The dissolved O$_2$ is consumed less than 0.8% within the test tube in agreement with low oxygen consumption observed in the experimental measurements. The low dissolved O$_2$ consumption results from the short residence time of the fuel flowing through the tubing. The calculated residence times are ~ 12 ms within the heated section, and ~ 20 ms for the entire tube length. In addition, the bulk fuel temperature gradually increases from 300 to 650 K within the heated section, while a constant temperature of 667 K is kept within the unheated portion as shown in Figure 4.10a. Thus the higher fuel temperature results in faster O$_2$ consumption in the unheated section than that in the heated section. In addition, F4177 fuel sample contains natural antioxidant species (AH and SH), which can delay oxygen consumption. Thus, the O$_2$ consumption rate increases in the unheated section. The figure shows that the oxygen profiles at the inner wall and tube center are nearly identical. Figure 4.11b shows the O$_2$ concentrations along the short tube. For this short length tube, the calculated residence
time is \( \sim 15 \) ms within the entire tube length, thus the dissolved O\(_2\) consumption is less than that in the long length tube. However, at the same axial distance, more O\(_2\) is consumed in the short tube than in the long tube due to higher heat flux along the short tube. For example, at \( x=0.1 \) m from the inlet, the O\(_2\) concentrations are 99.92\% and 99.99\% for the short and long tubes, respectively. Although this difference in the O\(_2\) concentration between the short and long tubes is small, it indicates the effect of the heat flux on the oxidation rate. Because the lower fuel bulk temperature and shorter residence time in the unheated section of the short length tube, the oxidation rate is lower along the short tube than along the long tube. In addition, Figure 4.11b shows a slight drop of the dissolved O\(_2\) at the inner wall near the inlet region for the short tube, resulting from higher interior wall temperature in the short tube followed by mixing of higher O\(_2\) concentration fuel from the tube center.

The O\(_2\) profiles in Figure 4.11a and 4.11b indicate that the O\(_2\) consumptions strongly depend on both the residence time and fuel temperature under the conditions of “rocket-like” heat fluxes and flow rates. The short residence time results in very little dissolved O\(_2\) consumption along the test tubes. In the experiment, the on-line GC measured the concentrations of the dissolved O\(_2\) as 100\% remaining at the outlet for both short and long tubes. The simulated O\(_2\) concentrations agree roughly with the measurement.
Figure 4.11 Simulated dissolved O\(_2\) (solid lines) and the insoluble (dashed lines) at the interior wall and tube center along (a) long tube and (b) short tube.
4.4.3.3 Measured and Simulated Deposits along the Long and Short Tubes

It is important to study the effect of high heat flux on surface deposit formation to enable the fuel system designer to use the cooling capacity of the fuel most efficiently while avoiding excessive deposit production. Previously, a global deposit sub-mechanism was developed to simulate thermal oxidative deposition over the temperature range 458 to 673 K.\(^\text{16}\) This deposition sub-mechanism demonstrated good agreement between simulations and experiments for deposits produced in this previous study over a range of fuel samples at relatively low heat flux conditions. Here, the global deposit sub-mechanism developed previously is employed without modification to simulate deposition under our high heat flux and high wall temperature conditions. The purpose of this work is to better understand the deposition process at these high heat flux conditions, and to examine the usefulness of the deposition sub-mechanism at these extrapolated conditions.

Here we have chosen to compare the simulated and measured deposit profiles on a normalized basis, where the simulated and measured deposits are normalized to their respective peak values. This normalization is performed to assess the ability of the simulation to correctly predict the deposition profiles while initially not being concerned with absolute deposit quantities. The normalized deposit profiles (simulated and measured) are plotted in Figures 4.12a and 4.12b for the long and short tubes, respectively. The figures show reasonable agreement in the measured and simulated deposit profiles for both tubes. For the both the long and short tubes, the simulations and measurements show a peak near the end of the heated section, with a drop in deposition upon entering the unheated tube, followed by an increase in deposits near the end of the
unheated section. The good agreement in deposit profiles between the simulation and measurement gives confidence in the ability of employing the deposit sub-mechanism for the current conditions, which are beyond the conditions for which it was developed.

It is important to note that the absolute magnitude of the simulated deposit prediction using this deposition sub-mechanism is not in good agreement between simulation and experiment, with the simulation being lower than the experiment by up to a factor of $6 \times 10^3$ (for the peak deposition in the long tube). This lack of agreement is not unexpected as the deposition sub-mechanism is a global mechanism that was developed for a particular set of fuels under lower heat flux and temperature conditions. One goal of this work is to obtain these comparisons between the simulation and experiments to allow development of improved deposition sub-mechanisms that can be used to predict deposition over a wide range of flow and temperature conditions. We have chosen not to modify the Arrhenius parameters in the deposition sub-mechanism to match the deposition of the current study, but rather use the differences between simulation and experiment to help determine future modifications required for a deposit sub-mechanism that is more globally applicable.
Figure 4. Comparison the measured and simulated deposits mass along (a) long tube and (b) short tube.
One important difference between the simulated and measured deposit profiles occurs near the tube entrance region for both the long and short tubes. The measured deposit profiles both show significantly higher normalized deposition than the simulations. We have previously shown that the wall temperatures in these regions are above the fuel supercritical temperature and thus fuel pyrolysis may occur in the near wall region. Simple kinetic calculations (assuming a global fuel pyrolysis activation energy of ~60 kcal/mol) show that the extremely short residence times (<1 msec) for which the fuel is exposed to these supercritical temperatures results in only minor extents of fuel pyrolysis. At this time it is unclear whether fuel pyrolysis at the near wall region of the tube entrance can be the cause of the increased deposition observed experimentally for both tubes. Future chemical kinetic mechanisms can combine pyrolytic reactions along with the current oxidative reaction scheme to further elucidate the chemistry occurring in the near wall regime.

Another interesting observation in the deposition profiles of both long and short tubes, is the increase in deposition near the end of the unheated section. This increase in deposition occurs despite the relatively low temperatures in this region, especially for the short tube (see Figure 4.10b). An examination of the profiles of the global “insolubles” species is instructive in determining the cause of this increased deposition. The insolubles species concentrations are plotted in Figures 4.11a and 4.11b for the long and short tubes, respectively. The plots show that for the long tube case, the insolubles continue to be produced in the unheated section, due to increased oxygen consumption. This is less apparent in the short tube, but this tube exhibits a higher level of insoluble production in the heated section due to the higher temperatures. It is apparent that the increase in
deposition in the unheated section of the long tube can be explained by the continued increased in the insolubles deposit precursor species in this section, which is caused by increased oxygen consumption at relatively high temperatures. The short tube simulation only shows a minor increase in deposition at the end of the unheated section despite a larger increase demonstrated in the measured profile. The short tube exhibits a significant cooling of the fuel when entering the unheated section. Cooling can result in the increased formation of insolubles due to decreased solubility at lower temperatures. The current deposit sub-mechanism does not consider this process of insoluble formation and thus may under predict deposition in cooled regimes. Future deposit sub-mechanisms may need to consider the effect of fuel cooling on insoluble formation. The extent of fuel cooling after heating depends on fuel system design, with some fuel systems having insignificant cooling due to fuel combustion soon after fuel heat exposure.
CHAPTER V

CONCLUSIONS

5.1 Summary

This study investigates jet fuel behavior which involved the complex interactions between the fluid dynamics, heat transfer and chemical reactions. The conclusions from these three topics are presented in this section. The recommendations for the future work are given in the next section of this chapter.

In Chapter 2, an investigation was conducted on the effect of a sudden expansion or contraction in flow path on surface deposition formed in heated cylindrical tubes. Both experiment and simulation show that, under isothermal laminar flow conditions, the peak deposit axial location in the tube is a strong function of the fuel oxidation rate in the flow direction. While the limited axial resolution of the experimental deposition measurements prevented observation of the effects of the step change on oxidation and deposition, the computational model was successfully used to detect excess deposition caused by the step changes in flow geometry. The model was also used to extrapolate to flow conditions that are experimentally inaccessible. The measurements and calculations were performed for conditions where the deposition peak occurs near the step change location to maximize the effect of the change in geometry on fuel flow. For the expansion case, the simulation predicts that an increase in deposition occurs in the wide secondary tube downstream of
the expansion due to a recirculation zone which increases fuel residence and oxidation reaction times. For the contraction case, the simulation predicts that insolubles species produced during the relatively long residence time in the wide primary tube, flow into the secondary tube via acceleration through the contraction throat. The high level of insolubles in the narrow secondary tube causes excess deposition even though oxidation reactions do not occur readily due to the short residence time in this narrow tube. In the expansion case, the excess deposition is less likely to create conditions where the deposit narrows the flow passage due to its occurrence in the wider secondary tube. For the contraction case, the excess deposition is a greater concern as it occurs in the narrow secondary tube and is more likely to result in flow restriction issues. Fuel system component designers need to consider the fuel and wall temperatures, flow rates, throttle changes, and the locations of changes in flow geometry to maximize fuel heat sink and minimize fuel surface deposition problems caused by fuel oxidative degradation.

Chapter 3 described simulations of the fluid dynamics and heat transfer involving a liquid hydrocarbon fuel in a single rotating heated test article. The three-dimensional unsteady flow simulations were performed in a rotating reference frame. The simulations were begun using an initial rotational speed of 200 rpm and, then, incrementally increased by 100 rpm with a relatively small time step (0.1 ms) such that converged solutions were obtained for each desired rotational speed. Simulations show the combined effects of centrifugal and Coriolis forces on the turbulent flow and heat transfer in a rotating environment. With the current boundary conditions, the flow is laminar when the test article is stationary. Rotation induces turbulent flow and promotes heat transfer along the flow path. The coupled effects of rotation, turbulent flow and heat
transfer result in a fuel temperature that increases with increasing rotational speed. A recirculation flow was observed in the flow path with bypass geometry. The recirculation flow increases with rotational speed, and thus increases the fuel residence time in the heated region. As a result, the heat transfer is increased.

In Chapter 4, an effort was made to study fuel heat transfer under the “rocket-like” conditions. The first challenge of this work was to select an appropriate turbulence model so that simulation results would correctly represent the fuel behavior. In the past, the standard $k$-$\varepsilon$ turbulence model (SKE) was used successfully to simulate high Reynolds number flow. For the current flow and heating conditions, a poor agreement was found for the SKE model incorporating a standard wall function (SKE-st), which used coarse grid spacing near the wall. The SKE model with a fine grid spacing of the enhanced wall function (SKE-en) provided a significant improvement over the SKE-st model. Thus, the grid density in the vicinity of the wall is important and fine grid spacing has to be used when large heat fluxes are imposed on the interior wall surface. However, simulations using the SKE-en model also showed an under-prediction of the fuel heat transfer compared with the measurement. The SST $k$-$\omega$ model predicted a reasonable bulk fuel temperature, but fails to predict the physical phenomena of the initial peak in the wall temperature which was observed in the experiments. The RNG turbulence model combined with the enhanced wall function (RNG-en) gives an accurate numerical solution for representation of the turbulent behavior under these high heat flux conditions. The simulated temperature using the RNG-en model yield reasonable heat transfer, which is reflected by the agreement with measured outlet fuel bulk temperature and by the capability of reproducing the measured exterior wall temperature. With the
RNG-en model, it was found that the large heat flux create a thin supercritical layer and the thickness of this layer increases with an increase of the heat flux. Simulations show a large radial temperature gradient between this supercritical layer and bulk fuel and the temperature gradient increases with the heat flux. With the large flow rate (Re > 100,000), the heat transfer significantly increases, which is demonstrated by the bulk fuel become supercritical at the end of heated section along the long tube, while the bulk fuel stay subcritical along the short tube. In addition, an oxidative chemical kinetic mechanism was incorporated into CFD model to study the effect of the heat flux and flow rate on the autooxidation reactions and surface deposition. The mechanism predicts that the dissolved O₂ is consumed less than 1% in the heated tubing due to the short residence time. Deposition is formed in the heated and unheated sections of the tube due to the higher bulk fuel temperature. Both of the simulations and experiments show that the deposits increase along the flow direction and the peak deposit locates at the highest interior wall temperature.

It was found that an initial peak in the wall temperature is caused by heat transfer deterioration (HTD) in the supercritical layer near the wall. Heat transfer deterioration has been defined as a condition in which the heat transfer from the wall is below that expected for “normal” subcritical convective heat transfer and is characterized by a sudden rise in the wall temperature. Experiments and simulations show that, the likelihood of HTD is associated with heat flux (q”) and mass flow rate flux (G). The degree of HTD increases as q”/G becomes larger. For JP-8 fuel upwards flowing in a cylinder tube at pressure of 5.5 MPa, the heat transfer is deteriorated in the supercritical layer when the parameter q”/G (q” is heat flux and G is mass flux) is greater than 0.55.
The viscosity dominates the peak in the wall temperature when HTD occurs. This important observation has an application for the high speed aircraft. The unexpected local maximum in the wall temperature may create a local maximum deposition on the interior wall surface. Further, the local maximum wall temperature has a potential to deteriorate the tube wall.

5.2 Recommendations

For the study of the effect of flow path changes on fuel deposition in chapter 2, future work needs to study other geometry changes that may be of interest for fuel systems, such as a sudden “elbow” change in flow geometry. It would also be interesting to determine if gradual changes in geometry and/or rounded corners can minimize the increased deposition that occurs at sudden passageway size changes. In addition, deposition experiments need to be performed under non-isothermal and turbulent flow conditions to confirm the general applicability. The study of turbulent conditions is especially desirable as aircraft fuel system flow is often in this regime, although higher flow rates usually imply lower fuel and wall temperatures and thus decreased deposition issues. Also, the current study does not determine the extent that a passageway is occluded. This requires knowledge of the density of the deposit whose value may change with the temperature at which it is produced and with the identity of the fuel. Ultimately, the fuel system designer is more concerned with the deposit volume and the fraction of tube blockage rather than the deposit mass per unit area as calculated here, so future experiments and models need to consider the deposit volume.
With regard to chapter 3 study of the effect of the rotation on the heat transfer as fuel passes through a heated rotating passage, the rotational speed is limited up to 3000 rpm due to convergence problems and the lack of measured boundary conditions. In future work as part of a larger study, the effects of higher rotational speed (~10,000 rpm) on the heat transfer should be investigated. For simplicity, circular tubing is used here for the flow path. It is recommended to model the complex geometry of test specimens, which can better represent the flow passages in future turbine blades. Furthermore, chemical reactions need to be incorporated into the CFD model to simulate the thermal stability for different fuels.

For the study of effect of high heat flux on the fuel behavior in Chapter 4, it is suggested to investigate HTD in laminar and transition flows with different fuel samples. Also, the effect of the antioxidant species on the oxidation rate needs to be evaluated under short residence time flow conditions. Due to the disagreement in deposition magnitudes between the measured and simulated, the global deposition sub-mechanism needs to be further studied so that can be used for over a wide temperature range. In modern military aircraft, the heated fuel can be re-circulated to the tank, thus it is important to investigate the effect of fuel cooling on the formation of the insolubles/deposition. Pyrolysis reactions can take place when liquid fuels are heated to the supercritical state and, thus, it is recommended to add pyrolytic kinetic mechanisms in the CFD simulation to better understand the deposit formation under rapid heating condition.


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APPENDIX

Photographs of Experimental Equipment

Figure A - 1 Near-Isothermal Flowing Test Rig (NIFTR) (Chapter 2 Experiments)

Figure A-1 shows the NIFTR system used in the experiments of Chapter 2 (see Figure 2.1). From left to right: syringe pumps and controller, furnace and the on line gas chromatograph (GC). On the upper right side is the temperature controller used to adjust the furnace temperature.
Figure A - 2 Swagelok Welder (SWS-M100-MS-13-202) (Chapter 2 Experiments)

Figure A-2a shows the tube welding system used to join the two different ID tubes. Figure A-2b shows the control panel used to edit the program and control the welding process.
Figure A-3 shows the tube dimensions and the 90 degree function at step. The darker color on the large inner diameter surface indicates the deposits distribution as reference in Figure 2.4. Figure A-3b and 3c shows images of the heavier and light deposits, respectively, through the SEM (Scanning Electron Microscope).
Figure A - 4 Test Chamber (Chapter 3 Experiments)

Figure A-4a shows the entire test chamber that will be used to validate the simulation results in the Chapter 3. Figure A-4b shows the rotating assembly (located inside the test chamber) as depicted in Figure 3.2. Figure A-4c shows the test specimen attached on the rotational blade (see Figure 3.3).
Figure A-5 shows the tube heated by resistive heating as depicted in Figure 4.1. The thermocouples were welded to the exterior tube wall to measure surface temperatures. A hot spot, bright red section of the tube, is clearly seen near the inlet.