Numerical Simulation of JP-10/Water Combustion at High Pressure

by

Raghav Sharma

Bachelors in Technology in Mechanical Engineering, Punjab Technical University

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This thesis was presented

by

Raghav Sharma

It was defended on

July 15, 2021

and approved by

Shervin Sammak, Ph.D., Assistant Professor, Department of Mechanical Engineering and Materials Science

Peyman Givi, Ph.D., Professor, Department of Mechanical Engineering and Materials Science

Arash Nouri, Ph.D., Assistant Professor, Department of Mechanical Engineering and Materials Science

Thesis Advisor: Shervin Sammak, Ph.D., Assistant Professor, Department of Mechanical Engineering and Materials Science
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Combustion at high pressures has the potential to increase the efficiency and usability of jet engines in the presence of high moisture. However, not a lot of research has been done in the domain of high pressure combustion owing to various challenges of performing experiments as well as simulations in these conditions. The studies that exist mostly explore the combustion of fuels such as methane and its hydrates. Also, which chemical reactions are the most dominating reactions in these cases hasn’t been explored much. In this work, combustion of a proper jet engine fuel, JP-10 is analyzed under high pressures in the presence of dry air as well as moisture by plotting temperature and axial velocity profiles in a 1-dimensional cross-flow diffusion flame setting using Cantera’s open source code. It is found that increasing pressure increases the extinction limit for the fixed amount of JP-10 being burnt in air. This finding proves that for given a high pressure device, the combustion of jet fuel can take place even if it contains higher amounts of moisture, hence, increasing its application range and usefulness, especially in extreme environmental situations. To determine the most dominant chemical reactions, sensitivity analyses are carried out for the various cases of pressure for both dry fuel as well as with moisture, near the extinction limits of the corresponding pressures. Hence, showing that an increase in pressure plays a significant role in altering the pathway that the combustion chemical reaction is following, proving that the role of the chemistry of the fuel cannot be ignored while developing high pressure combustion devices.

Keywords: High pressure combustion, JP-10, water-laden flame.
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Preface

The motivation of this work of research was to add knowledge to the domain of jet engines so that engines of higher efficiency can be developed. First of all, I would like to thank my advisor, Dr. Shervin Sammak, for introducing me to this topic and supporting me financially and more importantly, as a supportive and motivating mentor who provided the best possible guidance a student can ask for. Finally, I also would like to thank Dr. Albert To, without whom this work of research would not have been completed by me.

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"Not all those who wander are lost" - J.R.R. Tolkien
1.0 Introduction

High pressure combustion is a research area that is seeing an increased interest in the combustion community, especially in the last few years. The primary reason for this increase in interest is the fact that existing combustion devices operate on high pressure ranges, most of them well above the critical pressure range of the carbon-based fuels that are typically employed in various applications [1]. Furthermore, to meet the demand of extracting maximum efficiency out of the fuel being burnt, the operating pressure ranges have been increasing steadily for various applications of jet engine turbines. Operating pressures in the gas chambers of gas turbines have been increasing linearly for the last 50 years, and are expected to do so [2] in the coming future as well. In order to build new combustion devices that operate at increasingly high pressures, strong background research is needed in this domain.

However, it is not practical to simply extrapolate the extensive research and theory that exists for fuel combustion at low pressures [3]. At higher pressures, there is a significant difference between the physics at the macro as well as the micro-level behavior of the fuel as compared to the combustion behavior observed at room pressure (1 atm). For instance, if the operating pressure of the combustion chamber goes beyond the critical pressure of the fuel being burnt, which is usually the case for high-pressure combustion, the physical behavior of the atomized fuel itself changes. As the critical pressure is exceeded, the state of the fuel is simply referred to as “fluid”. This is because changes in temperature at fixed super-critical pressure do not result in phase change. Hence, during the process of fuel atomization, the breakup of the liquid core into droplets ceases abruptly, and there is a further increase in the pressure yield behavior due to the absence of surface tension and latent heat of the fuel [4].

The complexity posed by high operating pressure is observable even while developing simulation models. For instance, one of the computational requirements for turbulent flame Direct Numerical Simulation (DNS) is a detailed fuel combustion mechanism. Low pressure combustion kinetics include only the temperature dependency via the Arrhenius rate law and neglect pressure dependence on combustion pathways. However, it is well known that these
pathways are affected by pressure and high pressure combustion simulations must include pressure dependence. But such mechanisms which have been validated are very limited in number [5, 6], hence adding an extra layer of complexity when it comes to high-pressure combustion research.

Even from a purely experimental point-of-view, research in the domain of high pressure combustion is a major challenge [7]. It is very challenging to build actual experimental set-ups that operate at high pressures based on which actual physical and empirical laws for combustion can be inferred from. Most of the existing experimental studies usually address high-pressure atomizers and are primarily based on qualitative visualizations or relatively simple quantitative measurements [8–12]. This is because it is difficult to make in-situ measurements in highly pressurised combustion chambers [13]. Furthermore, most of these experiments avoid combustion due to further difficulties that come in due to an increase in pressure and heat in the system being investigated. However, there have been some studies that have been conducted for combustion under high pressure. Mayer et al., [12] conducted combustion experiments at high pressure (6 MPa). The findings of these experiments showed a significant difference in the overall behavior of the system under high pressure as compared to combustion at low pressures (1 atm). This fact provides further motivation for an independent investigation into high pressure combustion and proves that merely extrapolating results from low pressure combustion could prove to be erroneous. In the light of limited experimental data, the existence of simulation models that can predict the behavior of high pressure fuel combustion becomes even more critical.

Most of the high pressure combustion studies are for single component simple fuels, which are not complex in their molecular structure. Shimizu et al., [14], updated the pre-existing hydrogen-oxygen kinetic mechanism previously proposed by Kitano et al., [15] for high pressure values greater than 10 atm. They validate their update with experimental shock-tube analysis and measuring laminar flame speeds. Albert et al., [16], studied the phenomenon of combustion of methane in oxygen from 1 atm pressure to up to 100 atm for a counter-flow diffusion flame setup and even used the Soave-Redlich-Kwong equation of state to simulate real gas behavior. But both of these studies deal with fuels which are simple in their molecular structure, namely hydrogen and methane. In real-world applications such
as gas turbines, rocket engines, and even the Bradley trucks used by the US army, simple fuels like hydrogen and methane are not used. Instead, multi-component fuels such as A2 (Jet A), A1 (JP-8), single-component complex fuels such as JP-10 are typically used in jet-engine applications while RP2-2 and RP2-1 are distillate fuels, used in rocket engines, as per the information provided by the National Jet Fuels combustion program (NJCFP) [17].

Extensive research in the form of ignition-delay experiments and premixed flame-speed measurement tests has been performed for the development of kinetic mechanisms, obtaining thermochemical data, transport data, as well as characterizing the behavior of various real jet and rocket fuels namely JP-8, Jet-A, JP-5, RP2-1, RP2-2, JP-10, Shell A, Shell D, etc. All these real fuel models have been developed using the novel HyChem (Hybrid chemistry) approach. This approach was developed by the collaboration between combustion research groups of the University of Southern California (USC), Stanford University, and the University of Illinois at Chicago (UIC). The HyChem approach, as the name suggests is a hybrid approach as it combines the results of both experiments and chemical kinetic modeling.

The HyChem approach proposes that the oxidation of fuel can be split into two physical phenomena [18]:

1. Pyrolysis of fuel to form pyrolysis products
2. Oxidation of the pyrolysis products

Large hydrocarbon fuels undergo pyrolysis first, followed by the oxidation of pyrolysis products. These two processes are decoupled in both time and space. The second step is the rate-limiting step. Therefore, the composition of the pyrolysis products determines the overall oxidation rate of the fuel.

The fuel pyrolysis step is modeled by several experimentally-constrained lumped reaction steps. The experiments on which the lumped reaction steps are based include ignition delay experiments and determining flame speeds in cross-flow diffusion flames. While the oxidation of the pyrolysis products is modeled by a detailed foundational chemistry model. The detailed chemistry model chosen for the development of the various HyChem models is USC Mech II. [18–23]. But again, no extensive research has been done to simulate and analyze the behavior of these fuels under high pressure.
In an idealistic combustion scenario, the fuel is pure, in the sense that it is devoid of moisture and impurities. But in real-life cases, this is not possible. The fuel is burnt, for instance in a gas-turbine which will always contain some percentage of water in it. This percentage of water in a given amount of fuel can be minimized but not eliminated. Hence, in order to model real-life combustion behavior, the role of water in fuel cannot be ignored. In environments with heavy rainfall, the chances of water escaping into the combustion increase drastically, which has the potential of not only reducing the efficiency of a jet engine for instance but can also lead to failure of the engine. Also, fuel containing high amounts of water has the potential to provide a cleaner source of energy. For example, methane hydrates can contain up to 85% water and only 15% methane, so their combustion reduces the environmental impact of methane combustion significantly as a much lesser amount of methane (a green-house gas) is released, while providing comparable energy as that is provided by the combustion of pure methane of the same amount [24].

In order to study and quantify the behavior of water in fuels, one of the primary quantities analyzed in literature is the extinction limit. Extinction limit is defined as the upper value of water in a given amount of fuel, beyond which the fuel will not undergo combustion, for a given pressure and existing boundary conditions. The extinction limit proves to be a critical consideration to determine the optimum conditions for the working of any combustion system. Extinction limit has been studied in the past, but mostly in the low pressure range of 1 atm [25–27]. Sirignano et al., [16] did perform extinction analyses simulation under high pressures up to 100 atm for a counter-flow diffusion flame setting but, it was performed for methane mixed with water (40% water content) in the presence of oxygen, which is again a simple single-component fuel (methane). Lee et al., also studied the effects of pressure on the extinction limits of water-laden methane/air flames in a counter-flow, non-premixed setting. [28]. They demonstrated through kinetic simulations, as the pressure increased, so did the extinction limit for a given amount of fuel (methane, in this case). They also showed that with increasing pressure, the width of the flame also decreases, and the flame at higher pressures is dominated by physical effects rather than being dominated by chemistry. Such insights are useful for designing high-pressure combustion devices. But such insights exist mostly for simple single-component fuels. It will be of great practical importance to see
whether the results from the study of simple fuels hold for high pressure combustion, with moisture, for real fuels as well.

Sensitivity Analysis is defined as the study of how the uncertainty in the output of a mathematical model or system (numerical or otherwise) can be divided and allocated to different sources of uncertainty in its inputs [29]. In simple terms, it is a statistical analysis to determine by how much the output of a model or system is going to vary, given some variance in its inputs. A sensitivity analysis is used for the simplification of physical models, to investigate the robustness of the model predictions, to explore the impact of varying input assumptions, and to determine which input parameters have the maximum influence on the value of the final predicted output [30].

Combustion inherently is a highly complex phenomenon, characterized by the interaction and competition of various physical and chemical processes. In order to describe the chemical changes during combustion correctly, large kinetic mechanisms are needed. In order to make sense of the large number of input parameters and chemical reactions during combustion, sensitivity analysis has proven to be a useful tool in the past. Sensitivity Analysis has several useful applications when applied to combustion chemical models. Firstly, such an analysis reveals which are the main control parameters in the model. It then provides information about the chemical reactions that are driving the combustion forward or backward, and also by what comparative degree, as compared to the other reactions [31]. Secondly, detailed chemical reactions are too big for complex combustion simulations. Sensitivity analysis can identify the reactions in a kinetic mechanism that are the least significant and removing them simplifies the mechanism while maintaining a high degree of accuracy of the predictions as compared to a full-fledged kinetic model. [32–34]. Another popular method for mechanism reduction, the Principle Component Analysis (PCA), requires sensitivity analysis as its first step [31, 35, 36]. This first step involves the calculation of the normalized local sensitivity matrix, which is the collection of the normalized local sensitivities of the observed parameters with respect to the variations in the reaction coefficients of each reaction. The matrix is then decomposed by diagonal decomposition. By this decomposition step, the dimensional space defined by all the chemical reactions is transformed or simplified into a new space that is of much lower dimension but captures most of the variance or ”useful information” of the
system. Working in this much simpler space speeds up computations as it simplifies calculations. The transformed components obtained also allow for the rank-order the chemical reactions, which allows for the reduction of the full-kinetic mechanism which can be achieved by removing the reactions which add the least variance or "usefulness" to the system. More information about PCA for combustion kinetics can be found in [37].

Sensitivity analyses in general, are of two types, namely the local sensitivity analysis and the global sensitivity analysis [29, 31, 33]. To explain the concept better, consider a black-box system modelled by a continuous scalar function $\phi$. The input of this function is a $p$-dimensional random variable $X = (X^{(1)}, X^{(2)}, X^{(3)}...X^{(p)})$ and the output is defined by the variable $Y$ such as $Y = \phi(X)$. Local sensitivity analyses how a small perturbation near an input space value $x^0 = (x^0_1, ..., x^0_p)$ influences the value of $y = \phi(x^0)$. It consists in estimating

$$A_i = \frac{\partial y}{\partial x_i}(x^0_1, ..., x^0_p) \tag{1.1}$$

that characterizes the effect on the random value $Y$ of a perturbation on the input $X^{(i)}$ near a nominal value $x^0_i$. A global sensitivity analysis focuses on the variance of model output $Y$ and more precisely on how the input variability influences the variable output. It enables the researcher to determine which parts of the output variance are due to the different inputs with the estimation of Sobol indices [38]. For the case of combustion chemistry, a global sensitivity analysis takes into account the uncertainty in the input parameters, namely the uncertainty in the reaction coefficients of each of the chemical reactions in a given combustion reaction mechanism. [39, 40]. A local sensitivity analysis has the advantage of being computationally cheaper than a global sensitivity analysis for the same system and at the same time identifies the most significant mechanisms with reasonable accuracy. The local sensitivity analysis is the predominantly used sensitivity analysis method for providing scientific insights as well as in mechanism reduction approaches in the combustion research community [20, 21, 33]. A local sensitivity analysis is often performed as the first step in mechanism reduction of a given mechanism followed by more advanced reduction techniques such as Directed Relational Graph (DRG), Directed relational graph with error propagation (DRGEP), Path influx analysis (PFA), etc. [33].
The goal of this work of research is to contribute to the discussion of designing high-pressure devices for complex fuels which are already in use for devices as jet gas turbines and rocket engines. JP-10 fuel has been selected to serve as a suitable example for a complex real fuel. Kinetic combustion simulations are performed for JP-10 for a cross-flow non-premixed diffusion flame setup. The cross-flow diffusion flame set-up was chosen as there exists abundant literature on analytical, numerical, and experimental studies involving cross-flow diffusion flames [3, 41, 42]. Such flames are of fundamental interest because they approximate a one-dimensional character and because residence times within the flame zone can be easily varied, making them an ideal choice for fundamental research investigations.

To make the investigation applicable to real life results, the role of water content is also studied under varying pressure conditions from 1 atm to 70 atm. Extinction limits for one mole of JP-10 under different operating pressures are determined as well. Beyond the extinction limit, the fuel becomes so wet (or the water content is so high) that a flame cannot be formed. The goal of the above mentioned extinction analysis is to simulate a high-pressure jet turbine running in an environment with high humidity.

Finally, local sensitivity analyses are performed for various pressures ranging from 1 atm to 70 atm, for dry fuel as well wet fuel near the determined extinction limits to identify the most influential or dominating chemical reactions in each case. This is done by analyzing the variation of maximum temperature with the variation of the kinetic reaction constants \( \frac{\partial T_{\text{max}}}{\partial k_i} \) for each corresponding reaction in the mechanism.
2.0 Governing Equations and Numerical Method

High pressure combustion kinetic simulations were performed using the Cantera library [43]. The flame configuration selected to run all the simulations was the opposed flow diffusion flame configuration. The opposed flow configuration is the most suitable as the flame produced is a strained, laminar, one-dimensional flamelet with well defined dynamics [28]. The fuel that has been chosen for the combustion studies was JP-10. JP-10 is a commonly used jet fuel in the military for missile gas turbines and jet engines.

2.1 Opposed Flow Diffusion Flame

Assuming radial velocity $v$ is linearly proportional with $r$ direction, the two dimensional flow problem reduces to a one-dimensional problem and the behavior of the system and

\[\text{Figure 1: Schematic of opposed flow diffusion flame}\]

1The full Jupyter notebook used to generate the temperature profiles, velocity profiles, and sensitivity analyses can be found in the github repository https://web.stanford.edu/group/haiwanglab/HyChem/fuels/JP-10_spec.html
various flow variables can be determined by Ordinary Differential Equations (ODEs) with \( x \) as the spatial variable [28].

\[
\frac{\partial \rho u}{\partial x} + 2\rho V = 0, \tag{2.1}
\]

\[
\rho u \frac{\partial V}{\partial x} + \rho V^2 = -\Lambda + \frac{\partial}{\partial x} \left( \mu \frac{\partial V}{\partial x} \right), \tag{2.2}
\]

\[
\rho c_p u \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left( \Lambda \frac{\partial T}{\partial x} \right) - \sum_k j_k c_{p,k} \frac{\partial T}{\partial x} - \sum_k h_k W_k \omega_k, \tag{2.3}
\]

\[
\rho u \frac{\partial Y_k}{\partial x} = -\frac{\partial j_k}{\partial x} + W_k \omega_k, \tag{2.4}
\]

where \( \rho \) is the density, \( u \) is the axial velocity, \( v \) is the radial velocity, \( V = v/r \) is the scaled radial velocity, \( \Lambda \) is the pressure eigen value where \( \frac{d\Lambda}{dx} = 0 \), \( \mu \) is the dynamic viscosity, \( c_p \) is the heat capacity at constant pressure, \( T \) is the temperature, \( \lambda \) is the thermal conductivity, \( Y_k \) is the mass fraction of species \( k \), \( j_k \) is the diffusive mass flux of species \( k \), \( c_{p,k} \) is the specific heat capacity of species \( k \), \( h_k \) is the specific enthalpy of species \( k \), \( W_k \) is the molecular weight of species \( k \), and \( \omega_k \) is the molar production rate of species \( k \).

In this formulation, the species diffusive mass fluxes, \( j_k \), are computed according to a multi-component formulation,

\[
 j_k = \frac{\rho W_k}{W^2} \sum_i W_i D_{ki} \frac{\partial X_i}{\partial x} - \frac{D_k^T}{T} \frac{\partial T}{\partial x}, \tag{2.5}
\]

where \( W \) is the mean molecular weight of the mixture, \( X_i \) is the mole fraction for species \( i \), \( D_{ki} \) is the multi-component diffusion coefficient, and \( D_k^T \) is the Soret diffusion coefficient.

2.2 Numerical Simulations

Numerical simulations have been performed using Cantera [43]. Cantera is an open source, object oriented suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. Originally developed in C++, it has multiple interfaces
in Python, MATLAB, and even Fortran. Some of its prominent application areas include combustion, detonation, electrochemical energy, fuel cells, batteries, plasmas, and film deposition.

To solve the equations mentioned in the previous section, the steady-state version of the equations are discretized on a generally non-uniform 1-D mesh across the domain. Each of the system of equations are then solved by using a damped modified Newton method solution algorithm with internal time integration scheme. The general modified Newton step-by-step algorithm is outlined below [44]:

1. Make an initial guess for the quantity to be estimated, $x^0$. Set the iteration counter $k = 0$. Select a tolerance $\epsilon$ for the stopping criterion.
2. Calculate $c_i^{(k)} = \frac{\partial f(x^{(k)})}{\partial x_i}$ for $i = 1$ to $n$. If the magnitude of $c_i^{(k)} < \epsilon$, stop the iterative process. Otherwise, continue.
3. Calculate the Hessian matrix $H^{(k)}$ at the current point $x^{(k)}$.
4. Calculate increment in $x$ using the equation $\Delta x = -H^{-1}c$.
5. Update the initial guess as $x^{(1)} = x^{(0)} + \Delta x$
6. Repeat the calculations from Step 2 onward till convergence is reached. But the Hessian (Step 3) is not to be calculated again.

The implementation of the above algorithm is said to be damped because a damping coefficient is added to reduce the vibration of the numerical system and help with the convergence of the solution. Also an internal time integration term is added to the solution algorithm. This “artificial temporal term” is added to help with the convergence if the damping fails.

The overall system is solved by Cantera using the following steps:

1. Set a grid of equidistant points.
2. Solve with these grid points.
3. Damped modified Newton solver with internal time integration is used to compute the temperature slope and curvature with the set_refine_criteria as input.
4. The converged solution is then obtained as per the tolerances set in set_steady_tolerances.
5. If the solution algorithm does not converge, the mesh is refined. A point may be added if needed and some unnecessary points may be removed if needed.

6. The solution process again begins from Step 2 with this modified mesh.

All simulations cross-flow diffusion simulations in Cantera follow the following steps for programming and working with Cantera in Python:

1. Import relevant libraries (Cantera, Matplotlib, NumPy, Pandas, etc.)

2. Specify the input conditions namely the pressure, fuel and oxidizer inlet temperatures, the fuel and oxidizer mass flow rates, fuel and oxidizer inlet temperatures, and finally the width of the domain.

3. Gas object is created which takes the mechanism file (.cti) as input.

4. Temperature and pressure of the gas are initialized using this object and the input provided in step 1.

5. Cantera object CounterflowDiffusionFlame is created which takes the gas object and width of the domain as the input.

6. All the inputs specified previously are then passed to this object.

7. Then the solve command is initiated via the declared object.

8. Once the problem is solved, using the Cantera object, temperature or axial velocity curves are plotted using the Matplotlib library.

For this study, the one-dimensional counter-flow diffusion flame class was used to represent the flame domain. It consists of a fuel inlet on the left, the flow in the middle, and the oxidizer inlet on the right. All properties in this system are assumed to be dependent only on the axial direction. For all simulations, Soret Effect has been turned off and losses due to radiation have not been considered for the sake of simplicity.

2.2.1 Boundary Conditions

The inlet fuel temperature and the inlet air temperature were both taken to be at the room temperature of 300 K. The mass flow rate of air was taken to be at 0.72 kg/m²/s while that of the fuel is taken to be at 0.24 kg/m²/s. The distance between the fuel and air
inlets was taken as 2 cm. These chosen boundary conditions are the most commonly used in both simulation and experimental setups [28, 36]

In all the simulations performed, the air composition was 78% of nitrogen, 21% of oxygen, and 1% of Argon. The fuel being burnt in each case was 1 mol of JP-10 with variable amounts of water depending on the case being studied.

Results were generated and analyzed for varying values of pressure while keeping the above-mentioned conditions fixed. Combustion in jet engine combustion chambers typically occurs at the high pressure range of 35-40 atm. In order to perform a well-rounded study and observe behavior on either side of the working pressure, the pressure cases analyzed were for 1, 10, 20, 30, 40, 50, 60, and 70 atm values of pressure. For each pressure case, starting from dry fuel (no water content), water was added incrementally to the fuel till flame extinction was observed and the extinction limits were noted.

2.3 Reaction Mechanisms

In order to perform an accurate combustion simulation, the composition of species in a given fuel needs to be determined with high accuracy. Only if the composition is well-defined can a detailed chemistry model be developed, which uses the fuel composition as a part of the thermodynamic input. The task is an arduous one as the fuel may be composed of thousands of hydrocarbons and developing detailed reaction models for even a single hydrocarbon may reach a few thousand steps.

The HyChem approach proposes that the oxidation of fuel can be split into two physical phenomena: [18]:
1. Pyrolysis of fuel to form pyrolysis products
2. Oxidation of the pyrolysis products

Large hydrocarbons fuels undergo pyrolysis first, followed by the oxidation of pyrolysis products. These two processes are decoupled in both time and space. The second step is the rate-limiting step. Therefore, the composition of the pyrolysis products determines the
overall oxidation rate of the fuel. The JP-10 fuel model was developed using this approach by
the research groups mentioned in the introduction section [21]. The input file containing the
full mechanism was chosen for high accuracy for all the simulations in this work of research.

2.4 Local Sensitivity Analysis

The sensitivity coefficient that is determined in all cases, $\frac{\partial T_{\text{max}}}{\partial k_i}$, is of not much use
if used directly. The reason being that the rate coefficients belonging to different chemical
reactions will have different units. Hence, it is not possible to make any direct, hence fruitful,
comparisons. For the sake of comparison, normalized sensitivity coefficients are used instead
of the original coefficients. The normalized sensitivity coefficients $S_i$ for the $i$th reaction is
defined as:

$$S_i = \frac{\partial T_{\text{max}}}{\partial k_i} \frac{k_j}{T_{\text{max}}} = \frac{\partial \ln T_{\text{max}}}{\partial \ln k_i}$$ (2.6)

This is the quantity that was estimated in all the sensitivity analyses. This quantity was
calculated using the preexisting features in Cantera. The steps to perform a local sensitivity
analysis for any given system are outlined as follows:

1. The original maximum temperature of the system, $T_{\text{max}}^0$, is determined by performing a
simple counter-flow diffusion flame situation as described previously.
2. A perturbation value $dk$ is set. For all the cases in this research study, the perturbation
value chosen was 1e-2.
3. The first reaction coefficient is then perturbed by the perturbation constant defined in
the previous step.
4. The flame system is then solved again with the perturbed reaction coefficient.
5. The new maximum temperature $T_{\text{max}}$ obtained in this case is then stored.

2The Cantera input file for JP-10 can be found at the web address: https://web.stanford.edu/group/
haiwanglab/HyChem/fuels/JP-10_spec.html
6. From this new maximum temperature, the normalized sensitivity $S_m$ for the $mth$ reaction (where $m = 1$ for the first reaction) is calculated using the relation $S_m = \frac{T_{max} - T_{max}^0}{T_{max}^0 - dk}$

7. Steps 3-6 are repeated for all the remaining $m - 1$ reactions.

8. Once all the sensitivities are calculated, a few of the most sensitive reactions are plotted on a bar-plot by setting a threshold on the sensitivity values.
3.0 Results

3.1 Effect of Water Addition on Temperature and Velocity Profiles

Temperature and axial velocity profiles for the combustion of 1 mol of JP-10 fuel in dry air as well as with added water content to fuel (wet fuel) were determined. Water content was added to the fuel till the extinction limit is reached and the flame is extinguished. The simulations were performed for the pressures of 1, 10, 20, 30, 40, 50, 60, and 70 atm.

![Figure 2: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (1 atm)](image)

At all values of pressure, a common trend that was observed in Fig. 2-9 was that as more and more water was added to the fuel, there was a gradual decrease in both the peak temperatures and axial velocities as compared to the peak temperature and axial velocity values when the fuel was dry for a given pressure case. When the water content became so large that no flame could be formed, at that point, the extinction limit of the flame was said to have reached.

Another trend that can be observed in Fig. 2-9 is that across all the pressure values, was that when water was added continuously, there was a gradual shifting of the domain where the flame was being formed, for both the temperature and axial velocity plots. The
Figure 3: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (10 atm)

Figure 4: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (20 atm)
Figure 5: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (30 atm)

Figure 6: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (40 atm)
Figure 7: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (50 atm)

Figure 8: Variation in temperature (a) and velocity (b) by addition of water content at constant pressure (60 atm)
flame formation domain, along with the points in the domain where the peak values are observed, started shifting from left to right as the water content was added to the fuel till the extinction limit was reached (no flame was observed in such a case, only a flat line).

### 3.1.1 Effect of Pressure on Peak Temperature and Axial Velocity for Dry JP-10 Fuel

As can be observed in Fig. 10, for the case of dry air, the peak temperature of the flame was observed to be 1954.9 K at 1 atm. It increases steadily to 2236.8 K as the pressure was increased from 1 atm to 10 atm. After ramping up the pressure from 10 atm to 20 atm, there was only a slight increase in peak temperature from 2236.8 K to 2282.7 K. Beyond 20 atm, no increase in peak temperature occurs for any value of pressure. The value of peak temperature was observed to have become constant for any pressure range beyond 20 atm.

As can be observed in Fig. 10, a similar trend was observed in the case of the maximum value of axial velocity as well. At 1 atm, the axial velocity was found to be -0.35 m/s. It decreased to -0.041 m/s as the pressure was increased from 1 atm to 10 atm. After ramping up the pressure from 10 atm to 20 atm, there was only a slight decrease in peak temperature
Figure 10: Variation of peak temperature for dry air under varying pressure

Figure 11: Variation of peak axial velocity for dry air under varying pressure
from -0.041 m/s to -0.021 m/s. Beyond 20 atm, not much decrease in peak axial velocity occurred for any value of pressure. The value of peak axial velocity is observed to have become constant for any pressure range beyond 20 atm.

3.2 Extinction Limit as a Function of Pressure

![Graph of Combustion of 1 mole of JP-10](image)

Figure 12: Extinction limit vs. pressure for 1 mol of JP-10 combustion

Fig. 12 shows that as the pressure kept on increasing, so did the extinction limit for the combustion of 1 mol of JP-10 in air. This indicates that higher the pressure, more the the moisture content that the system can tolerate for a successful combustion of fuel.

As indicated in Fig. 13, as the pressure kept on increasing, the slope of the extinction limit curve kept on decreasing and it is strongly hinted that it will show asymptotic behavior at a certain higher value of pressure.
3.3 Sensitivity Analysis Results

3.3.1 Sensitivity Analysis of Dry Air

Sensitivity analyses were carried out for the combustion of JP-10 fuel in dry air for the pressure cases of 1, 10, 20, 30, 40, 50, 60, and 70 atm pressure. The parameter for which sensitivity was observed is the peak temperature of the flame at a given pressure without any water added to the fuel.

For the case of 1 atm, as shown in Fig. 14, the most sensitive reaction was the reduction of oxygen molecule to form hydroxyl species and mono-molecular oxygen. The second most sensitive reaction was the formation of water, $H + O_2 \leftrightarrow O + OH$. The decomposition of the JP-10 molecule into simpler products (pyrolysis) was the 11th most sensitive reaction, $C_{10}H_{16} \rightarrow 0.866C_2H_4 + 0.0693C_3H_6 + 0.952C_5H_6 + 0.08242C_6H_5CH_3 + 0.351373C_6H_6 + 0.01CH_3 + 1.79H + 0.407143H_2 + 0.2aC_3H_5$. 

Figure 13: Slope of extinction limit with respect to pressure vs. pressure for 1 mol of JP-10 combustion
For the cases of 10, 20 and, 30 atm pressure, as shown in Fig 15-17, the most sensitive reaction was the formation of water in the presence of an inert molecule, \( H + OH + M \leftrightarrow H_2O + M \). For the case of 20 atm (Fig. 16) and 30 atm (Fig. 16), the pyrolysis of the JP-10 molecule was the fourth most-sensitive and fifth-most sensitive reaction, \( C_{10}H_{16} =\rightarrow 0.866C_2H_4 + 0.0693C_3H_6 + 0.952C_5H_6 + 0.08242C_6H_5CH_3 + 0.351373C_8H_6 + 0.01C_9H_3 + 1.79H + 0.407143H_2 + 0.2aC_3H_5 \), respectively.

For all the higher pressure ranges, from 40 atm to 70 atm, as seen in Fig. 18-21, The most sensitive reaction in the entire mechanism was the reaction of Hexene with hydroxyl ion to form phenol and hydrogen ion. \( C_6H_6 + OH \leftrightarrow C_6H_5OH + H \). The reaction of formation of water was still highly sensitive at 40, 50, and 70 atm, but not for 60 atm, \( H + OH + M \leftrightarrow H_2O + M \).

### 3.3.2 Sensitivity Analysis of Wet Fuel Near Extinction Limit

Sensitivity analyses were also carried out for the combustion of JP-10 fuel in the presence of water added to the fuel in dry air, for the pressure cases of 1, 10, 20, 30, 40, 50, 60, and 70 atm pressure. The amount of water added was corresponding to the amount very close to the extinction limit.
Figure 15: Normalized sensitivities \( \frac{\partial T_{\text{max}}}{\partial k} \) for the most sensitive reactions at 10 atm for combustion of 1 mol dry JP-10 in air.

Figure 16: Normalized sensitivities \( \frac{\partial T_{\text{max}}}{\partial k} \) for the most sensitive reactions at 20 atm for combustion of 1 mol dry JP-10 in air.
Figure 17: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 30 atm for combustion of 1 mol dry JP-10 in air.

Figure 18: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 40 atm for combustion of 1 mol dry JP-10 in air.
Figure 19: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 50 atm for combustion of 1 mol dry JP-10 in air.

Figure 20: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 60 atm for combustion of 1 mol dry JP-10 in air.
Figure 21: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 70 atm for combustion of 1 mol dry JP-10 in air

For the pressure cases of 1 and 10 atm, as seen in Fig. 15-16, the most sensitive reaction was found to be the reduction of the oxygen molecule into oxygen ion and hydroxyl ion, $H + O_2 \leftrightarrow O + OH$. The oxidation of carbon monoxide by hydroxyl ion to form carbon dioxide, $CO + OH \leftrightarrow CO_2 + OH$ was found to be a highly sensitive reaction for these pressure cases as well.

For the higher pressure ranges of 20, 30, 40, 50, 60, and 70 atm, as shown in Fig. 17-22, the most sensitive reaction near the extinction limit shifts from $H + O_2 \leftrightarrow O + OH$ to $HO_2 + OH \leftrightarrow H_2O + O_2$, that is the formation of water and the oxygen molecule from hydrogen dioxide and hydroxyl ion. The oxidation of carbon monoxide by hydroxyl ion to form carbon dioxide, $CO + OH \leftrightarrow CO_2 + OH$ was found to be a highly sensitive reaction for these pressure cases as well.
Figure 22: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 1 atm for combustion of 1 mol JP-10 near extinction limit (6 mol $H_2O$)
Figure 23: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 10 atm for combustion of 1 mol JP-10 near extinction limit (20 mol $H_2O$)
Figure 24: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 20 atm for combustion of 1 mol JP-10 near extinction limit (28.5 mol $H_2O$)
Figure 25: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 30 atm for combustion of 1 mol JP-10 near extinction limit (32 mol $H_2O$)
Figure 26: Normalized sensitivities \( \frac{\partial T_{\text{max}}}{\partial k} \) for the most sensitive reactions at 40 atm for combustion of 1 mol JP-10 near extinction limit (40 mol \( H_2O \))
Figure 27: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 50 atm for combustion of 1 mol JP-10 near extinction limit (42 mol $H_2O$)
Figure 28: Normalized sensitivities ($\frac{\partial T_{\text{max}}}{\partial k}$) for the most sensitive reactions at 60 atm for combustion of 1 mol JP-10 near extinction limit (48 mol $H_2O$)
Figure 29: Normalized sensitivities $\left( \frac{\partial T_{\text{max}}}{\partial k} \right)$ for the most sensitive reactions at 70 atm for combustion of 1 mol JP-10 near extinction limit (50 mol $H_2O$)
4.0 Discussion

In order to establish the behavior of a sample jet engine fuel, JP-10, under high pressure and moisture, for real-life jet engine applications, 1D cross-flow diffusion flame simulations were carried out using the open source code Cantera. It was found that in the case of dry air, as the operating pressure was increased, the peak temperature and the peak axial velocity also increased till the pressure of 20 atm. Beyond 20 atm, the peak temperature and axial velocity values were approximately constant. It was also observed that, at a given operating pressure, there is a gradual shift in the domain of flame formation for both temperature and axial velocity curves as the water content is added continuously till the extinction point is reached, beyond which the flame is extinguished. Another observation that is deduced from the curves is, for a given pressure, as the water content is added to the fuel continuously, the peak temperature and axial velocity values also decrease gradually, till the point of extinction, beyond which no flame is possible. It was also observed that higher the pressure, the higher the extinction limit for a constant amount of fuel that is being burnt.

In addition to generating temperature and axial velocity curves, Cantera was used to perform local sensitivity analyses with peak temperature as the output or observed metric. The sensitivity analyses were carried out for dry air combustion for all the cases of operating pressure. It was observed that for the case of 1 atm pressure, the most sensitive reaction was the reduction of the oxygen molecule to form hydroxyl ion and mono-molecular oxygen. For the higher pressure cases of 10, 20, and 30 atm, the reaction with the highest sensitivity was the formation of water from the combination reaction of hydroxyl ion and hydrogen ion. For all the pressure cases beyond 30 atm, the most sensitive reaction was found to be the reaction of hexene with hydroxyl ion to form phenol and hydrogen ion. Finally, a series of sensitivity analyses were again carried out for all the pressure cases, the only difference being that the fuel contained water content very close to the extinction limit. For the operating pressure range from 1 atm to 20 atm, the most sensitive reaction was found to be the reduction of the oxygen molecule into oxygen and hydroxyl ions. Beyond this pressure range, the most sensitive reaction was found to be the formation of water and the
oxygen molecule from hydrogen dioxide and the hydroxyl ion. It can clearly be observed from both physical and chemical standpoints, that pressure clearly alters the behavior of the flame formed. The increase in peak temperature observed for the case of dry air is also observed by Sirignano et al., [16] for the combustion of methane in a cross-flow diffusion flame setting. But unlike their flame, whose peak temperature values kept on increasing with pressure, the peak temperature value becomes constant after 20 atm for the case of combustion of JP-10 flame. This deviation in behavior can be attributed to the fact that the fuel being burnt is JP-10, a complex fuel, unlike methane, which is a simple fuel. This observation for the peak temperature for the combustion of JP10 is also seen to extend to the case of peak axial velocity values. Similar to Sirignano et al.,’s real methane flame combustion under high pressure, there is a shift from left to right in the flame profile for both temperature and axial velocity cases for a given pressure. This can be attributed to the fact that the fuel is coming in from the left nozzle and air from the right nozzle. When water is added to the fuel stream, this added water gives extra weight, hence extra momentum, to the fuel stream while the momentum of the air-stream remains the same for all cases. The resultant of this added momentum in the fuel stream, shifts the overall profile of the flame towards the air-stream nozzle and away from the fuel-stream nozzle. Also, a gradual decrease in the peak temperature and axial velocity is observed as the water content keeps on increasing for a given pressure. This can be attributed to the fact that the added water acts as a heat sink and this heat sink effect keeps on increasing till the extinction point is reached. It is beyond this point of extinction that the minimum temperature needed for combustion is simply not achievable as the heat sink effect of water starts fully dominating the system. This phenomenon was also observed by Rankin et al., [28] for a similar case of combustion of water-laden methane in a cross-flow diffusion flame setting while trying to predict the extinction limits of methane hydrates. Finally, it is observed that as the pressure of the system is increased, so is the extinction limit. This observation agrees with Rankin’s extinction limit analysis of water-laden methane at high pressure. This observation has the potential to give designers of high-pressure devices, such as jet engines freedom to design systems that are operable in extremely moist or rainy environments. Such a combustion chamber that operates at higher pressure values, will also be useful where highly dry fuel
is difficult to procure. The sensitivity analyses for both dry JP-10 as well as the fuel near extinction limit shows that by varying only the pressure, there is a shift in the trend of the most sensitive reaction. This provides a strong indication that by simply varying the pressure, there is a significant change in the reaction being followed by the combustion of a given fuel, proving there is a strong effect on the chemistry by the pressure as well. Hence proving that the chemistry of the fuel also plays a key role in developing high pressure devices and cannot be overlooked.
5.0 Limitations and Future Work

5.1 Limitations

The following limitations are identified pertaining to the research carried out:

1. The sensitivity analysis carried out is a local sensitivity analysis. Since the kinetic rate equation is a highly non-linear term (containing the exponential constant), it is not able to accurately capture what is the effect of the input variance on the output variance [32, 45].
2. JP-10 is mostly single component jet fuel ($C_{10}H_{16}$). There is no answer to the question of whether the same trends will be observed for multi-component jet fuels such as Jet-A.
3. Sensitivity analysis was carried with only the maximum temperature as the dependent metric. Looking at different dependent metrics will provide a more holistic picture of the dominating reactions in a given case.

5.2 Future Work

Based on the results and discussion, the following future work is proposed:

1. For a better sensitivity analysis, global sensitivity analysis can be employed instead of the currently used local sensitivity analysis [29, 38, 39].
2. Repeat the study with different fuel models other than JP-10, such as Jet-A. Hy-Chem models already exist for Jet-A [18]. This will allow for the confirmation of whether the extinction limit and sensitivity trends observed in this research are dependent or independent of the fuel used.
3. Selecting other dependent metrics such as fuel concentration and flame speed, along with maximum temperature for sensitivity analysis can tell us which of these metrics is more suitable for determining the sensitivity for our study. This approach was followed by
Turanyi for the case of hydrogen combustion [46]. He found that flame speed had a higher value of sensitivity as compared to fuel concentration, hence establishing that the flame speed is a better metric to determine the order of dominating reactions in the combustion reaction.

4. Principle Sensitivity Analysis (PCA) may also be used to determine the dominant chemical reaction in a given combustion simulation [35, 37].
Bibliography


