Modelling and Analysis of Flare Stack Thermal Radiation on Offshore Oil and Gas Facilities

By

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Abstract
This research studied the capabilities of RANS-based computational fluid dynamics to model large scale 2-phase propane jet flares with considerations for thermal radiation, soot development, and other key flare properties. The goal of this work was to determine how modest CFD could be used in the generation and evaluation of large scale jet flares that are often only studied experimentally. Measurements of incident thermal radiation to remote targets, soot volume fraction, and relevant flare geometries are reported based on the CFD models produced and compared to various analytical and experimentally derived models.

The CFD study was completed using the commercial suite of tools from ANSYS, namely ICEM CFD 18 and Fluent 18. Emphasis was put on evaluating the pre-existing models within the solver. The standard $k$-$\varepsilon$ turbulence model was used in this study due to its support from literature, and performance in preliminary tests. A probability density function approach was used to model the non-premixed combustion, and the 2-step soot model was used to predict soot production. The P-1 radiation model was used as it is an economical, non-raytracing model that allows for the inclusion of radiation from soot.

The CFD results were compared to a solid flame model as well as empirical models and measurements. The CFD predicted soot volume fraction in the flare between $2.7 \times 10^{-7}$ and $4.9 \times 10^{-7}$ depending on the flare boundary temperature selected. Incident thermal radiation was found to agree strongly with a solid flame model; ranging from $1.6 \frac{\text{kw}}{\text{m}^2}$ at a 2m distance, to $0.11 \frac{\text{kw}}{\text{m}^2}$ at 15m. Agreement with experimental radiometer data was weak, with the CFD results predicting much lower levels of thermal radiation. Average surface emissive power of the flare was determined to be $100.3 \frac{\text{kw}}{\text{m}^2}$ using literature based techniques and agreed well with various empirical models from literature. The radiative signature of the flare was also studied for crosswinds of up to 6m/s, showing expected increases in incident radiation to downstream targets - up to $9.1 \frac{\text{kw}}{\text{m}^2}$ in the near field for 6m/s winds.
Acknowledgements

I would like to thank my supervisor, Dr. A. M. Birk, for his wealth of knowledge and support throughout this project. His passion for engineering and academics is motivating and appreciated.

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Table of Contents

Abstract ................................................................................................................................. ii
Acknowledgements ............................................................................................................. iii
Table of Contents ................................................................................................................ iv
List of Figures ....................................................................................................................... vii
List of Tables ......................................................................................................................... xii
Nomenclature ....................................................................................................................... xiii

1. Introduction ....................................................................................................................... 1
   1.1. Objectives .................................................................................................................. 3
   1.2. Scope .......................................................................................................................... 3

2. Theory and Literature Review ....................................................................................... 4
   2.1. 2-Phase Combustion .................................................................................................. 4
       2.1.1. Atomization and Droplet Size ........................................................................... 4
       2.1.2. Droplet Combustion ....................................................................................... 7
   2.2. Thermal Radiation .................................................................................................... 9
       2.2.1. Weighted-sum-of-Gray-Gases-Model ............................................................... 12
       2.2.2. Participating Medium .................................................................................... 13
   2.3. Soot Production ....................................................................................................... 14
   2.4. CFD Overview ......................................................................................................... 18
       2.4.1. Turbulence ......................................................................................................... 19
       2.4.2. Non-Premixed Combustion ............................................................................. 23
       2.4.3. Discrete Phase Modelling .............................................................................. 25
       2.4.4. Soot Modelling .............................................................................................. 27
       2.4.5. Radiation Modelling ...................................................................................... 28
   2.5. Solid Flame Modelling ............................................................................................ 30

3. Numerical Methodology ............................................................................................... 34
   3.1. CFD Studies Overview ............................................................................................ 34
   3.2. Computational Domain ........................................................................................... 34
       3.2.1. Domain Geometry ......................................................................................... 34
       3.2.2. Mesh Generation ............................................................................................ 36
   3.3. Boundary Conditions .............................................................................................. 39
       3.3.1. Pressure Inlet ................................................................................................ 40
       3.3.2. Pressure Outlet .............................................................................................. 40
       3.3.3. Wall ............................................................................................................... 41
3.3.4. Velocity Inlet ........................................................................................................... 41
3.3.5. Discrete Phase Interactions ................................................................................. 41
3.3.6. Species Definitions .............................................................................................. 41
3.3.7. Thermal Definitions ............................................................................................. 41
3.4. Solver Settings ........................................................................................................ 42
  3.4.1. Discretization Scheme ......................................................................................... 42
  3.4.2. Pressure-Based Solver ......................................................................................... 42
3.5. Physical Models ........................................................................................................ 43
  3.5.1. Turbulence Model ............................................................................................... 43
  3.5.2. Discrete Phase Model ......................................................................................... 43
  3.5.3. Injection Model .................................................................................................. 44
3.6. Solution Generation .................................................................................................. 44
  3.6.1. Initialization and Interpolation ........................................................................... 45
  3.6.2. Under-Relaxation .............................................................................................. 45
  3.6.3. Solution Convergence ....................................................................................... 46
4. Results and Discussion .................................................................................................. 50
  4.1. Flare Geometry ..................................................................................................... 50
  4.2. Soot Characteristics .............................................................................................. 53
  4.3. Thermal Radiation .................................................................................................. 57
    4.3.1. Solid Flame Models ......................................................................................... 61
    4.3.2. Experimental Based Models .......................................................................... 62
    4.3.3. Surface Emissive Power .................................................................................. 65
  4.4. Swirling Flow .......................................................................................................... 66
  4.5. Crosswind Flows .................................................................................................... 76
5. Conclusions .................................................................................................................. 79
  5.1. Flare Geometry ..................................................................................................... 79
  5.2. Soot Characteristics .............................................................................................. 80
  5.3. Thermal Radiation .................................................................................................. 80
  5.4. Swirling and Crosswind Flows ............................................................................. 81
6. Recommendations .......................................................................................................... 82
  6.1. Exhaustive CFD Model Studies ............................................................................ 82
  6.2. Experimentation ..................................................................................................... 83
  6.3. Flare and Nozzle Configurations ......................................................................... 83
  6.4. Swirling Flows ....................................................................................................... 83
References ........................................................................................................................ 85
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. Supplementary Literature</td>
<td>88</td>
</tr>
<tr>
<td>A.1. Thermal Hazard Measurement</td>
<td>88</td>
</tr>
<tr>
<td>A.2. Nozzle Design</td>
<td>89</td>
</tr>
<tr>
<td>B. Computational Models and Codes</td>
<td>92</td>
</tr>
<tr>
<td>B.1. EES Flash Calculations</td>
<td>92</td>
</tr>
<tr>
<td>B.2. Swirling Boundary Condition</td>
<td>95</td>
</tr>
<tr>
<td>C. Additional CFD Material</td>
<td>100</td>
</tr>
<tr>
<td>C.1. Grid Independence Study</td>
<td>100</td>
</tr>
<tr>
<td>C.2. Sample Script</td>
<td>103</td>
</tr>
</tbody>
</table>
List of Figures

Figure 1-1: Flares produced from an offshore flare boom. A “peacock” style burner head is used to disperse waste fuel over a larger area [1].................................................................................................................. 1

Figure 1-2: (left) Water spray shielding used to cool and protect the back side of a ship [3]. (right) Physical wall thermal barrier on a raised flare boom arm [4]................................................................. 2

Figure 2-1: Visualization of how velocity impacts the atomization of a simple fluid jet [5]. ...................... 5

Figure 2-2: Results from the 2mm nozzle trial at X=95mm, (a) 5 bar, (b) 11 bar [7]. ................................. 7

Figure 2-3: Basic schematic of a single fuel droplet combusting [10] ....................................................... 8

Figure 2-4: Radial variations of temperature and species partial pressures in the 2-film model [8]. ........... 9

Figure 2-5: Absorption spectra for various gases in the Earth’s atmosphere [11]................................. 11

Figure 2-6: Total emittance of carbon dioxide in a mixture of total pressure P = 1atm [12]....................... 11

Figure 2-7: Total emittance of carbon dioxide pressure corrections for varying total pressures [12]. ...... 12

Figure 2-8: Band overlap corrections for a mixture of carbon dioxide and water vapour. Gas temperatures are 400K, 810K, and 1200K, from left to right respectively [12]................................................................. 12

Figure 2-9: A schematic showing the absorption, scatter, and transmission of radiation along a path in a participating medium [13]..................................................................................................................... 14

Figure 2-10: A highly luminous oil boom flare producing a large amount of soot. Buoyancy effects cause an upward deflection of the flare [1].............................................................................................................. 15

Figure 2-11: Soot diameter and volume fraction for the two flame trials. Measurement ports indicate the streamwise location of the measurements with 2 corresponding to the flame base, and 5 near the flame tip [14].................................................................................................................................................. 17

Figure 2-12: Soot formation as a function of excess oxygen (equivalence ratio) and oxygen concentration in the combustion air, dilution with nitrogen. Bold lines represent constant oxygen concentration but variable velocity, dashes lines represent variable oxygen concertation with constant velocity [15]......... 18
Figure 2-13: Ratio of radiant flame length and equivalent flame diameter for varying fuel mass flows and orifice diameters [22].................................31

Figure 2-14: Atmospheric transmissivity predicted using the Brzustowski model for various values of relative humidity. .................................................................33

Figure 2-15: Configuration B-32 used to determine the relevant view factor for flare calculations. ....33

Figure 3-1: Dimensioned diagram of the computational domain with labeled axes.........................35

Figure 3-2: Dimensioned diagram of the concentric rings on the base plane of the domain. Radius dimensions are given for each ring with ring 1 being the innermost, increasing outwardly to ring 6 ....35

Figure 3-3: A sample surface mesh of the base surface showing increasing cell density at the inner rings. .............................................................................................................36

Figure 3-4: Two density regions along the centerline of the domain limit cell size and growth.........37

Figure 3-5: A central vertical plane of the volume mesh. Two density zones are clearly visible with increased cell density. Inflation layers seen on the lower floor surface.................................................38

Figure 3-6: Horizontal plane showing the increased mesh density around the central core flame region. 38

Figure 3-7: Inflation layer cells stacked on the base surface add necessary detail to capture boundary layer flows.................................................................39

Figure 3-8: Boundary conditions used..................................................................................40

Figure 3-9: Location of the liquid fuel injection in the computational domain (not to scale)..............44

Figure 3-10: The temperature monitors (red) and thermal radiation monitors (grey) in the domain....47

Figure 3-11: Centerline temperatures developing and converging during solution generation. Monitor labels correspond to the vertical distance above the ground plane in meters. .........................48

Figure 3-12: Soot volume fraction developing during solution generation..................................48

Figure 3-13: Net mass flow through the boundaries of the domain during solution generation........48

Figure 3-14: Incident thermal radiation to the targets at varying distances from the centerline of the domain developing during solution generation..................................................49

Figure 4-1: The flare volume defined by the 600K iso-surface inside the computational domain....51
Figure 4-2: Comparing the size for the three iso-surface defined flare volumes ........................................... 52
Figure 4-3: Temperature contour of the flare .......................................................... 52
Figure 4-4: Contour of soot volume fraction along a vertical center plane showing the local maximum concentration in the flare relative to the computation domain .......................................................... 54
Figure 4-5: Soot volume fraction and temperature distribution displayed inside the 600K iso-surface flare. .......................................................... 55
Figure 4-6: Three-dimensional rendering of the predict soot results. The volume is defined by a constant soot volume fraction of $1 \times 10^{-6}$ .......................................................... 56
Figure 4-7: Incident thermal radiation from the CFD results. The monitored targets at 2m, 4m, etc. are highlighted .......................................................... 57
Figure 4-8: Contour plot of incident radiation from the CFD analysis .......................................................... 58
Figure 4-9: Center-plane contour plot of thermal radiation flux distribution. Highest levels of radiation occur inside the hottest part of the flame where soot concentration is highest .......................................................... 59
Figure 4-10: Four geometrically similar reference lines used to measure incident radiation around the flare .......................................................... 60
Figure 4-11: Comparing the normalized radiation data for each reference line .......................................................... 60
Figure 4-12: Comparing the CFD results with three temperatures of solid flame models. Emissivity of $\varepsilon = 0.45$ was used for each solid flame .......................................................... 61
Figure 4-13: Comparing the CFD results with three emissivity values of solid flame models. Flame temperature of 1400K was used for each solid flame .......................................................... 62
Figure 4-14: Incident radiation raw data and fits for the experimental trials [23]. .......................................................... 63
Figure 4-15: CFD Results compared with Zhang’s experimental work .......................................................... 64
Figure 4-16: Comparing surface emissive power for the CFD model and solid flame model .......................................................... 65
Figure 4-17: Streamlines of velocity originating from the swirling velocity inlet. Maximum tangential swirl velocity of 1m/s .......................................................... 67
Figure 4-18: Lines used to evaluate tangential velocity at various heights above the inlet velocity boundaries. ................................. 68

Figure 4-19: Tangential swirl velocity profile for 1 m/s maximum swirl strength. Legend indicates vertical distance above the boundary. ........................................... 69

Figure 4-20: Tangential swirl velocity profile for 3 m/s maximum swirl strength. Legend indicates vertical distance above the boundary. ........................................... 70

Figure 4-21: Tangential swirl velocity profile for 5 m/s maximum swirl strength. Legend indicates vertical distance above the boundary. ........................................... 70

Figure 4-22: Streamlines of velocity above the 3 m/s swirling velocity inlet .................................................. 71

Figure 4-23: Streamlines of velocity above the 5 m/s swirling velocity inlet .................................................. 71

Figure 4-24: Tangential velocity contour for a maximum swirl strength of 1 m/s. The recirculation zone is not present at the lower speed. .................................................. 72

Figure 4-25: Tangential velocity contour for a maximum swirl strength of 3 m/s. The recirculation zone can be seen above the boundary plane. Tangential velocity degrades rapidly downstream. .................. 73

Figure 4-26: Tangential velocity contour for a maximum swirl strength of 5 m/s. The recirculation zone is significant above the boundary plane. Tangential velocity degrades rapidly downstream. .................. 73

Figure 4-27: Temperature monitors for the 3 m/s swirl case. Rapidly changing and deteriorating temperature values indicate solution convergence and stabilization issues. ........................................ 74

Figure 4-28: Temperature monitors for the 1 m/s swirl case. Stabilization of the solution is improved over the higher speed cases, but is not ideal. Continuing temperature development indicates changing flare characteristics ................................................................. 75

Figure 4-29: Comparing the thermal radiation profile from the low speed swirl and base cases. ............ 75

Figure 4-30: Crosswind direction vectors. The crosswind produced blows the flare directly overhead of the reference line used to capture incident thermal radiation. ............................................................... 76

Figure 4-31: Flame deflection for each crosswind speed studied ............................................................... 77
Figure 4-32: Measured incident radiation convergence for solution generation of the 4 m/s crosswind trial.

Figure 4-33: Comparing the incident thermal radiation profiles for various crosswind speeds.

Figure A-1: Characteristic patterns of various spray nozzles. Full cone, hollow cone, fan from left to right [5].

Figure B-1: Simplified schematic of the propane system showing the two states.

Figure B-2: T-s diagram of the isentropic propane flash from saturated liquid. Diagram is not to scale.

Figure B-3: Normalized tangential velocity profile for the swirling boundary condition.

Figure B-4: Normalized tangential velocity profiles for N=3.

Figure B-5: Normalized tangential velocity profiles for N=5.

Figure B-6: Normalized tangential velocity profiles for N=7.
List of Tables

Table 1-1: Qualitative risk descriptions of varying thermal radiation levels (HSE 2006) .............................. 2
Table 2-1: Fuel droplet measurements, 2mm nozzle. Error reported as 8% for velocity measurements, and 13% for diameter measurements. Altered from [7] ........................................................................................................ 6
Table 2-2: Fuel droplet measurements, 5mm nozzle. Error reported as 8% for velocity measurements, and 13% for diameter measurements. Altered from [7] ........................................................................................................ 6
Table 2-3: Optical properties to consider for thermal radiation .......................................................................... 10
Table 2-4: Experimentally determined propane soot radiation characteristics[13] ................................................. 16
Table 2-5: Classification of RANS turbulence models .......................................................................................... 21
Table 4-1: Geometric flame properties from iso-surfaces of varying temperatures .............................................. 51
Table 4-2: Comparing the soot volume fraction for each iso-surfaced defined flare body ..................................... 56
Table 4-3: Power correlations of radiation with distance for the experimental trials [23] ................................. 63
Table 4-4: Comparison of five emissive power models from literature .............................................................. 66
Table 4-5: Swirling boundary velocity inputs for the cases studied ...................................................................... 67
Table A-1: Fatality rate as a function of exposure time for varying radiation strengths [2] ......................... 89
Table A-2: Classification of pressure-atomizing nozzles. Arrows indicate fuel flow direction [5] ............ 91
Table A-3: Classification of twin-fluid nozzles. Arrows indicate flow direction [5] ........................................ 92
Table B-1: EES results for a 4mm nozzle diameter case .................................................................................... 94
Table B-2: Calculated flow rates for various lab type nozzle diameters ............................................................ 95
Table C-1: Recorded metrics used in the CGI study ......................................................................................... 102
Table C-2: Results from the independence study .......................................................................................... 102
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
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</tr>
</thead>
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<tr>
<td>$A_p$</td>
<td>Particle Reference Area</td>
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<td>2-D Flare Area</td>
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<td>Throat Area</td>
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\( h \)  
Representative Cell Size

\( I(\vec{r}, \vec{s}) \)  
Incident Radiation

\( I_b(\vec{r}) \)  
Emitted Radiation

\( I_{target} \)  
Thermal Radiation to Target

\( K \)  
Circulation Strength

\( k \)  
Turbulent Kinetic Energy

\( k \)  
Thermal Conductivity

\( l \)  
Length Scale

\( L \)  
Characteristic Length

\( L \)  
Radiant Flame Length

\( M \)  
Soot Mass Concentration

\( \dot{m} \)  
Mass Flow

\( N \)  
Soot Particle Number Density

\( N_{norm} \)  
Normalization Constant

\( Nu \)  
Nusselt Number

\( N_g \)  
Number of Gray Gases

\( n \)  
Refractive Index

\( Pr \)  
Prandtl Number

\( P_{crit} \)  
Critical Pressure

\( p \)  
Partial Pressure

\( p \)  
Order of Fit

\( P_{\varphi}(\psi) \)  
Probability Density Function

\( P(f) \)  
Weighted Probability Density Function

\( q_r \)  
Radiation Flux

\( Re \)  
Reynolds Number

\( r \)  
Air Fuel Mass Ratio

\( r \)  
Radial Distance

\( \vec{r} \)  
Ray Path

\( S \)  
Path Length

\( S \)  
Radiation Source Term

\( s \)  
Sign Correction Function

\( \vec{s} \)  
Direction Vector

\( \vec{s}' \)  
Scatter Direction Vector
\(Sc\)  
Schmidt Number

\(Sh\)  
Sherwood Number

\(S_m\)  
Mass Flow Source Term

\(t\)  
Time

\(T\)  
Temperature

\(U\)  
Velocity

\(\bar{u}_p\)  
Particle Velocity

\(\bar{u}_g\)  
Continuous Phase Velocity

\(u_i\)  
Velocity Component

\(u,v,w\)  
Cartesian Velocities

\(v\)  
Velocity Scale

\(V\)  
Thermal Dose

\(V_\theta\)  
Tangential Velocity

\(V_m\)  
Mean Droplet Velocity

\(V_{soot}\)  
Soot Volume

\(V_{flame}\)  
Flame Volume

\(We\)  
Weber Number

\(w_i\)  
Dimensionless Weighting

\(X\)  
Streamwise Displacement

\(X\)  
Target Distance

\(X\)  
Quality

\(x,y,z\)  
Cartesian Coordinates

\(Y_{soot}\)  
Soot Mass Fraction

\(Y\)  
Probit Function

\(\alpha\)  
Absorptivity

\(\alpha\)  
Under-Relaxation Factor

\(\beta_v\)  
Evaporation Coefficient

\(\beta_\lambda\) or \(\beta\)  
Extinction Coefficient

\(\Gamma\)  
Circulation

\(\Gamma_\varphi\)  
Scalar Diffusivity

\(\Gamma_t\)  
Turbulent Diffusivity

\(\delta_{ij}\)  
Kronecker Delta

\(\varepsilon\)  
Emissivity
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</tr>
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</table>
1. Introduction

Offshore oil drilling platforms are used to extract and process oil before it is brought to shore for refining. These platforms are fitted with flare booms to burn off excess products during the extraction process. While the specific geometry and style of these flare booms can vary greatly, there is always concern about the dangerous levels of thermal radiation that the flares emit to onboard personnel and ship hardware. A mixture of mainly methane, propane, and butane, the petroleum waste products are often flared as a liquid under fuel rich combustion conditions, resulting in highly sooty flares and dangerous levels of thermal radiation.

Health and safety standards dictate the level or duration of exposure to thermal radiation workers can experience. For example, the Health and Safety Executive in the United Kingdom suggests that workers without additional protection should not work in locations receiving more than 1.6 \( \frac{\text{kW}}{\text{m}^2} \) of incident thermal radiation, with 4.7 \( \frac{\text{kW}}{\text{m}^2} \) representing the maximum allowable level of thermal radiation where emergency actions lasting up to several minutes may be required [2]. For open air jet flares like the ones seen on oil platforms, surface emissive power can reach upwards of 400 \( \frac{\text{kW}}{\text{m}^2} \) during peak burning, posing a significant risk to both workers and ship structures. Further explanation of the characterization of thermal radiation
risks is provided in A.1. Table 1-1 provides a qualitative description of thermal radiation risk levels to unprotected personnel.

*Table 1-1: Qualitative risk descriptions of varying thermal radiation levels (HSE 2006).*

<table>
<thead>
<tr>
<th>Radiation Strength (kW/m²)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Received from the sun at noon in summer.</td>
</tr>
<tr>
<td>2</td>
<td>Minimum to cause pain after 1 minute of exposure.</td>
</tr>
<tr>
<td>5</td>
<td>Will cause pain in 15-20 seconds and burns after 30 seconds of exposure</td>
</tr>
<tr>
<td>6</td>
<td>Rapid pain development, protection needed for prolonged exposure.</td>
</tr>
<tr>
<td>12+</td>
<td>Significant chance of fatality during exposure, protection necessary.</td>
</tr>
</tbody>
</table>

To help control the levels of radiation, ships are often fitted with physical walls, or water spray shielding. These systems require additional structural and/or pumping considerations when designing a flare boom, which increase initial costs and maintenance requirements.

*Figure 1-2: (left) Water spray shielding used to cool and protect the back side of a ship [3]. (right) Physical wall thermal barrier on a raised flare boom arm [4].*
1.1. Objectives
The objective of this project is to investigate the radiative properties of large scale 2-phase flares using computational fluid dynamics (CFD), and study how thermal radiation levels are effected by flame properties such as geometry, soot levels, and swirl. The methodology developed during this study can lead to further developments in modelling more complex flare stack projects. More specifically, key objectives include:

i) develop a modest RANS based CFD based model of a 2-phase propane jet flare
   a. use CFD to model and predict soot production
   b. use CFD to model and predict thermal radiation levels around the flare

ii) determine the effect of cross winds and swirling flows on flame properties and radiation levels

iii) compare the CFD model results with solid flame model results and experimental data

1.2. Scope
Computational studies were limited to the use of ANSYS ICEM 18.0 for mesh generation and ANSYS Fluent 18.0 for solution generation. The scope of the project was to investigate and use preexisting physical models, models for soot generation, liquid fuel combustion, and radiation. Altering these models beyond the basic physical constants was outside the scope. Turbulence modelling was limited to two-equation RANS models, as is common in literature and many industrial applications.

Validation with simplified models and public domain experimental data is the result of limitations in the availability of appropriate testing facilities. Large scale jet flares testing requires considerable time, funding, and safety considerations, in addition to highly trained operations personnel and specialty testing facilities.
2. Theory and Literature Review

2.1. 2-Phase Combustion

The primary focus of this research is to investigate the characteristics of spray combustion, specifically a hydrocarbon jet flare. Spray or 2-phase combustion is the combustion of dispersed liquid fuel droplets in air.

2.1.1. Atomization and Droplet Size

The process of forming a spray is known as atomization and is achieved by pumping a fluid (fuel) through a spray nozzle that enables the dispersion of the liquid fuel. Spray combustion nozzles aim to control the fluid droplet size and fuel dispersion to maximize combustion efficiency and limit emissions. An overview of typical nozzle designs is provided in A.2.

While spray pattern is mostly a control of the physical nozzle, the atomization of liquid fuel is highly dependent on flow variables related mostly to velocity. Spray atomization can be broken down into two types; primary atomization that occurs near the nozzle, and secondary atomization that occurs further downstream. The main stresses responsible for droplet-break up are inertial, viscous, and surface tension.

Relevant dimensional groups include the Reynolds number $Re$, and Weber number $We$ which relate the inertial to viscous forces, and inertial to surface tension forces respectively. For fluid density $\rho \left[ \frac{kg}{m^3} \right]$, velocity $U \left[ \frac{m}{s} \right]$, dynamic viscosity $\mu \left[ \frac{kg}{m \cdot s} \right]$, surface tension $\sigma \left[ \frac{N}{m} \right]$, and characteristic length $L \left[ m \right]$, the dimensional groups are defined.

\[
Re = \frac{\rho U L}{\mu} \quad \text{(2.1)}
\]

\[
We = \frac{\rho U^2 L}{\sigma} \quad \text{(2.2)}
\]
Increased $Re$ and $We$ promote finer and more rapid atomization of a sprayed liquid [5]. Figure 2-1 shows how the atomization of a simple jet is effected by the velocity of the jet $U_L$ relative to the surrounding gas $U_g$.

For uses in combustion, difficulty arises with the specification of required atomization characteristics. Spray characterization is usually conducted under cold conditions, thus the effects of combustion heat on droplet vaporization and breakup need to be determined. Additionally, measurement of the flow conditions in close proximity to the nozzle exit is difficult. These limitations can make theoretical modelling and simulation challenging. As a result, averaged spray conditions taken from downstream are usually used to define the flow. For most engineering application, a simplifying assumption is made that droplets are spherical. This assumption is valid when droplet collision effects are small, and the Weber number is low, $We < 5$. Under these conditions, droplet size can be adequately specified a single parameter $D$, the droplet diameter [5].

Droplet diameter and fuel volatility both effect the combustion characteristics. A highly volatile fuel atomized into very small droplets will produce a flame structure only mildly influenced by the effects of the 2-phase flow. An experiment conducted with tetralin ($C_{10}H_{12}$) sprays showed that
droplet sizes less than 10µm resulted in flame characteristics not distinguishable from single phase gas flames [6].

There is particular interest in the behavior of propane fuel in 2-phase jets for use in future experimentation and research. A plethora of academic papers are available that study 2-phase propane jets focusing on both combustion and droplet mechanics. A study by E. Hervieu and T. Veneau was completed to investigate the size and velocity of liquid propane droplets produced by a range of nozzle diameters and operating pressures [7]. Table 2-1 and Table 2-2 below show the experimental measurements from a 2mm nozzle trial and 5mm nozzle trial where $X$ is the downstream displacement from the nozzle, $V_m$ is the mean droplet velocity, $D_{32}$ is the Sauter mean diameter and $D_{10}$ is the arithmetic mean diameter. The Sauter mean diameter is defined as the diameter of a droplet with the same ratio of volume to surface area as the entire spray [7].

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Pressure (bar) & 5 & 11 & 17 \\
\hline
$X$ (mm) & 30 & 60 & 95 & 30 & 60 & 95 & 30 & 60 & 95 \\
\hline
$V_m$ (m/2) & 41.9 & 25.9 & 17.3 & 34.4 & 26.2 & 25.4 & - & 23.5 & 24.2 \\
\hline
$D_{32}$ (µm) & 49.5 & 38.5 & 35.8 & - & 30.2 & 25.2 & - & 26.6 & 23.7 \\
\hline
$D_{10}$ (µm) & 34.8 & 26.7 & 24.6 & - & 23.7 & 16.4 & - & 18.8 & 17.1 \\
\hline
\end{tabular}
\caption{Fuel droplet measurements, 2mm nozzle. Error reported as 8\% for velocity measurements, and 13\% for diameter measurements. Altered from [7].}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Pressure (bar) & 5 & 11 & 17 \\
\hline
$X$ (mm) & 30 & 60 & 95 & 30 & 60 & 95 & 30 & 60 & 95 \\
\hline
$V_m$ (m/2) & 36.7 & 35.8 & 29.0 & 31.9 & 26.0 & 31.8 & - & - & 24.5 \\
\hline
$D_{32}$ (µm) & - & 48.5 & 52.8 & - & 31.2 & 27.0 & - & - & 29.8 \\
\hline
$D_{10}$ (µm) & - & 37.4 & 41.7 & - & 25.0 & 18.5 & - & - & 22.5 \\
\hline
\end{tabular}
\caption{Fuel droplet measurements, 5mm nozzle. Error reported as 8\% for velocity measurements, and 13\% for diameter measurements. Altered from [7].}
\end{table}
Figure 2-2 below presents all of the collected data from the 2mm nozzle trial at 95mm downstream, with pressures of 5 bar and 11 bar. Measurements were taken with a Phase Doppler Particle Analyzer; a device capable of simultaneously measuring droplet size and velocity inside the jet, based on phase Doppler interferometric theory.

As expected, increasing pressure for the same nozzle results in finer atomization, and faster velocities of the liquid. An additional pattern to recognize is that droplet size decreases with streamwise displacement (with some outliers). This is to be expected due to secondary atomization effects that happen after ejection.

2.1.2. Droplet Combustion

Burning of fuel droplets occurs as the fuel is evaporated from the liquid surface and combusted in the oxidizing atmosphere around it. The rate at which this occurs is generally determined by the rate of heat transfer from the flame front to the fuel droplet surface. For most models, the liquid surface is assumed to
be at the boiling temperature of the fuel being used, but studies of burning liquid temperature fields indicate that the liquid surface is slightly below the normal boiling temperature [8]. After sudden initial heating, the droplet reaches an equilibrium at wet bulb temperature (below boiling) and vapourization occurs at the surface [9]. In the simplest case, the combustion around a droplet is considered spherical. Oblong or egg-shaped flames are the result of convective effects due to the relative motion between the droplets and surrounding gas. For very small droplets, these effects are diminished and the spherical model is more accurate. Figure 2-3 details the basic spherical combustion model of a single fuel [10]

![Diagram of a single fuel droplet combusting](image)

**Figure 2-3: Basic schematic of a single fuel droplet combusting [10]**.

This spherical model can be described as a 2-film model; one film being between the droplet surface and the infinitely thin reaction zone (flame front), and the second film being between the flame front and the surrounding oxidizing atmosphere. In the first film, heat transfer from the flame front to the liquid surface vaporizes the fuel. In the second film, oxygen diffuses to the reaction zone as combustion products and heat are transported to the surrounding atmosphere. Figure 2-4 visualizes the distributions of temperature and partial pressures ($\rho$) in the 2-film model.
Ultimately, the most important parameter for engineering applications is the mass-burning rate of the fuel droplets as it controls the rate of heat release during combustion. Initially defined for non-combustion related experiments, the \( D^2 \)-evaporation law defines the rate of change of droplet diameter and has been verified for both combusting and non-combusting applications [8].

\[
D^2 = D_o^2 - \beta_v t
\]

(2.3)

Here \( D \) is the droplet diameter at time \( t \), \( D_o \) is the initial droplet diameter, and \( \beta_v \) is termed the evaporation coefficient which is determined experimentally.

2.2. Thermal Radiation

Thermal radiation is the transfer of heat energy through electromagnetic radiation. Of interest to this study is the radiation emitted from a body due to its temperature. The concept of a black body, a theoretical ideal emitter and absorber of thermal radiation, describes the maximum thermal radiation a body can emit over all wavelengths. The total emissive power of a black body \( e_{bb} \left[ \frac{W}{m^2} \right] \) depends only on temperature \( T \) [K] and is described with the Stefan-Boltzmann law, where \( \sigma = 5.67 \times 10^{-8} \left[ \frac{W}{m^2\text{K}^4} \right] \) is the Stefan-Boltzmann constant.
For non-ideal, real world bodies, only a fraction of this total possible radiation is emitted. This depends on the material’s emissivity $\varepsilon$. Key optical properties to consider when dealing with thermal radiation are summarized in Table 2-3.

Table 2-3: Optical properties to consider for thermal radiation.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon$</td>
<td>Emissivity</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Absorptivity</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Reflectivity</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Transmissivity</td>
</tr>
</tbody>
</table>

A surface or body is described as being gray if its optical properties do not vary with wavelength. In reality, most studied materials have optical properties that vary with temperature, wavelength, and incident radiation direction. The simplifying assumption that of gray radiation can be appropriate for some engineering applications, but experimentation and empirical data are used to confirm the validity of the gray assumption. A gaseous volume such as one in a combusting system will emit, reflect, absorb, and transmit thermal radiation depending on its temperature and chemical composition. The gases that are present in the combustion of a hydrocarbon fuel are not gray but rather selective absorbers and emitters. A selective absorber or emitter’s optical properties vary with wavelength as seen in Figure 2-5 which shows the absorptivity spectra of various greenhouse gases.
When modeled as gray, a gas’s properties are dependent on temperature, total pressure, partial pressure of the gas, and path length through the gas. Individual gray gas properties are available in published charts validated by experiment. An example of such a chart is shown in Figure 2-6 for carbon dioxide.

Figure 2-5: Absorption spectra for various gases in the Earth’s atmosphere [11].

Figure 2-6: Total emittance of carbon dioxide in a mixture of total pressure $P = 1$ atm [12].
Additional data can be used to account for different pressures. Furthermore, when multiple gases are present in a mixture band overlap must be considered such that the spectral emissivity or absorptivity do not exceed the theoretical maximum of that of a black body. Figure 2-7 and Figure 2-8 provide examples of published data used for corrections in pressure and band overlap respectively.

![Figure 2-7: Total emittance of carbon dioxide pressure corrections for varying total pressures [12].](image1)

![Figure 2-8: Band overlap corrections for a mixture of carbon dioxide and water vapour. Gas temperatures are 400K, 810K, and 1200K, from left to right respectively [12].](image2)

In a simple example of a carbon dioxide and water vapor mixture, the resulting gray gas emittance $\varepsilon_g$ is calculated with species ‘x’ emittance $\varepsilon_x$, pressure correction $C_x$, and band overlap correction $\Delta \varepsilon$.

$$\varepsilon_g = C_{CO_2} \varepsilon_{CO_2} + C_{H_2O} \varepsilon_{H_2O} - \Delta \varepsilon$$

2.2.1. Weighted-sum-of-Gray-Gases-Model

In combustion processes where complex mixtures of reacting gases are present, it becomes exceedingly difficult to model the spectral properties and resulting levels of radiation. To simplify this challenge, the
Weighted-sum-of-Gray-Gases-Model or WSGGM is used which replaces an integration of spectral properties of a mixture with a summation of a set of $N_g$ gray gases to simulate the mixture’s non-gray spectral properties. For the $i^{th}$ gas weighting $w_i$, absorptivity $\alpha_i$, and a path length partial pressure product $pL$, the gray gas emittance is defined [12].

\[
\varepsilon_g = \sum_{i=1}^{N_g} w_i (1 - e^{-\alpha_i pL})
\]  

(2.5)

\[
w_i > 0 \sum_{i=1}^{N_g} w_i = 1
\]  

(2.6)

Each weighting can be compared to the fraction of the black body energy spectrum for which the $i^{th}$ gas’s absorptivity is approximately $\alpha_i$. Various literature resources are available detailing versions of the WSGGM that account for specific partial pressures, or the presence of unburnt hydrocarbon fuels in the mixture. These models rely on empirically determined constants and validation.

2.2.2. Participating Medium

Radiation emitted from a gaseous volume will pass through the surrounding fluid medium. This leaving radiation intensity is then absorbed and scattered along any given path, resulting in only a portion of the initial radiation intensity being transmitted. In such cases when the absorption and/or scatter are significant, the fluid is said to be a participating medium. Radiation interactions are described and measured in terms of the medium’s absorption coefficient $\kappa_\lambda$ [m$^{-1}$], scatter coefficient $\sigma_{s,\lambda}$ [m$^{-1}$], and their sum – the extinction coefficient $\beta_\lambda = \kappa_\lambda + \sigma_{s,\lambda}$. The optical thickness of a medium $\tau_\lambda$ is defined when the extinction coefficient is integrated along a path length $S$. For $\tau_\lambda \gg 1$ the medium is said to be optically thick, indicating rapid attenuation. For $\tau_\lambda \ll 1$ the medium is optically thin and approaches non-participation.
Optical thickness in a flame body increases as the combustion becomes less ideal, resulting in more soot production. Combustion products such as carbon dioxide, and water vapor readily absorb thermal radiation, and particulate matter such as soot causes scatter. Figure 2-9 shows the aforementioned radiation interactions in a participating medium.

\[
\tau_\lambda = \int_0^s \beta_\lambda ds
\]  

(2.7)

2.3. Soot Production

Soot is a suspended mass of impure carbon particles resulting from an incomplete combustion process. The formation of soot is an important topic not only for environmental considerations, but also thermal radiation concerns. For a clean burning flame with near stoichiometric combustion, thermal radiation contributions come mainly from H₂O and CO₂ as other products have low concentrations or are mostly transparent to radiation, such as O₂ or N₂. These flames are called non-luminous as they produce little visible light, and have low emissivity. As combustion becomes less ideal, the incomplete combustion results in a luminous flame, with production of soot (carbon solids) and carbon monoxide gas. Balanced chemical equations of complete and incomplete combustion of propane are shown below.
Complete: \( \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \) \hspace{1cm} (2.8)
Incomplete: \( 2\text{C}_3\text{H}_8 + 7\text{O}_2 \rightarrow 2\text{CO}_2 + 8\text{H}_2\text{O} + 2\text{CO} + 2\text{C} \) \hspace{1cm} (2.9)

The presence of soot in a flame has a strong impact on the thermal radiation as soot particles radiate like small black bodies and dominate the thermal emissions. Soot emits a continuous spectrum in the visible and infrared regions resulting in radiation emissions double or triple of that of the gasses alone [13].

![Image of a highly luminous oil boom flare producing a large amount of soot. Buoyancy effects cause an upward deflection of the flare](image)

**Figure 2-10**: A highly luminous oil boom flare producing a large amount of soot. Buoyancy effects cause an upward deflection of the flare [1].

The amount of soot in a given flame is described by the soot volume fraction \( f_v \) which is dependent on the volume of the flame \( V_{\text{flame}} \) and the volume of soot present in the flame \( V_{\text{soot}} \). For hydrocarbon diffusion flames, soot volume fraction is typically between \( 10^{-8} \) to \( 10^{-5} \) [13].

\[
f_v = \frac{V_{\text{soot}}}{V_{\text{flame}}} \hspace{1cm} (2.10)
\]

Individual soot particles typically have diameters of \( 0.005 \mu\text{m} \) to \( 0.08 \mu\text{m} \) but can group together to form agglomerations or filaments up to \( 0.3 \mu\text{m} \) in size [13]. Experimental measurements of soot characteristics are notoriously hard to complete as probes used to gather soot for analysis cause additional agglomeration and alter soot characteristics. The specific mechanisms governing the growth of soot particles are not well understood and as a result, soot production and radiation models rely mainly on experimental data.
The production of soot is highest in fuel rich areas with large temperature gradients [8]. Reducing the zones where these conditions arise is an effective way to limit soot production. This can primarily be done by enhanced mixing of the fuel stream and surrounding air, ultimately making the combustion more ideal by reducing fuel rich zones. Wide spread nozzles with fine atomization disperse fuel over a greater area improving combustion quality. Active devices can also be used to pump in additional combustion air.

The effects of excess air on soot production was studied in a 2017 paper by Bäckström et al [14]. In this study, the size distribution, volume fraction, and optical properties of soot in a small scale propane flame were measured. Two flame trials were completed, with flame B having limited air compared to that of flame A. The decrease in available air is not quantified, so a numerical relation to soot production cannot be made directly. Figure 2-11 shows the measurements of average soot diameter and soot volume fraction for each flame trial. Limiting combustion air resulted in soot particles up to four times larger, and volume fractions nearly three orders of magnitude times larger.

Table 2-4: Experimentally determined propane soot radiation characteristics [13].

<table>
<thead>
<tr>
<th>Wavelength [µm]</th>
<th>Index of Refraction</th>
<th>Extinction Coefficient</th>
<th>Absorption coefficient per Particle Volume Fraction [µm⁻¹]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4358</td>
<td>1.57</td>
<td>0.46</td>
<td>9.29</td>
</tr>
<tr>
<td>0.4500</td>
<td>1.56</td>
<td>0.50</td>
<td>9.83</td>
</tr>
<tr>
<td>0.5500</td>
<td>1.57</td>
<td>0.53</td>
<td>8.44</td>
</tr>
<tr>
<td>0.6500</td>
<td>1.56</td>
<td>0.52</td>
<td>7.07</td>
</tr>
<tr>
<td>0.8065</td>
<td>1.57</td>
<td>0.49</td>
<td>5.34</td>
</tr>
<tr>
<td>2.5</td>
<td>2.04</td>
<td>1.15</td>
<td>2.34</td>
</tr>
<tr>
<td>3.0</td>
<td>2.21</td>
<td>1.23</td>
<td>1.75</td>
</tr>
<tr>
<td>4.0</td>
<td>2.38</td>
<td>1.44</td>
<td>1.24</td>
</tr>
<tr>
<td>5.0</td>
<td>2.07</td>
<td>1.72</td>
<td>1.30</td>
</tr>
<tr>
<td>6.0</td>
<td>2.62</td>
<td>1.67</td>
<td>0.727</td>
</tr>
<tr>
<td>7.0</td>
<td>3.05</td>
<td>1.91</td>
<td>0.484</td>
</tr>
<tr>
<td>8.5</td>
<td>3.26</td>
<td>2.10</td>
<td>0.357</td>
</tr>
<tr>
<td>10.0</td>
<td>3.48</td>
<td>2.46</td>
<td>0.271</td>
</tr>
</tbody>
</table>
In a 1973 paper, Sjögren states that the decisive factor of soot formation is the relative velocity between the larger droplets in the fuel spray and the combustion air [15]. Smaller droplets in a spray have enough time to evaporate completely ahead of the flame front, and burn as a premixed flame. Larger droplets in the spray do not evaporate completely, and burn as individual droplets producing soot. To control this, the larger droplet flames can be extinguished. This is achieved if the velocity between the droplets and air exceeds the critical extinction velocity. A specific extinction velocity is determined by the droplet diameter and composition of combustion air. Extinction velocity rises with increasing oxygen concentration in the combustion air and falls to zero if the oxygen concentration is reduced to 14%-16%, with nitrogen as a diluent [15]. Figure 2-12 shows the experimental results comparing oxygen equivalence ratio, air velocity, and soot formation. These tests were performed with an oil burner and thus additional experimentation could be require for differing fuel types and sprays.
Figure 2-12: Soot formation as a function of excess oxygen (equivalence ratio) and oxygen concentration in the combustion air, dilution with nitrogen. Bold lines represent constant oxygen concentration but variable velocity, dashes lines represent variable oxygen concentration with constant velocity [15].

2.4. CFD Overview

Computational Fluid Dynamics (CFD) is the use of numerical methods to produce solutions of governing fluid dynamics equations. Primarily, this includes the Navier-Stokes equations which consist of a continuity equation, a momentum equation, and an energy equation [16].

\[
\frac{\partial p}{\partial t} + \nabla \cdot (\rho u_i) = 0 \tag{2.11}
\]

\[
\rho \frac{du_i}{dt} = \rho g - \nabla p + \nabla \cdot \tau_{ij} \tag{2.12}
\]

\[
\rho \frac{d\hat{u}}{dt} + p(\nabla \cdot u_i) = \nabla \cdot (k \nabla T) + \Phi \tag{2.13}
\]

Where \(\Phi\) is the viscous-dissipation function:

\[
\Phi = \mu \left[ 2 \left( \frac{\partial u}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + 2 \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 \right] \tag{2.14}
\]
And $\tau_{ij}$ is the viscous stress tensor:

$$
\tau_{ij} = \begin{bmatrix}
\tau_{xx} & \tau_{yx} & \tau_{zx} \\
\tau_{xy} & \tau_{yy} & \tau_{zy} \\
\tau_{xz} & \tau_{yz} & \tau_{zz}
\end{bmatrix}
$$

(2.15)

A common method to obtaining approximate solutions to these equations is the finite volume approach. The finite volume method approximates the solution to these partial differential equations by discretizing a continuous fluid domain into a finite number of smaller volumes known as cells. The Navier-Stokes equations are solved algebraically for each cell volume. Fluxes are conserved on boundaries between neighboring cells and the extents of the fluid domain where boundary conditions are set and must be satisfied.

2.4.1. Turbulence

The primary parameter in determining a given flows level of turbulence is the Reynolds number which describes the ratio of inertial forces to viscous forces within the fluid.

$$
Re = \frac{\rho u L}{\mu}
$$

Low Reynolds number flows are laminar and exhibit streamlines that follow smooth paths. As Reynolds number increases, and surpasses the so-called critical Reynolds number, the flow transitions to turbulence and becomes dominated by the complex and random nature of eddies and velocity fluctuations. Flow parameters experience irregular fluctuations over time. In turbulent flows, there is a rapid mixing of heat and momentum, and kinetic energy is dissipated due to the fluid viscosity.

The Navier-Stokes equations hold for both laminar and turbulent flows, so solving turbulent flows with these equations directly is possible. This approach is called Direct Numerical Simulation (DNS), but for most applications the complex nature of turbulence makes the computational requirements uneconomical.
To reduce the computational power needed to numerically approximate turbulent flows, a variety of
turbulence models have been developed which estimate the effects of turbulence. These models are
classified as either Large Eddy Simulation (LES), first-order closure, or second-order closure – the latter
two models belonging to the Reynolds-Averaged Navier-Stokes (RANS) category. LES simulations
directly compute larger scale eddies which are more energetic than small scale eddies and are the primary
transporter of flow characteristics through a fluid domain. Small scale eddies are spatially filtered from the
Navier-Stokes equations and their contributions are approximated through a sub-grid model. This
simplification reduces the computational power needs compared to DNS, but complex flows still require
highly detailed grids and powerful computing hardware making LES uneconomical for some applications.

To further simplify the approximation of turbulent flows, RANS based simulations average the Navier-
Stokes equations in time. This is accomplished through Reynolds decomposition where a given flow
variable $\phi$ is decomposed into a mean component $\bar{\phi}$ and a fluctuating component $\phi'$.

$$\phi = \bar{\phi} + \phi' \quad (2.16)$$

The terms for velocity and pressure are decomposed and substituted into the Navier-Stokes equations.
Taking a time average results in the Reynolds-Averaged Navier-Stokes equations for continuity and
momentum.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{u}_i) = 0 \quad (2.17)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_i} = - \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial}{\partial x_i} (- \rho u_i' u_j') \quad (2.18)$$

Additionally, for an arbitrary scalar quantity $\varphi$ such as temperature or species concentration, a time
averaged transport equation is derived where $\Gamma_\varphi$ is the scalars diffusivity.

$$\frac{\partial \bar{\varphi}}{\partial t} + \nabla \cdot (\bar{\varphi} \bar{u}_i) = \frac{1}{\rho} \nabla \cdot (\Gamma_\varphi \Delta \bar{\varphi}) - \frac{\partial u_i' \varphi}{\partial x_i} \quad (2.19)$$
The time averaging introduces new terms in the momentum equations called the Reynolds stresses. These new terms \( -\rho \bar{u}'\bar{u}' \) are the products of fluctuating velocities due to the momentum transfer caused by turbulent eddies. In long form, there are three normal stresses \( \tau_{xx} = -\rho \bar{u}'^2 \), \( \tau_{yy} = -\rho \bar{v}'^2 \), and \( \tau_{zz} = -\rho \bar{w}'^2 \), and three shear stresses \( \tau_{xy} = \tau_{yx} = -\rho \bar{u}'\bar{v}' \), \( \tau_{xz} = \tau_{zx} = -\rho \bar{u}'\bar{w}' \), \( \tau_{yz} = \tau_{zy} = -\rho \bar{v}'\bar{w}' \).

These Reynolds stress terms require additional equations for closure which come from the various forms of RANS turbulence models. These models are classified by the amount of additional transport equations they introduce as seen in Table 2-5. The algebraic stress and Reynolds stress models are second-order closure models and will not be used or discussed in depth in this research. These models calculate the Reynolds stresses directly using their governing equations which requires more computational power. More common in industry are the first-order closure models, with the \( k-\epsilon \) model and mixing length model being comprehensively validated [17].

<table>
<thead>
<tr>
<th>Additional Transport Equations</th>
<th>Model Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Mixing length model</td>
</tr>
<tr>
<td>1</td>
<td>Spalart-Allmaras model</td>
</tr>
<tr>
<td>2</td>
<td>( k-\epsilon ) model, ( k-\omega ) model, Algebraic stress model</td>
</tr>
<tr>
<td>7</td>
<td>Reynolds stress model</td>
</tr>
</tbody>
</table>

First-order closure models operate on the assumption that the turbulent Reynolds stresses are proportional to mean rates of deformation; an idea proposed by Boussinesq in 1877 and formally called the Boussinesq hypothesis:
\[ \tau_{ij} = (-\rho \overline{u_i' u_j'}) = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \]  

(2.20)

where \( k = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) \) is the turbulent kinetic energy, \( \mu_t \) is the turbulent viscosity, and \( \delta_{ij} \) is the Kronecker delta used to account for both the normal and shear Reynolds stresses. Similarly, the arbitrary scalar quantity \( \varphi \) undergoes turbulent transport proportional to the gradient of its mean value, where \( \Gamma_t \) is the turbulent diffusivity.

\[ -\rho \overline{u_i' \varphi'} = \Gamma_t \frac{\partial \overline{\varphi}}{\partial x_i} \]  

(2.21)

The \( k\)-\( \epsilon \) model uses two additional equations to find the turbulent viscosity \( \mu_t \); one for turbulent kinetic energy \( k \), and one for turbulent dissipation \( \epsilon \). The velocity scale \( v \) and length scale \( l \) related to the large-scale turbulence are defined with \( k \) and \( \epsilon \).

\[ v = k^{1/2} \]  

(2.22)

\[ l = \frac{k^{3/2}}{\epsilon} \]  

(2.23)

The turbulent viscosity is then formulated, where \( C_\mu \) is a dimensionless model constant.

\[ \mu_t = C_\mu \rho vl = C_\mu \rho \frac{k^2}{\epsilon} \]  

(2.24)

The individual transport equations for \( k \) and \( \epsilon \) contain an addition five constants and the standard model uses constants determined through vigorous fitting of experimental data. Qualitatively, the transport equations take the form:

\[ \text{Rate of Change} + \text{Transport by Convection} = \text{Transport by Diffusion} + \text{Rate of Production} - \text{Rate of Destruction} \]

Values of \( k \) and \( \epsilon \) must be given along boundary conditions, and are usually based on empirical data, or approximated with turbulence intensity and characteristic length values.
Later developments of the standard k-ε model include the renormalization group (RNG) and realizable sub-models. These models offer better performance than the standard model k-ε model for certain characteristic flows. The RNG k-ε model includes an additional term in the equation for turbulent dissipation which makes it a more robust option for rapidly strained flows such as swirling flows. The realizable k-ε model uses an altered formulation for turbulent viscosity where \( C_\mu \) is no longer constant, and is dependent on the turbulent kinetic energy, turbulent dissipation, and the mean stress and rotation rates. The realizable model boasts improved performance in predicting flows with strong adverse pressure gradients, recirculation, and separation.

2.4.2. Non-Premixed Combustion

In CFD, combustion processes are determined by the underlying governing models for heat and mass transfer, as well as additional models for reaction chemistry, radiative heat transfer, resulting species concentrations, etc. Of particular interest in this study are the models used to predict the non-premixed combustion of liquid fuel sprays. This includes the use of the discrete phase model (DPM) and non-premixed combustion model.

Non-premixed combustion includes flows where the fuel enters the reaction zone unmixed with the oxidizer (air). In particular, this study focuses on flows where liquid fuel is injected into ambient air where the mixing and eventual combustion take place. The non-premixed model simplifies the thermochemistry of combustion to be dependent on a single scalar parameter \( f \) called the mixture fraction. This parameter denotes the localized mass fraction of unburnt fuel elements in all of the combustion species. By assuming equal diffusion constants of each species, the chemistry is reduced to a single mixture fraction transport equation. This assumption is acceptable in flows where molecular diffusion effects are insignificant in comparison to turbulent convection.

For mixture thermal conductivity \( k \), specific heat \( C_p \), Prandtl number \( Pr \), turbulent viscosity \( \mu_t \), and source term of mass flow \( S_m \):
\[ \frac{\partial}{\partial t} (\rho \bar{f}) + \nabla \cdot (\rho u_i \bar{f}) = \nabla \cdot \left( \frac{k}{C_p} + \frac{\mu_t}{Pr} \nabla \bar{f} \right) + S_m \] (2.25)

The mixture fraction of the system can be described using the equivalence ratio of the combustion $\emptyset$, and the mass ratio of air to fuel $r$. This allows the mixture fraction to be calculated for fuel-rich, or fuel-lean combustion conditions.

\[ f = \frac{\emptyset}{\emptyset + r} \] (2.26)

\[ \emptyset = \frac{(fuel/air)_{actual}}{(fuel/air)_{stoichiometric}} \] (2.27)

To predict the effects of the turbulent thermochemistry, a probability density function (PDF) approach is used. This is a statistical method used to determine the mean values for fluctuating scalars, specifically the mixture fraction. For an arbitrary flow scalar $\varphi$, the distribution function $F_{\varphi}(\psi)$ and probability density function $P_{\varphi}(\psi)$ are defined.

\[ F_{\varphi}(\psi) = Prob\{ \varphi < \psi \} \] (2.28)

\[ P_{\varphi}(\psi) = \frac{dF_{\varphi}(\psi)}{d\psi} \] (2.29)

$Prob\{ \varphi < \psi \}$ denotes the probability that $\varphi$ is smaller than a given value $\psi$. The PDF also has the following properties.

\[ a) \quad P_{\varphi}(\psi) \geq 0 \] (2.30)

\[ b) \quad \int_{-\infty}^{\infty} P_{\varphi}(\psi) d\psi = 1 \] (2.31)
For use in combustion problems, a density-weighted PDF for the mixture fraction \( \tilde{p}(f) \) is defined in terms of the unweighted function \( p(f) \) from which any density-averaged scalar quantity can be calculated.

\[
\tilde{p}(f) = \frac{\rho(f)}{\bar{\rho}} p(f)
\]  
(2.32)

\[
\bar{\phi} = \int_{0}^{1} \phi(f) \tilde{p}(f) df
\]  
(2.33)

2.4.3. Discrete Phase Modelling

To model the presence of discrete dispersed phase, specifically the liquid fuel droplets used in combustion, the Euler-Lagrange approach is used. The dispersed droplets are tracked through the continuum of fluid (air) which is governed by the Navier-Stokes equations. Considerations for energy, mass, and momentum transfer between the two phases are also determined. For larger scale spray combustion processes such as jet flares, the dispersed liquid droplets occupy a low volume fraction when compared to the fluid domain. In this case droplet-droplet interactions are negligible and the model is further simplified. The trajectory of dispersed droplets are determined using a force balance which depends on the dispersed phase Reynolds number \( Re \), particle momentum response time \( \tau_v \), and a drag coefficient \( C_D \) [18].

\[
\frac{\partial \tilde{u}_p}{\partial t} = \frac{1}{\tau_v} C_D Re |\tilde{u}_p - \tilde{u}_g| + \frac{\tilde{g}(\rho_d - \rho_g)}{\rho_d}
\]  
(2.34)

\[
\tau_v = \frac{\rho_p d_p^2}{18 \mu_g}
\]  
(2.35)

\[
Re = \frac{\rho_g d_p |\tilde{u}_p - \tilde{u}_g|}{\mu_g}
\]  
(2.36)

\[
C_D = \frac{F_D}{\frac{1}{2} \rho_g |\tilde{u}_p - \tilde{u}_g|^2 A_p}
\]  
(2.37)
Where $\vec{u}_p$ is the particle velocity, $\vec{u}_g$ is the continuous phase velocity, $\vec{g}$ is acceleration due to gravity, $\rho_p$ and $\rho_g$ are the fluid densities for the discrete and continuous phases respectively, $d_p$ is the particle diameter, $\mu_g$ is the continuous phase dynamic viscosity, and $A_p$ is the particle reference area. The momentum response time $\tau_v$ relates to the time required for a particle to respond to velocity changes in the continuous phase.

Additional models for droplet breakup, drag, and other mechanics are a prominent field of study for CFD developers. While these areas will not be covered in this study, but a brief overview of droplet evaporation is included due to its significance to the combustion process. A liquid fuel droplet will undergo evaporation due to the temperature difference between the droplet surface and the continuous phase (air). An energy balance on a particle is described as a function of thermal response time $\tau_T$, Sherwood number $Sh$, Nusselt number $Nu$, Prandtl number $Pr$, and Schmidt number $Sc$. This equation considers the heat transferred to the particle due to the temperature difference, and the resulting heat transfer away from the particle due to vapourization mass transfer [18].

$$\frac{dT_p}{dt} = \frac{Nu}{2\tau_T} (T_g - T_p) + \frac{Sh}{2} \frac{Pr}{\tau_T Sc} \frac{h_L}{C_{p,p}} (\omega_{A,\infty} - \omega_{A,s})$$

(2.38)

$$Nu = 2 + 0.6Re^{\frac{1}{2}}Pr^{\frac{1}{3}}$$

(2.39)

$$Sh = 2 + 0.6Re^{\frac{1}{2}}Sc^{\frac{1}{3}}$$

(2.40)

$$Sc = \frac{\nu_g}{D_v}$$

(2.41)

$$Pr = \frac{C_{p,g}h_g}{k_g}$$

(2.42)

$$\tau_T = \frac{\rho_p C_{p,p} d_p^2}{12k_d}$$

(2.43)

Where $T$ is the temperature, $C_p$ is the specific heat, and $k$ is the thermal conductivity of either the particle or continuous phase as denoted by the subscripts $p$ and $g$ respectively. $h_L$ is the latent heat of vapourization.
of the particle, $\omega_{A,\infty}$ and $\omega_{A,s}$ are the mass fractions of droplet species vapour in the free stream and at the droplet surface respectively, $\nu_g$ is the kinematic viscosity of the continuous phase, and $D_v$ is its thermal diffusivity. The Nusselt number and Sherwood number here are defined using the Ranz-Marshall and Froessling correlations for forced convection respectively [18].

2.4.4. Soot Modelling

Computational soot models are often categorized based on their complexity and required computational power. Models can be described as empirical, semi-empirical, and detailed, with detailed models requiring the most processing power and detailed underlying chemistry models. Most models were developed for specific combustion applications and therefore care must be taken to ensure the model is appropriate for differing combustion conditions.

The one-step model is an empirical model developed by Khan et. al, purposed for and validated with direct injection diesel combustion engines [19]. This model estimates soot formation based on fuel partial pressure, activation temperature, equivalence ratio, and several empirically determined constants. Another common empirical model, the two-step model, was developed by Tenser et al. for acetylene diffusion flames [20]. This model firstly estimates the rate of production of radical nuclei and then calculates soot generation on the nuclei. This requires two transport equations to be solved for each scalar quantity; the nuclei concentration and resulting soot concentration. Both the one-step and two-step models determine net soot production based on the difference between the rate of soot formation and the rate of soot combustion. The two-step model considers nuclei concentration when determining the rate of soot formation, however the one-step model determines soot formation directly from an empirical expression. Both the one-step and two-step models are limited to turbulent combustion and being empirical in nature, the validity of the models must be compared with experimental results. The empirical constants can be altered to encompass a wider range of combustion studies, but results should be considered qualitative at best until compared with experiment.
The Moss-Brookes model was developed for methane flames and was later adapted to the Moss-Brookes-Hall method to allow for considerations of other hydrocarbon fuels. Two transport equations are solved for soot mass fraction $Y_{soot}$ and normalized nuclei concentration $b_{nuc}^*$ where $\sigma$ is the turbulent Prandtl number for either soot or nuclei transport, $M$ is the soot mass concentration, $N$ is the soot particle number density, and $N_{norm}$ is a normalization constant of $10^{15}$ particles.

\[
\frac{\partial}{\partial t} (\rho Y_{soot}) + \nabla \cdot (\rho \vec{u} Y_{soot}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_{soot}} \nabla Y_{soot} \right) + \frac{dM}{dt} \tag{2.44}
\]

\[
\frac{\partial}{\partial t} (\rho b_{nuc}^*) + \nabla \cdot (\rho \vec{u} b_{nuc}^*) = \nabla \cdot \left( \frac{\mu_e}{\sigma_{nuc}} \nabla b_{nuc}^* \right) + \frac{1}{N_{norm}} \frac{dN}{dt} \tag{2.45}
\]

This model considers sources of nucleation and surface growth, and sink terms such as coagulation and oxidation when determining the soot mass concentration source $\frac{dM}{dt}$ and soot particle production rate $\frac{dN}{dt}$.

These terms also use multiple soot and model constants that have been determined through experimentation [21]. The Moss-Brookes models require the use of the PDF method to model the turbulence-chemistry interactions.

### 2.4.5. Radiation Modelling

Computational radiation modelling is important for problems where radiative heat transfer is expected to be large compared to that due to convection or conduction as a result of radiation’s fourth-order dependence on temperature. Discussed here are only the radiation models that are compatible with the other necessary models for modelling 2-phase combustion. Some other necessary model requirements are being able to include soot contributions to thermal radiation, consider 3D domains with participating medium, and have modest computational requirements.

As discussed in 2.2, gaseous combustion products and soot particles produce high levels of thermal radiation. While the radiation model is not directly coupled to the flow field, there is a strong indirect coupling with spatially distributed flow variables like temperature and species concentration. The absorption, scattering, and emission of thermal radiation in the fluid medium results in a radiative source...
The radiative transfer equation (RTE) governs the radiative heat transfer along a ray path at position $\vec{r}$ on the direction of vector $\vec{s}$.

$$\frac{dI(\vec{r}, \vec{s})}{ds} = \kappa I_b(\vec{r}) - \beta I(\vec{r}, \vec{s}) + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}') \Phi(\vec{s} \cdot \vec{s}') d\Omega'$$

(2.46)

Where $I(\vec{r}, \vec{s})$ is the incident radiation, $I_b(\vec{r})$ is the emitted radiation, $\kappa$ is the absorption coefficient, $\beta$ is the extinction coefficient, $\sigma_s$ is the scatter coefficient, $\vec{s}'$ is the scattering direction vector, $\Phi$ is a phase function, and $\Omega'$ is solid angle. The last term is the in-scattering integral which accounts for incoming scattered radiation from all directions through an integration over a unit sphere (solid angle of $4\pi$ steradians). Qualitatively, this equation can be described as follows:

$$\text{Rate of change of radiation per unit path length} = \frac{\text{Emitted radiation}}{\text{path length}} - \frac{\text{Absorbed and out-scattered radiation}}{\text{radiation}} + \frac{\text{In-scattered radiation}}{\text{radaiton}}$$

The P-1 radiation model offers a differential solution to the RTE using a series expansion of the radiation intensity along a given path. Truncating the series to a set number of terms results in a finite formulation that can be solved iteratively. This approach avoids the use of raytracing, greatly reducing necessary computational power. More specifically, the P-1 model uses a series expansion in terms of spherical harmonics truncated after the first term, hence the “1”. This is the simplest case of the more general P-N model and is a common choice for industrial applications.

For absorption coefficient $a$, scatter coefficient $\sigma_s$, incident radiation $I$, and a phase function $\Phi$, the radiation flux $q_r$ is obtained and simplified.

$$q_r = -\frac{1}{3(a + \sigma_s) - \Phi \sigma_s} \nabla I$$

(2.47)

$$\Gamma = -\frac{1}{3(a + \sigma_s) - \Phi \sigma_s}$$

(2.48)

$$q_r = -\Gamma \nabla I$$

(2.49)
The transport equation of the incident radiation is defined with refractive index $n$, the Stefan-Boltzmann constant $\sigma$, and a radiation source term $S$. Local radiation intensity is determined by solving this equation.

$$\nabla \cdot (\Gamma \nabla G) - aG + 4an^2\sigma T^4 = S$$

(2.50)

Further modifications to the P-1 model allow it to consider the effects of suspended second phase particles. Scatter is assumed to be exclusively from the dispersed phase and is dependent on the equivalent emission of the particles $E_p$, which is calculated based on particle projected area, temperature, and emissivity. The resulting transport equation for incident radiation is defined where $a_p$ is the equivalent absorption coefficient.

$$\nabla \cdot (\Gamma \nabla G) + 4\pi \left( an^2 \frac{\sigma T^4}{\pi} + E_p \right) - (a + a_p)G = 0$$

(2.51)

2.5. Solid Flame Modelling

The use of a solid flame model for experimental validation of a thermal radiation analysis is common in literature [22] [23]. In creating a solid flame model, the flame geometry is often simplified to a geometric shape with constant thermal properties. If the flame is complex, the geometry may be broken down into several zones, each with unique thermal properties. Determining the geometric shape of best fit requires a measurement of the real flame geometry. In experimental studies, flame bodies are often determined by the visible boundaries of the flame i.e. what can be seen by a human eye or digital camera. If a thermal imager is used, the geometry is determined by an isotherm; an enclosed area/contour of the flame where the temperature is at or above a given temperature. The choice of what temperature to use for the outer limit of the isotherm varies from application to application, and studies in literature of propane flares typically use values from 600K-800K based on a comparison with visual images [23]. Once the geometric model is made, emissive power and thermal fluxes can be calculated with view factors and an estimation of the flame’s emissivity.
The most common approach for jet flares is to use a cylindrical model. This type of flame is simple enough that a one-zone model may be used, as higher order models (2-zone or 3-zone) do not significantly improve the estimation of thermal fluxes [22]. The dimensions of the cylinder used to model a flare are defined by the radiant flame length \( L \), and the equivalent flare diameter \( D_{eq} \). The radiant flame length is determined from the measured (vertical) length of the isotherm selected. The equivalent flare diameter is selected such that the resulting rectangular projected area of the cylinder is equal to that of the 2-D flare area, \( A \).

\[
D_{eq} = \frac{A}{L}
\]  
(2.52)

This model was compared with experimental tests of varying mass flows and orifice diameters to determine that the following general relation can be applied [22]. This relation is shown graphically \((R^2 = 0.9)\) below in Figure 2-13.

\[
L = 7 \cdot D_{eq}
\]  
(2.53)

![Figure 2-13: Ratio of radiant flame length and equivalent flame diameter for varying fuel mass flows and orifice diameters [22].](image)

It is noted that this relation is more accurate for higher mass flows which would be common for full-scare flare testing, making it a simple and reliable way to produce a solid flame model from a single measurement of radiant flame length.
Once the cylindrical geometry is created, the resulting thermal radiation calculations can be completed. The thermal flux to a target, $I_{\text{target}}$, is obtained as the product of the geometrical view factor $F$, the flare’s average surface emissive power $E$, and the atmospheric transmissivity $\tau$. The flare model is treated as a gray radiating body allowing the emissive power to be calculated based on the flare’s emissivity $\varepsilon$, its temperature $T$, and the Stefan-Boltzmann law.

$$I_{\text{target}} = F E \tau$$

$$E = \varepsilon \sigma T^4$$

The determination of flare emissivity and temperature for use in these equations is not intuitive. Even with experimental data, the selection of emissivity and flare temperature in literature is seemingly just a reasonable guess. The determination of a flare’s emissivity is a trivial task if one assumes the radiation is grey (as the solid flame model does), but this assumption is often met with skepticism during review despite its accuracy. Nevertheless, the solid flame model is used frequently to validate experimental data. For example, flare values of $T = 1300K$ and $\varepsilon = 0.45$ produce good results for vertical propane jet fires as confirmed by several authors [22], [23].

The atmospheric transmissivity is estimated using a model suggested and validated by Brzustowski and Sommer which uses the relative humidity $H$, and the distance from the target to the cylindrical flare’s surface [24].

$$\tau = 0.79 \left[ \frac{100}{H} \right]^{\frac{1}{16}} \left[ \frac{30.5}{X} \right]^{\frac{1}{16}}$$
The view factor is a purely geometric property that quantifies the fraction of radiation that leaves one surface and reaches another. In the case of a flare, the view factor of interest is that which describes the radiation that leaves the cylindrical flare surface and reaches the target a chosen distance away. View factors for simple 2-D and 3-D geometrical setups can be found in a variety of databases and textbooks with accompanying equations. Configuration B-32 of the exhaustive online database produced by Howell is used to calculate the view factor between an arbitrary cylindrical flare, and a remote target [25].
3. **Numerical Methodology**

The main objective of this project is to develop a modest RANS based CFD based model of a simplified 2-phase propane jet flare and document the methodology used. With considerations for combustion, radiation, soot production, etc. this model utilizes many of the capabilities of modern CFD programs. This chapter details the decisions made, challenges found, and procedures developed during this process.

3.1. **CFD Studies Overview**

For this study, the ANSYS 18 suite of CFD programs was used. Geometry and mesh construction was completed using ICEM CFD 18. This study used unstructured, tetrahedral meshes. Solution generation was completed with Fluent 18 and the use of the Centre for Advanced Computing’s Frontenac Cluster. Typical cases were run with sixteen Intel Xeon E5-2650 cores and 64 gigabytes of memory. Post processing of results and generation of graphics was completed with CFD-Post 18.

3.2. **Computational Domain**

3.2.1. **Domain Geometry**

The fluid domain in this project is quite simple, and there is no complicated hardware or surfaces. Thus, the domain could be easily created in ICEM without the use of additional modelling software. The rectangular domain was constructed with dimensions of 32m x 32m x 40m as shown in Figure 3-1. A series of circular regions in the center of the base plane of the domain were included to allow for grid refinement and swirl conditions as described further in B.2. The dimensions of these circular areas are shown in Figure 3-2. The dimensions and number of rings were calculated based on a method described in B.2.
Figure 3-1: Dimensioned diagram of the computational domain with labeled axes.

Figure 3-2: Dimensioned diagram of the concentric rings on the base plane of the domain. Radius dimensions are given for each ring with ring 1 being the innermost, increasing outwardly to ring 6.
3.2.2. Mesh Generation

The main goal of the meshing process is to produce a mesh that can fill the domain and eventually capture flow details with appropriate accuracy. For this study, tetrahedral (tetra) mesh elements were used to fill the domain. While not as efficient at filling space as hexahedral elements, tetra meshes are quick to generate based on limited user defined parameters, simplifying the overall meshing process. Tetra elements are also easier to generate around areas of increasing cell density, resulting in smoother cell transitions.

A surface mesh is first generated and smoothed prior to volume meshing. With the prescribed geometry, this is simply the six surfaces of the box domain. Node spacing on each curve is manually specified to ensure smooth transitions and refinement around areas of interest, namely the center of the base plane - near where fuel injection will occur. Figure 3-3 shows a sample surface mesh around this area of interest. The patch-dependent meshing scheme is used which builds the mesh based on the defined curve nodes and other parameters such as maximum cell size. The resulting surface mesh is smoothed based on cell quality, a measurement relating to a cell’s aspect ratio.

Prior to volume meshing, two density regions were introduced along the vertical centerline of the domain. Density regions limit cell size and growth rate based on user defined constants. This allows the user to accurately control cell size and detail in areas without curves. A larger density region was included to
capture the flame region in addition to a smaller region around the area of liquid fuel injection as shown in Figure 3-4.

![Figure 3-4: Two density regions along the centerline of the domain limit cell size and growth.](image)

To generate the subsequent volume mesh, the Delaunay meshing scheme is used. The Delaunay method uses a bottom-up approach, requiring a pre-existing closed surface mesh to build the volume mesh from. This method proved more efficient than other volume mesh schemes, producing meshes in a few minutes. Figure 3-5 and Figure 3-6 show the details of volume mesh with mesh cut planes. Additionally, inflation layers were applied to the base surface to better capture any boundary layer development. Inflation layers are thin prism cells that extend normal to a wall surface (in this case, the bottom plane) with the intention on providing the necessary detail to capture boundary layer velocity gradients. Figure 3-5 and Figure 3-7 show the inflation layers interiorly and exteriorly.
Figure 3-5: A central vertical plane of the volume mesh. Two density zones are clearly visible with increased cell density. Inflation layers seen on the lower floor surface.

Figure 3-6: Horizontal plane showing the increased mesh density around the central core flame region.
It is noted that a cylindrical domain could also be used for this study. A cylindrical domain of similar dimensions and cell distribution was found to reduce the total cell count by only 3 percent due to the majority of cells lying in the high density region in the center of the domain. To ensure adequate mesh density, a grid independence study was completed using the Grid Convergence Index Method [26]. The details of this study are provided in C.1. The largest/densest mesh studied had approximately 3.4 million cells and was used for the full CFD analysis.

3.3. Boundary Conditions

CFD problems are defined in terms of initial and boundary conditions. Boundary conditions define the flow variables and thermal properties at the extents of the domain. Figure 3-8 shows the boundary conditions used for this study on each surface. The inner circular region’s boundary conditions varied through different tests as described below, and are thus described as either a velocity inlet, or wall.
3.3.1. Pressure Inlet

The outer four surfaces of the domain were set as pressure inlets with ambient air properties to create atmospheric condition from which air can be entrained into the domain. Defining the boundary as an inlet does not stop flow from exiting through the boundary though – reversed flow is allowed and accounted for. Total gauge pressure is defined with ambient temperature (300K), and a turbulence intensity of 1% to simulate standing air. Flow is forced to move across the boundary in the normal direction, so care must be taken to position boundaries far enough away as to not force unphysical streamline curvature in the region of interest. Earlier tests with a smaller computational domain were affected by this issue, but the domain described in Figure 3-1 was adequately dimensioned to prevent any unphysical behavior.

3.3.2. Pressure Outlet

The upper surface of the domain was set as a pressure outlet, representing an exit plane to open atmospheric conditions. Static pressure is defined on the plane and all other flow variables are subsequently calculated during solution generation. Additional temperature and turbulence values are set (standard atmospheric conditions) in the case of reversed flow which would enter the domain. Similar to pressure inlets, flow must enter normal to the boundary, and reversed flow is allowed.
3.3.3. Wall

The base of the domain was set as an adiabatic, no-slip wall boundary. Default conditions for roughness treatment were used, which assume smooth surfaces. Wall treatment in this project is not of large concern due to the combusting flow being free from interactions with walls.

3.3.4. Velocity Inlet

To study the effects of swirl, a swirling velocity boundary condition was used. The details and development of the model used are detailed in B.2. For these cases, the inner circular regions were defined as velocity inlet boundaries. On this boundary, temperature, gauge pressure, and turbulence intensity (increased to 5% for swirling cases) are defined as well as a velocity vector. By using a cylindrical coordinate system, inlet velocity is defined based on radial, tangential, and axial velocity according to the required swirl condition.

3.3.5. Discrete Phase Interactions

Interactions with the discrete phase are also defined on each boundary. In this study, discrete phase particles never reach the boundaries, so these conditions do not affect the solution. Out of necessity, the wall condition was defined as reflect, which considered a completely elastic collision, and the pressure inlet/outlet conditions were set as escape, which terminates particle trajectories.

3.3.6. Species Definitions

Each non-wall boundary must have defined parameters considering the combustion and soot processes. This includes defining mean mixture fraction, fraction variance, soot mass fraction, and soot nuclei particle density. As all of the non-wall boundaries are modelling standard atmospheric conditions, all of these values were set at zero. All of the combustion products are thus calculated from the liquid fuel source and subsequent combustion process alone.

3.3.7. Thermal Definitions

Each of the boundary conditions were set such that not heat flux was generated, and the internal emissivity values were set to 0. This ensures that radiation generated within the domain comes solely from the flare.
As stated previously, the temperature was held at a constant 300K for the atmospheric air boundaries to represent ambient conditions.

3.4. Solver Settings

This chapter will provide descriptions of the discretization, solving, and coupling schemes used within Fluent 18. Solutions were generated with the double precision, steady solver.

3.4.1. Discretization Scheme

A discretization scheme is necessary to solve differential equations over a finite volume domain. Discretization is used to approximate flow variable derivatives using cell face and cell center values, producing approximate algebraic equations for each element. For all computational studies in this project, a second-order scheme was used for pressure, with a second-order upwind scheme for all other variables. Second-order schemes are suggested for cases where flow is not aligned with the mesh as is the case with all tetrahedral meshes [27]. Second-order upwind schemes use a Taylor series expansion about a cell’s centroid to compute face values based on the upwind centroid values and the gradient between cells. The use of second-order discretization schemes was also suggested in the studied literature [28] [29] [30].

3.4.2. Pressure-Based Solver

A pressure-based solver was used in this research and is required for the PDF combustion and soot models. Specifically, a coupled pressure-based solver was used. The coupled algorithm solves the system of pressure and momentum-based continuity equations simultaneously, rather than sequentially as a segregated solver does. A coupled approach usually results in improved rate of convergence in terms of iteration count, but individual iterations require more memory. The coupled solver showed greatly improved solution generation when compared to the segregated scheme in early tests in terms of convergence and solution time, and was thus used throughout this research.
3.5. Physical Models

3.5.1. Turbulence Model

In this study the standard k-ε turbulence model was used. In literature, the k-ε family of models are used almost exclusively for CFD flare studies given their high level of industrial application and validation [31] [28] [30] [32]. More specially, the realizable and standard models see the most usage. During initial CFD testing, standard k-ε model proved to provide the best results in the least amount of time. The realizable k-ε model was able to produce results comparable to the standard k-ε model, but solution generation times were often over three times as long as compared to the standard model. As part of the scope of this work is to keep the CPU requirements modest, the standard k-ε model is therefore more desirable in this study. The RNG k-ε model was also tested but a converged solution was never reached due to poor flame development and an unstable nature of the monitored flare measurements. For these reasons, the standard k-ε model was selected.

3.5.2. Discrete Phase Model

For this project, the modelling of the discrete phase was intentionally simplified to include only the physical models necessary to produce the jet flares. Advanced models such as particle collisions, lift forces, and breakup were not included to lower the computational requirements. For such large scale flares, the complicated small scale interactions of fuel particles are not considered due to the low volume fraction as described in 2.4.3. Understandably, particle interactions with the continuous phase are included, with evaporation of the liquid phase particles fueling the combustion process. Particle tracking was included for a maximal length of 1 meter, by which time combustion had occurred. The shape and thermal properties of a large flare are almost entirely dependent on simply the physical injection properties as described in 3.5.3.

A discrete-phase iteration interval is defined which allows the user to control the frequency at which the source is updated and released particles are tracked. If set too low, frequent DPM updates can slow down solution generation, and if too high, a solution may diverge between DPM iterations. For this study, a DPM iteration interval of 15 was used which functioned well in preliminary trials and avoided divergence issues.
3.5.3. Injection Model

Discrete phase injections are modeled in Fluent based on defining geometric and flow variables. The liquid fuel injection was modeled as a 30 degree cone comprised of 15 individual particle streams, pointing vertically (+Z) and located a set distance above base of the domain’s center. This distance was set at 0.85m for direct comparison with literature sources. The velocity, mass flow, and injection diameter are all set to match expected experimental conditions. The calculations of these variables is described in detail in B.1. The liquid propane droplets were set to have a uniform diameter of 10 micron.

![Figure 3-9: Location of the liquid fuel injection in the computational domain (not to scale).](image)

3.6. Solution Generation

The initialization, generation, and monitoring of solutions was perhaps the most difficult and time-consuming aspect of this research. With such a complicated mixture of various CFD models, ensuring all parameters of interest developed properly was a great challenge. Many iterative studies were done to determine best practice for developing solutions efficiently. Besides descriptions of basic solver settings and boundary conditions, literature on the CFD process of modelling flares or similar combustion processes
is limited. The process discussed here for solution generation was based largely on trial and error in addition to suggestions from other CFD users, literature, and Fluent guides.

3.6.1. Initialization and Interpolation

Before beginning iterations, initial values are applied to the domain from which the solution is then generated. For simple cases such as a pipe flow, a constant velocity can be applied across the domain to approximate the “initial guess” of the solution. For the jet flare case under study, there is not an effective way to initialize the flow with considerations for combustion, soot, temperature, etc. so the domain was initialized as still, ambient air. This fundamental challenge of the solution generation process requires that the flame must “push” its way through the domain, initially igniting near the injection and propagating through the domain in a pseudo-transient fashion until it is fully formed, and the time average solution is reached. Depending on the mesh density, the development of a full flame in the initial phase of solution generation was slow. To avoid this for each case studied, interpolation can be used. Interpolation allows the solution data of one mesh to be applied to a different mesh of the same domain dimensions. For example, solution data of a coarse 1 million cell mesh can be interpolated onto a much denser mesh of 5 million cells and serve as the initialization of a new solution on the denser mesh. This effectively eliminates the solution time where the flame propagates through the domain, thus speeding up the overall solution.

3.6.2. Under-Relaxation

To control the rate of change of flow variables while iterating, under-relaxation factors (URFs) are used. Simply put, a given variable $\phi$ is dependent on the old value $\phi_{old}$, its calculated change $\Delta \phi$, and the user specified URF for that variable $\alpha$.

$$\phi = \phi_{old} + \alpha \Delta \phi$$

When URFs are low, the convergence of a variable can be thought to have higher “inertia” - it will be less prone to fluctuations. The coupled solver also uses an under-relaxation of entire equations to further
stabilize convergence. If a certain variable is found to diverge or fluctuate, lowering the URFs can lead to better results.

Determining appropriate URFs for this project was mainly done through trial and error, relying on user experience, and taking suggestions from literature where available. For example, lowering the URFs for pressure, density, and momentum had a positive, stabilizing effect on early flame development, eliminating divergence issues experienced prior to these changes. A sample of the URFs used in this study is provided in C.2.

3.6.3. Solution Convergence

Convergence in generally achieved when scaled residuals for each equation were allowed to reach a specific value. Due to the nature of the initialization though, relying on scaled residuals alone for this study could often be deceiving. To more accurately determine the convergence of a solution, flow properties were monitored to confirm that a flame was developed, and that measurements of soot, radiation, and net mass flow were not changing with additional iterations. More specifically, temperature monitors along the centerline of the flame were used to determine when the flare had fully developed. A total of six temperature monitors were placed along the vertical centerline of the domain at 2m, 3m, 4m, 5m, 7m, and 9m, which provided temperature values throughout the length of the flame. Remote targets to record incident thermal radiation were defined 0.5m above the ground surface at distances of 2m, 4m, 6m, 10m, and 15m, from the fuel injection location. The location of these monitors are shown in Figure 3-10. Net mass flow out of the domain was monitored to ensure conservation laws were met, as well as the volume fraction of soot present in the domain.
Figure 3-10: The temperature monitors (red) and thermal radiation monitors (grey) in the domain.

Figure 3-11 provides an example of how a solution develops through the monitored centerline temperatures. The solutions starts with no flame (ambient temperature), a flame develops, and is eventually stabilized. URFs are lowered at set intervals in the solution to help dampen oscillations in the solution. Figure 3-12 through Figure 3-14 show the progression of the solution from the other monitors used. Note that the fuel mass flow in this case was 0.1kg/s which results in a net mass flow of 0.1kg/s out of the domain (negative).
Figure 3-11: Centerline temperatures developing and converging during solution generation. Monitor labels correspond to the vertical distance above the ground plane in meters.

Figure 3-12: Soot volume fraction developing during solution generation.
Figure 3-13: Net mass flow through the boundaries of the domain during solution generation.

Figure 3-14: Incident thermal radiation to the targets at varying distances from the centerline of the domain developing during solution generation.
Reviewing the monitor data also allows for optimization in the amount of iterations needed to reach the desired results. For example, the above solution could be run with only 16000 iteration to the same level of convergence. Reviewing the monitor data was an effective way to evaluate solution quality, and quickly see some of the key flare properties under study. When all of the metrics of interest are not changing with further iterations, the solution can be said to be complete, and exported for further analysis.

4. Results and Discussion

4.1. Flare Geometry

The geometry of the flare is important for determining several other key flame characteristics. For example, the flame volume and surface area are used to determine the average soot concentration and surface emissive power of the flare respectively. Additionally, an estimation of the flame dimensions (specifically radiant flame length) must be used for comparison with a solid flame model. To determine the flames surface area and volume, and iso-surface of constant temperature was used. Surfaces of 600K, 700K, and 800K were selected as there is variation among literature. This results in three varying flame volumes and surface areas for a given mass flow. The volume of the flame is calculated by the total cell volume enclosed by the each iso-surface. The radiant flame length is taken as the total height (z-coordinate) of each iso-surface. Additionally, the 2-dimensional projected areas (onto the x and y planes) are averaged and the equivalent flare diameter is subsequently calculated as described in 2.5. Table 4-1 summarizes the key geometric properties obtained from the three iso-surfaces. With radiant flame length and equivalent flare diameter, the resulting cylindrical flare volume to be used in the solid flame model was also calculated. In each case, the resulting solid flame was larger than that determined by the iso-surface by 7.9%, 10.2%, and 12.7% for the 600K, 700K, and 800K boundary flares respectively.
Table 4-1: Geometric flame properties from iso-surfaces of varying temperatures.

<table>
<thead>
<tr>
<th>Geometric Measurement</th>
<th>600K Flame Boundary</th>
<th>700K Flame Boundary</th>
<th>800K Flame Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame Surface Area [m²]</td>
<td>34.6</td>
<td>27.0</td>
<td>22.4</td>
</tr>
<tr>
<td>Flame Volume [m³]</td>
<td>7.50</td>
<td>5.09</td>
<td>3.70</td>
</tr>
<tr>
<td>Radiant Flame Length [m]</td>
<td>11.62</td>
<td>10.13</td>
<td>9.22</td>
</tr>
<tr>
<td>Equivalent Flare Diameter [m]</td>
<td>0.94</td>
<td>0.84</td>
<td>0.76</td>
</tr>
<tr>
<td>Resulting Cylindrical Flame Volume [m³]</td>
<td>8.09</td>
<td>5.61</td>
<td>4.17</td>
</tr>
</tbody>
</table>

Figure 4-1 and Figure 4-2 are provided below showing the size of the 600K iso-surface flare volume relative to the computational domain, and each of the flares relative to one another. A temperature contour plot is provided below in Figure 4-3 showing a 2-dimensional plane through the center of the flare.

![Image](image.png)

*Figure 4-1: The flare volume defined by the 600K iso-surface inside the computational domain.*
Figure 4-2: Comparing the size for the three iso-surface defined flare volumes.

Figure 4-3: Temperature contour of the flare.
It is noted that the flares produced are not always perfectly symmetrical as one might expect from a time averaged solution. This is a result of the unstructured meshing used, the non-axisymmetric geometry, as well as very small (less than 0.5m/s) air velocities that developed around the flare. These small currents caused very minor asymmetries in the flare but did not have an effect on the flare parameters of interest, and thus were considered negligible.

4.2. Soot Characteristics

Soot characteristics of flares (e.g. soot volume fraction) are notoriously hard to measure experimentally. The collection of soot data with a physical apparatus causes conglomeration of soot particles which skews the data. Optical methods such as using a thermal imager are another option but often rely on simplifying assumptions that can lead to skepticism of the results. The soot models used in CFD applications have been created and validated for a small range of experimental conditions.

It is important to note that soot characteristics of flames are often best studied in a temporal way. Soot concentration and production in real flames is not a steady quantity, but something that fluctuates as a flame burns. Local areas of high temperature and fuel rich conditions will create puffs of soot and happen repeatedly throughout the flare. A time averaged approach to modelling soot in CFD should not be seen as a real physical representation of soot in a real flare, but rather an approximation of what can be expected in terms of average volume concentration.

Many of the soot models used in CFD have limitations and restrictions as to what models can be used in conjunction with them. For example, the two-step soot model which was used in this study is limited to pressure-based solvers, with non-premixed combustion. Considering all of this, is not uncommon to find that many researches limit studies of soot characteristics to experimentation of small lab scale flares. However, the goal of this project is to test the capabilities of the built in soot models of ANSYS Fluent and thus an effort was made to produce meaningful results despite the limitations.
The CFD soot volume fraction results are shown below in Figure 4-4. A full scale vertical center plane contour shows the location of the soot compared to the computational domain. Figure 4-5 shows the 600K defined flame area containing the produced soot. Comparing the location of highest soot density to the temperature contour of the same area shows that the highest volumetric amount of soot resides in the core of the flame, where temperatures are hottest. This area is also starved for oxygen as it is in the center of the flare body with the least access to the surrounding combustion air. The peak soot volume fraction was determined to be just over $f_v = 8.0 \times 10^{-6}$.

*Figure 4-4: Contour of soot volume fraction along a vertical center plane showing the local maximum concentration in the flare relative to the computation domain.*
Figure 4.5: Soot volume fraction and temperature distribution displayed inside the 600K iso-surface flare.

Figure 4-6 provides a three-dimensional graphic of the area of high soot concentration. An iso-surface of constant soot volume fraction was created for $f_v = 1 \times 10^{-6}$ to enclose the bulk of the predicted soot. Several contours are provided within the volume to further show how the soot is distributed in the central area. The 2-step soot model estimates soot production based on flame characteristics like temperature, but also on chemical composition inside the flare. Because of this, the soot pattern follows an elliptical shape rather than precisely following the temperature contour. It is also noted that the soot is not shown to propagate downstream and into the atmosphere as one would expect for a real flare. The 2-step soot model predicts soot based on a balance between the rate of soot formation and the rate of soot combustion and does not predict how soot particles propagate downstream. This limitation results in soot being predicted in only the areas where the necessary soot production conditions are met.
Figure 4-6: Three-dimensional rendering of the predict soot results. The volume is defined by a constant soot volume fraction of $1 \times 10^{-6}$.

The determination of the average volume fraction of soot is dependent on the flame volume that is used. As described in 4.1, the selection of an iso-surface of constant temperature to define the flare results in a varying flame volume. Volume integrations of the three flares (defined by the 600K, 700K, and 800K iso-surfaces) were completed to see the respective average volume fraction of soot in each flare. Table 4-2 summarizes the results.

<table>
<thead>
<tr>
<th>Measurement</th>
<th>600K Flame Boundary</th>
<th>700K Flame Boundary</th>
<th>800K Flame Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame Volume [m$^3$]</td>
<td>7.5</td>
<td>5.1</td>
<td>3.7</td>
</tr>
<tr>
<td>Resulting Soot Volume Fraction [10$^{-7}$]</td>
<td>2.7</td>
<td>3.8</td>
<td>4.9</td>
</tr>
</tbody>
</table>
4.3. Thermal Radiation

The results from the CFD work were compared to a solid flame model with the geometry determined in 4.1. A MATLAB code was written to complete the solid flame calculations for incident thermal radiation at varying distances from the flare. As described in 2.5, an estimation of flare emissivity and temperature are needed to complete the solid flame calculations. The values suggested from literature of $T = 1300$ K and $\varepsilon = 0.45$ were used for the solid flame model. In addition, a sensitivity study of the solid flame model was done by changing these values. Figure 4-7 below shows the results from the CFD analysis. The remote target distances used to monitor the radiation levels during solution generation are marked. These five targets in relation to the domain are seen in Figure 3-10.

![Incident thermal radiation from the CFD results. The monitored targets at 2m, 4m, etc. are highlighted.](image)

*Figure 4-7: Incident thermal radiation from the CFD results.*

*The monitored targets at 2m, 4m, etc. are highlighted.*
Contour plots of incident radiation are provided in Figure 4-8 and Figure 4-9. The results show expected radiation patterns in the computational domain, with thermal flux decreasing radially about the central vertical axis. Across the center plane, the thermal flux is highest inside the flame body, surrounding the area of highest soot concentration. This is expected as the high temperature soot particles dominate the radiative emissions from the flare.

*Figure 4-8: Contour plot of incident radiation from the CFD analysis.*
Ideally, incident radiation should only be a function of radial distance to the flame assuming measurements are taken from the same height. To account for the unstructured, non-axisymmetric nature of the mesh, incident thermal radiation was measured along four geometrically similar lines around the flare axis to evaluate how the radiation data varies based on location in the domain. These four lines are shown below in Figure 4-10. Each line is 0.85m above the base of the domain, and extends from 2m to 15m from the flare axis. Incident radiation data was taken along each line and normalized against the mean of the measurements. Figure 4-11 shows that the deviation from the mean increases with distance from the flare axis, which is expected as the mesh coarsen radially. Line 1 and Line 4 represent the largest degree of disagreement with a ~9% difference at a distance of 15m.
Figure 4-10: Four geometrically similar reference lines used to measure incident radiation around the flare.

Figure 4-11: Comparing the normalized radiation data for each reference line.
4.3.1. Solid Flame Models

The CFD results were compared to three versions of the solid flame model, each having a different flame temperature. The base case of $T = 1300K$ as suggested by literature was used, in addition to a 1400K and 1500K solid flame. Each case used the suggested emissivity of $\varepsilon = 0.45$. The geometry was identical for each case and was based on the 600K boundary flare as described in Table 4-1. Figure 4-12 shows the direct comparison to the CFD results. The 1300K solid flame produces thermal flux values lower than the CFD results which are up to 65% larger in the 4m range. The 1400K line has the best agreement with the CFD results in the near field (2m-3m) and far field (10m+). Between these distances, the CFD results are up to 26% greater than the 1400K solid flame model predicts, and approach the 1500K line around 5m.

![Figure 4-12: Comparing the CFD results with three temperatures of solid flame models. Emissivity of $\varepsilon = 0.45$ was used for each solid flame.](image)

To similarly test the effects of varying flame emissivity in the solid flame model, three values of $\varepsilon = 0.35$, 0.45, and 0.55 were tested for a flame temperature of 1400K. Figure 4-13 displays the results of the analysis. The low emissivity flame ($\varepsilon = 0.35$) has poor agreement with the CFD results compared to the other emissivity values. In the 4m-8m the CFD results are best represented by the $\varepsilon = 0.55$ model.
4.3.2. Experimental Based Models

The CFD results were also compared to the experimental results from Zhang’s 2015 paper *Experimental Study on Propane Jet Fire Hazards: Thermal Radiation*. In this study, the thermal radiation of propane jet flares (liquid and gaseous) was studied experimentally with the use of a thermal imager and seven radiometers. Unfortunately, the fuel flow rate for the liquid propane was not recorded so a direct comparison cannot be made. Of the four liquid fuel trials completed, it is stated that the flare ranged from ~8.5m in the first trial to ~13.2m in the last as measured by the visible flame length [23]. The CFD flare has a radiant flame length of 9.22m-11.62m depending on the iso-surface used as described in Table 4-1. In lieu of other relevant flare characteristics, one could assume that the CFD flare mass flow would lie within the range of experimental trials.

Zhang fit the radiation intensity data form the flares using a power correlation of the form $I = ax^b$ where $I \left[\frac{\text{kW}}{\text{m}^2}\right]$ is the intensity, $x[\text{m}]$ is the distance from the flare axis to the radiometer and $a$ and $b$ are constants.
determined by the fit. Table 4-3 summarizes the obtained correlations for each of the experimental trials. The raw data from the radiometers, and the fitted curves are shown together in Figure 4-14.

\[ I = 3877x^{-2.96} \]
\[ I = 4669x^{-3.0} \]
\[ I = 2043x^{-2.6} \]
\[ I = 1183x^{-2.3} \]

<table>
<thead>
<tr>
<th>Test Number</th>
<th>Power Correlation Fit</th>
<th>( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>( I = 3877x^{-2.96} )</td>
<td>0.81</td>
</tr>
<tr>
<td>12</td>
<td>( I = 4669x^{-3.0} )</td>
<td>0.81</td>
</tr>
<tr>
<td>13</td>
<td>( I = 2043x^{-2.6} )</td>
<td>0.87</td>
</tr>
<tr>
<td>21</td>
<td>( I = 1183x^{-2.3} )</td>
<td>0.91</td>
</tr>
</tbody>
</table>

The experimentally determined curves were compared to the CFD data as seen in Figure 4-15. The agreement between the results is poor. Zhang’s fits were only plotted over the range they were initially calculated for, as extrapolating the curves to 2m results in radiative fluxes upwards of \( 575 \, \text{kw/m}^2 \), an unrealistically high number for a flare of this size.
It is worth noting that the radiometers used in the experimental trials had ranges of $30 \text{ kW/m}^2$, $120 \text{ kW/m}^2$, and $300 \text{ kW/m}^2$ although it is not specified what the radiometer range was for each individual measurement. It is reasonable to assume that the larger range radiometers were used closer to the flame. The error on these radiometers is not stated in the paper, but similar models from the same manufacturer have posted uncertainties of $\pm 3\%$ of the range. For a $300 \text{ kW/m}^2$ radiometer, an associated error could be upwards of $9 \text{ kW/m}^2$ which is larger than the measurements taken in the experimental trials.

Additionally, wind speeds of $2.2 \pm 0.7 \text{ m/s}$ are reported with a direction between NNE and NNW. Assuming the worst case scenario where the wind is directly toward the radiometers, and the speed is the maximum recorded speed of $2.9 \text{ m/s}$, this would still not account for the large disagreement between the results. The effects of crosswinds are presented in 4.5, and Figure 4-33 shows head-on cross winds effect the levels on incident radiation. Comparing these results with the above clearly shows that crosswinds cannot fully explain the disagreement.
4.3.3. Surface Emissive Power

The surface emissive power of the flare is determined based on equation (2.55. With known geometry, a model for transmissivity, and the CFD based incident radiation results, emissive power can be derived. This method is used throughout literature with experimental measurements in place of CFD based results. Figure 4-16 shows the calculated surface emissive power compared to that of the solid flame model which is a constant for a given flame temperature. The CFD model produces distance-dependent results, indicating an unideal nature of the P1 radiation model used. The P1 model over predicts or under predicts the surface emissive power compared to the solid flame model depending on where the incident thermal radiation measurement is taken along the reference line. Variance in emissive power measurements over a distance is also common in experimental work. Across the distance measured, the largest disagreement corresponds to 19% of the solid flame value. The average surface emissive power over the same distance for the CFD model is $100.3 \text{ kW/m}^2$ compared to $98.0 \text{ kW/m}^2$ for the solid flame model.

![Figure 4-16: Comparing surface emissive power for the CFD model and solid flame model.](image-url)
A linear correlation or power correlation for radiant flame length \( L \) and surface emissive power \( E \) is commonly used in literature to characterize experimental work with turbulent propane flares. While these models do not provide strong correlations to experimental work (low \( R^2 \) values), several models are compared below from various authors with varying levels of agreement [33] [23] [31]. Radiant flame length from the 600K boundary flare results is used here to compare the models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Surface Emissive Power [kW/m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD (average)</td>
<td>100.3</td>
</tr>
<tr>
<td>Solid Flame</td>
<td>98.0</td>
</tr>
<tr>
<td>( E = 25.7L^{0.65} ) (Gomez)</td>
<td>126.6</td>
</tr>
<tr>
<td>( E = 28.37L^{0.51} ) (Zhang)</td>
<td>99.1</td>
</tr>
<tr>
<td>( E = 13L^{0.76} ) (Sonju)</td>
<td>83.8</td>
</tr>
<tr>
<td>( E = 10L + 22 ) (Gomez)</td>
<td>138.2</td>
</tr>
<tr>
<td>( E = 7.8L + 10 ) (Sonju)</td>
<td>100.6</td>
</tr>
</tbody>
</table>

4.4. Swirling Flow

To first test the capabilities of the concentric ring swirl boundaries, trial runs were completed without combustion taking place in the domain. The purpose of these tests was to evaluate the quality of the swirl produced, and ensure that the boundary conditions were working as intended. Details about the code used to initialize the boundary conditions are explained in B.2. For the cases evaluated in this section, the boundary conditions were applied over six different concentric regions as described in Figure 3-2. Table 4-5 summarizes the velocity definitions used on the swirling velocity boundaries. It is noted that all the velocities were defined with constant tangential velocity except the inner core region which was defined
with constant angular velocity. Throughout all of the swirling flow trials, an updraft (z-direction) velocity of 1m/s was used to propagate the swirl downstream.

Table 4.5: Swirling boundary velocity inputs for the cases studied.

<table>
<thead>
<tr>
<th>Maximum Speed [m/s]</th>
<th>Inner Core [rad/s]</th>
<th>Ring 1 [m/s]</th>
<th>Ring 2 [m/s]</th>
<th>Ring 3 [m/s]</th>
<th>Ring 4 [m/s]</th>
<th>Ring 5 [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.6</td>
<td>0.9</td>
<td>0.7</td>
<td>0.5</td>
<td>0.3</td>
<td>0.1</td>
</tr>
<tr>
<td>3</td>
<td>16.7</td>
<td>2.7</td>
<td>2.1</td>
<td>1.5</td>
<td>0.9</td>
<td>0.3</td>
</tr>
<tr>
<td>5</td>
<td>27.8</td>
<td>4.5</td>
<td>3.5</td>
<td>2.5</td>
<td>1.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Evaluation of streamlines, and velocity profiles indicated that the swirling boundary condition produced stable results. Figure 4-17 shows the streamlines of the swirling flow in the computational domain for a maximum tangential velocity of 1m/s.

Figure 4-17: Streamlines of velocity originating from the swirling velocity inlet. Maximum tangential swirl velocity of 1m/s.

Tangential velocity was evaluated along lines at various vertical offsets from the velocity inlet boundary conditions. Figure 4-18 shows a sample of the lines that were used for the velocity profiles. The lines were
2.5m in length which allowed the full profile to be captured, including a 0.7m length radially into the domain to see how the swirl propagated outward.

![Diagram showing tangential velocity lines](image)

*Figure 4-18: Lines used to evaluate tangential velocity at various heights above the inlet velocity boundaries.*

The lowest swirl speed tested was a maximum tangential velocity of 1m/s. Figure 4-19 shows how the velocity profile developed from the inlet condition, upward to a height of 12m. As expected, the swirl degrades and slows down as it travels away from the forced inlet conditions. The non-continuous steps in velocity boundary profile also smoothen out due to viscous forces as the air is mixed downstream.
For higher swirl velocity inlet conditions (3m/s and 5m/s), the velocity profiles rapidly change above the inlet condition near the core of the swirl. Figure 4-20 and Figure 4-21 show the swirl velocity profile development in the first 1m above the inlet condition. From the central axis to 0.5m radially, the profile degrades rapidly. This is due to the centrifugal nature of the flow at the higher swirl velocity. The flow is thrown out radially from the inlet and a strong recirculation/vacuum zone is created above the boundary plane. This is shown visually in Figure 4-22 and Figure 4-23; as the swirl strength increases up to 5m/s, the streamlines show that the air moves radially immediately following the boundary plane. The central vortex area has a larger radius to accommodate the inner recirculation zone.
Figure 4-20: Tangential swirl velocity profile for 3m/s maximum swirl strength. Legend indicates vertical distance above the boundary.

Figure 4-21: Tangential swirl velocity profile for 5m/s maximum swirl strength. Legend indicates vertical distance above the boundary.
Figure 4.22: Streamlines of velocity above the 3m/s swirling velocity inlet.

Figure 4.23: Streamlines of velocity above the 5m/s swirling velocity inlet.
Contours of tangential velocity along a central cut-plane also show the development and scale of the recirculation zone. Figure 4-24 through Figure 4-26 compare these contours for each swirl case. In the 3m/s and 5m/s cases, the higher tangential velocity does not propagate any meaningful distance downstream. After the initial distance where the recirculation zone appears, the swirl maintains a maximum tangential velocity of less than half the initial maximum.

Figure 4-24: Tangential velocity contour for a maximum swirl strength of 1m/s. The recirculation zone is not present at the lower speed.
Figure 4-25: Tangential velocity contour for a maximum swirl strength of 3m/s. The recirculation zone can be seen above the boundary plane. Tangential velocity degrades rapidly downstream.

Figure 4-26: Tangential velocity contour for a maximum swirl strength of 5m/s. The recirculation zone is significant above the boundary plane. Tangential velocity degrades rapidly downstream.
Issues arose with the swirling flows when the discrete phase (liquid fuel) and combustion models were reintroduced. Convergence was difficult to obtain for the swirling combusting flows for higher speed swirls. As the swirl speed increased, flare development and stabilization deteriorated. Figure 4-27 shows the temperature monitors used to evaluate the solution development.

![Temperature monitors for the 3m/s swirl case. Rapidly changing and deteriorating temperature values indicate solution convergence and stabilization issues.](image1.png)

A low speed (1m/s) swirl case was completed with somewhat adequate convergence, but showed no notable differences from the no swirl case. Figure 4-28 shows the temperature development of this low speed swirl case. Small changes in the key flare characteristics (less than 10% change) were observed, but the poor overall convergence of the solution must be considered. The jet momentum was too great to that of the slower swirling flow for flare characteristics/geometry to meaningfully change. Figure 4-29 compares the incident radiation profile from the base case and the low speed swirling case. The maximum difference between the two corresponds to about 8% at the 2m mark. No meaningful data was obtained from the higher speed swirling flows (3m/s and 5m/s) due to the poor solution development.
Figure 4-28: Temperature monitors for the 1m/s swirl case. Stabilization of the solution is improved over the higher speed cases, but is not ideal. Continuing temperature development indicates changing flare characteristics.

Figure 4-29: Comparing the thermal radiation profile from the low speed swirl and base cases.
4.5. Crosswind Flows

The effect of crosswinds on the flare were studied to quantify how the radiation levels change depending on the geometry and location of the flare relative to a local target. In a real world scenario, a sudden change in wind can cause the flare to bend toward working personnel suddenly introducing a large thermal radiation risk. To simulate flows of varying crosswind strength, a velocity inlet boundary condition was applied to one wall of the domain and the opposite boundary was set as a pressure outlet. The crosswind was applied perpendicular to the measurement line simulating the worst-case scenario where the wind blows the flare directly towards an observer, resulting in the largest thermal hazard. Figure 4-30 shows the crosswind direction, and the reference line used to measure the incident radiation. This line is the same geometry as that used in 4.3 so a direct comparison to the previous results can be made.

![Crosswind Direction Vectors](image)

*Figure 4-30: Crosswind direction vectors. The crosswind produced blows the flare directly overhead of the reference line used to capture incident thermal radiation.*
Five different crosswind speeds were tested to cover a realistic range – 0.5m/s, 1m/s, 2m/s, 4m/s, and 6m/s. Similar ranges of crosswind speeds have also been used in literature for studying jet in crossflow phenomena [28]. The resulting deflected flares are shown below in Figure 4-31. It is noted that as the crosswind speed increased, the flare geometry became less stable. While small perturbations were seen in the temperature monitors used in the solution generation, the thermal radiation data converged well. A sample of the incident radiation convergence for the 4 m/s trial is provided below in Figure 4-32.

Figure 4-31: Flame deflection for each crosswind speed studied.
The incident thermal radiation along the reference line was collected for each case and compared to the base (no crosswind) flare as shown below in Figure 4-33. As expected, the incident thermal radiation increases as the flare is directed toward the reference line, thus increasing the view factor. The 6 m/s line produces a local maxima near the 2m mark, indicating that the part of the flare that provides the most thermal radiation is directly overhead. Further increases in crosswind speed could result in a decrease in received thermal radiation to the 2m target assuming the combustion and flare geometry remains stable. At 0.5 m/s, the cross wind has little impact on the radiative properties of the flare, increasing the incident radiation at 2m by about 7%.
5. Conclusions

The computational results of this study show that the RANS based CFD methods discussed can be used to produce and study largescale liquid propane jet flares and include considerations for soot, thermal radiation, and crosswind effects. The ANSYS suite of CFD tools was used for each step of the study, and proved to be appropriate for flares of the scale studied. While most studies of this nature are limited to experimentation and simplified models (solid flame, geometric relations), the results of this work show that CFD based models can be a useful tool and compliment experimental work by providing a unique way to flare determine flare characteristics that typical experimental methods cannot.

5.1. Flare Geometry

The CFD flare model allows for key geometric measurements to be taken based on an iso-surface of constant flame temperature. Measurements of radiant flame length, equivalent flare diameter, surface area, and volume can all be determined to construct a solid flame model, or compare with experimental thermal
imager data. Extracting these dimensions from experimental data alone can be difficult due to the temporal nature and often low resolution of thermal imagers. In this work, the geometric data extracted from the CFD model was used to define a solid flame model with a high level of agreement. Crosswind effects were also taken into consideration and the resulting flame deflection was observed. These results are can be useful for the design of industrial flaring rigs where crosswinds are common.

5.2. Soot Characteristics

A time averaged approach to modelling soot in CFD should not be seen as a physical representation of soot in a real flare, but rather an approximation of what can be expected in terms of average volume concentration. The results in this study were used to obtain a measurement of average soot volume fraction as defined by a varying flame boundary. The soot volume fraction was determined to be $2.7 \times 10^{-7}$, $3.8 \times 10^{-7}$, and $4.9 \times 10^{-7}$ for the 600K, 700K, and 800K iso-surface bound flares respectively. The CFD results also showed the highest soot concentrations to be present in the core of the flare, where temperature is hottest and oxygen is sparse.

5.3. Thermal Radiation

The thermal radiation modelling provided useful results for mapping the incident thermal radiation around the flare. In particular, the P1 model used in this study was found to produce results comparable to a solid flame model approach. The CFD based modelling of thermal radiation is valuable for producing numerical results not limited by measurement devices, and continuous contours of thermal radiation - something that can’t be done in an experimental study. Using literature based methods for solid flame modelling, the CFD was compared and validated using a solid flame model. A sensitivity analysis was preformed to see how the agreement between the two models changes as solid flame parameters like temperature and emissivity were altered. The CFD results were within the range of solid flame cases studied, and had strongest agreement in the 4-8m range.
Comparing the CFD work to experimental results from literature was difficult due to the lack of documentation of the source mass flow rate, and other relevant parameters. Comparing the CFD model of this work to the work of Zhang’s 2015 paper resulted in poor agreement. It is difficult to assess the level of error without further information about the fuel source, and the measurement devices used (radiometers). Zhang’s results seem to be unnaturally high for a flare of the size studied, and the agreement between the solid flame model and CFD indicates this as well. Zhang compares this work to a solid flame model using the same methodology used in this paper, but only the normalized data is presented in comparison with the experimental results – not the raw data from the solid flame model. Considering the crosswinds recorded also do not create a large enough difference to account for the disagreement observed.

The surface emissive power was also determined from the CFD based on the thermal radiation measurements, and a methodology commonly found in literature. An average surface emissive power of $100.3 \frac{\text{kw}}{\text{m}^2}$ was calculated over the measurement range, though this value varied by up to 19% over the same range. This result has good agreement with several experimentally determined models relating to flame length.

5.4. Swirling and Crosswind Flows

A swirling boundary condition was developed to produce a swirling flow around the flare as described in B.2. The CFD results for the swirling flow alone (no flare) showed that at higher speeds (3-5m/s) a recirculation zone developed, and degraded the swirl strength downstream. Introducing the liquid fuel combustion into the solution resulted in very poorly converged solutions, and in the higher speed cases, no meaningful data could be recovered. For the low speed case (1m/s), the results were not significantly different to the no swirl case, and the unstable nature of the solution’s convergence indicates that the results were not ideal.

Crosswind flows were simulated in CFD with success and data comparing the crosswind speed and incident thermal radiation was collected. As expected, the thermal radiation received increases as the flare is blown
towards the target. At a low wind speed of 0.5m/s, the effect was negligible, but at higher speeds upwards of 6m/s, the incident radiation to close targets increases significantly. This information is important in the design and implementation of thermal radiation shielding on oil rigs where high winds speeds are common.

6. Recommendations

6.1. Exhaustive CFD Model Studies

The scope of this work was to develop an approach in ANSYS Fluent to model the flares of interest. This involves a large number of built in models, each with their own limitations and assumptions. It would be beneficial in future work to further examine each of these models in detail for the use of studying large scale 2-phase propane jet flares.

During the literature review process for this work, two concepts became evident:

1. The study of large scale 2-phase jet flares is almost entirely based on experiments and solid flame models.
2. Most of the ANSYS Fluent models used to produce the results of this work were designed or validated for small, lab scale fires.

The modelling of liquid fuel combustion, radiation, and soot development is difficult as it involves such a high number of models working in tandem. It can be overwhelming and expensive, and thus it is reasonable to see why many researches limit their work to experimentation. Due to the complexity of each of the models being used, the scope of this project was limited to developing a CFD methodology based on the preexisting models and evaluating their capabilities. It would be valuable to have a study that comprehensively examined each model individually. Such a study would ideally focus on a single simple flare, and preform a sensitivity analysis on one of the models being used. In this study, many models were disqualified due to inherent limitations and incompatibilities with other models being used. This limited the pool of potential models somewhat, but the work presented here is only meant to be a showing of the basic implementations of the models used, not a full optimization.
6.2. Experimentation

An experiment was not included in this study due to the time and resource limitations. A comparison to a detailed experiment would provide the best means of validating the CFD models used. The experiment should be planned in such a way to ensure that all CFD relevant measurements are taken such as mass flow, precise radiometer locations, and injection (nozzle) properties. The use of appropriate ranged radiometers, and a thermal imager (or more) would provide the most accurate experimental measurements for validation.

In the literature reviewed for this work, there is a distinct lack of papers that compare experimental results, a CFD model, and a solid flame model. This type of broad comparison would be both unique and useful for further developing the CFD methodology used here.

6.3. Flare and Nozzle Configurations

There are a variety of commercial flaring systems available with unique nozzles that result in interesting flare patterns. The peacock burner shown in Figure 1-1 is just one example of how a system can distribute fuel for flaring. By distributing the fuel through multiple nozzles or in a unique pattern, the geometric view factor is changed and thus the thermal radiation to an observer also. The vertical flare configuration studied in this work represents a very simple case, but the methodology produced can be used for more complex configurations by altering the fuel injection parameters. Using CFD to investigate the effects of various flare distributions would provide interesting insight into how nozzle geometry could be used to lessen thermal radiation risks for a given mass flow rate of fuel.

6.4. Swirling Flows

The progress made in this work toward a swirling flow solution showed that a free-vortex model of swirling flow can be created in Fluent. The errors associated with introducing combustion into the domain were not resolved. Further research into this area could result in a more detailed and interesting study on how a swirling flow may affect the flare’s radiative signature and stability in crosswinds. The stability of the swirling flows without combustion present suggests that the issue is not a result of the flow modelling, but rather is likely to due to limits in the combustion modelling, or coupling between the various models at
work. Further research into the limitations and capabilities of the combustion models could result in better solution convergence, especially with the high speed swirling flows. Ideally, results in this area of study could lead to the design and development of a physical device that can produce high speed swirling flows for use in experimental studies or industrial applications.
References


A. Supplementary Literature

A.1. Thermal Hazard Measurement

A thermal radiation risk is often described in terms of a received thermal dose. 

\[ V = I^4t \]  

(A.1)

The thermal dose \( V \) \( \left[ \frac{(\text{KW}^4)}{\text{m}^2 \text{s}} \right] \) is dependent on the incident radiation flux \( I \) \( \left[ \frac{\text{KW}}{\text{m}^2} \right] \) and the exposure time \( t \) [s]. To account for differing levels of protective clothing or other levels of mitigation, the modified effective thermal dose \( V' \) can be used. The effective dose relies on a dimensionless protection factor \( \emptyset \) such that \( V' = V\emptyset \). For example, a fully clothed individual would have a protection factor of ~0.5. Usage of the thermal dose is an effective way to categorize a thermal risk, as it takes into account both the radiation strength and exposure time. Health and safety guidelines can then limit the thermal dose for workers near a thermal hazard. Receiving a thermal dose of 80-200 would likely result in pain, with more significant injuries or first degree burns occurring at 200-800. With a thermal dose of 1000-2000 there is a high likelihood of severe burns, and significant chance of fatality occurs at 2000+ [2].

There are several empirically determined probit (probability estimate) functions used to estimate fatality rates of thermal hazards. One such function developed by Tsao and Perry in 1979 takes the form 

\[ Y = -12.8 + 2.56\ln V \]  

[35]. From this the probability of death \( P \) is then determined with the use of the error function.

\[ P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y-5} \frac{e^{-t^2}}{2} dt \]  

(A.2)

This can be used to create a matrix to evaluate thermal radiation risk depending on radiation strength and exposure time. Table A-1 is an example of such a matrix calculated from the above probit model considering unprotected human skin. Other commonly used models include the Eisenberg model, Lees model, or TNO...
The experimental radiation sources used to develop each model having varying levels of ultraviolet and infrared radiation, so matching the model to the application of interest with yield the best results. Tsao and Perry suggest that ultraviolet radiation requires about 2.2 times more than the equivalent amount of infrared radiation to produce similar thermal risk/damage [2].

Table A-1: Fatality rate as a function of exposure time for varying radiation strengths [2].

<table>
<thead>
<tr>
<th>Exposure Time [s]</th>
<th>Fatality Rate [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10 kW/m²</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>11</td>
</tr>
<tr>
<td>40</td>
<td>31</td>
</tr>
<tr>
<td>50</td>
<td>53</td>
</tr>
<tr>
<td>60</td>
<td>71</td>
</tr>
</tbody>
</table>

A.2. Nozzle Design

The design and effectiveness of spray nozzles vary depending on the application. In this section, some of the basic nozzle designs will be discussed. This will include the typical applications, advantages, and limitations of various common nozzle types. The primary purpose of spray nozzles is to control the atomization of the liquid – in this case the fuel for combustion. Differing nozzle types will produce differing droplet sizes and dispersion effects. The selection of an appropriate nozzle will usually depend on material properties, cost requirements, and project specifications about the combustion required. Spray nozzles are often evaluated according to the distribution of droplet size produces, spray angle, and spray pattern (full cone, hollow cone, fan, etc.). Figure A-1 shows the distinct spray patterns of various nozzle types. Cone shaped sprays are most common in combustion related applications.
The fuel type used can also affect the spray characteristics so experimental testing is necessary for appropriate nozzle selection. In general, spray nozzles are often broadly classified into two categories; \textit{pressure-atomizing nozzles} and \textit{twin-fluid nozzles}. In pressure-atomizing nozzles, liquid fuel passes through the nozzle and is atomized by the kinetic energy of the liquid as it passes through a significant pressure drop. These nozzles are most widely used as it is more energy efficient at producing surface area than twin-fluid types. Droplet size is controlled directly with pressure; as fluid pressure increases, kinetic energy increases and the droplet size decreases [5]. Table A-2 characterizes common types of pressure-atomizing nozzles.
Table A-2: Classification of pressure-atomizing nozzles. Arrows indicate fuel flow direction [5].

<table>
<thead>
<tr>
<th>Nozzle Type</th>
<th>Schematic</th>
<th>Spray Pattern</th>
<th>Common Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plain Orifice</td>
<td></td>
<td>Hollow Cone</td>
<td>Diesel engines</td>
</tr>
<tr>
<td>Pintle Nozzle</td>
<td></td>
<td>Full cone or multiple cones</td>
<td>Diesel engines, gas turbines</td>
</tr>
<tr>
<td>Swirl Nozzle (with spillback)</td>
<td></td>
<td>Hollow cone or Full cone</td>
<td>Furnaces, gas turbines</td>
</tr>
<tr>
<td>Impinging jet</td>
<td></td>
<td>Fan spray</td>
<td>Cleaning equipment, rocket engines</td>
</tr>
</tbody>
</table>

Twin-fluid nozzles atomize liquid fuel through the interaction of high velocity gas (usually air) and the liquid fuel. These nozzles have two separate streams for each medium and the atomization occurs where the streams mix. Compared to the single streamed counterparts, twin-fluid nozzles are capable of finer atomization, especially at low fuel flow rates and off-design operation. This type of spray nozzle is further classified into internal mixing and external mixing types. Intuitively, internal mixing nozzles contact the fluid streams inside the nozzle before ejection where shearing between the streams initializes atomization. External mixing nozzles contact the fluid streams outside the nozzle, post ejection. Internal mixing nozzles typically produce finer droplet sizes and use less atomizing gas than external ones, with air to water mass ratios ranging from 0.01 to 0.3 [5]. Table A-3 shows the two classifications of twin-fluid nozzles.
Table A-3: Classification of twin-fluid nozzles. Arrows indicate flow direction [5].

<table>
<thead>
<tr>
<th>Nozzle Type</th>
<th>Schematic</th>
<th>Spray Pattern</th>
<th>Common Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal Mixing</td>
<td><img src="image" alt="Internal Mixing Schematic" /></td>
<td>Hollow cone or full cone</td>
<td>Furnaces, gas turbines</td>
</tr>
<tr>
<td>External Mixing</td>
<td><img src="image" alt="External Mixing Schematic" /></td>
<td>Hollow cone</td>
<td>Furnaces, gas turbines</td>
</tr>
</tbody>
</table>

It is noted that there are other non-standard styles of atomizer nozzles not covered directly in this section. Examples of this could include ultrasonic atomizers (popular in medical fields) which use high frequency vibrations to atomize fluids in the fluid nozzle or rotary atomizers (popular in agriculture) that use rotating components to form a spray. These types of nozzles are not common in combustion related applications and have been omitted.

B. Computational Models and Codes

B.1. EES Flash Calculations

An EES (Engineering Equation Solver) model was developed to determine an acceptable mass flow rate of propane for a plain orifice nozzle of various diameters. This allows for appropriate inlet conditions to be set for the injection model in Fluent. A homogeneous equilibrium model was used which considers both the vapour and liquid propane at the same velocity. This model was selected for its simplicity. Other models such as the frozen liquid model, or models that include slip could be used for more detailed results, but the purpose of the tool was to get an appropriate estimate for typical experimental conditions. During an experiment, mass flow rate is likely to be determined directly from the apparatus and accompanying monitors, so the use of the EES model would be unnecessary.
In this model, saturated liquid propane in a reservoir at ambient temperature (state 1) exits a nozzle through an isentropic pressure drop with constant stagnation enthalpy (state 2). The flow at the nozzle becomes choked at a critical pressure ratio resulting in a maximum mass flow rate for a given nozzle diameter. The critical pressure ratio of the propane was determined to be $P_{crit} = 0.835$ using an iterative approach. Figure B-1 shows a simple drawing of the system being modelled. A T-s diagram of the system is shown in Figure B-2 (not to scale).

![Simplified schematic of the propane system showing the two states.](image1)

**Figure B-1:** Simplified schematic of the propane system showing the two states.

![T-s diagram of the isentropic propane flash from saturated liquid. Diagram is not to scale.](image2)

**Figure B-2:** T-s diagram of the isentropic propane flash from saturated liquid. Diagram is not to scale.

The area of the nozzle throat $A_t$ is calculated as a circle with diameter $d_t$.

$$A_t = \frac{\pi d_t^2}{4} \quad (B.1)$$
In state 1, the saturated liquid propane has a quality of \( X_1 = 0 \), and a temperature of \( T_1 = 20^{\circ}C \). The remaining thermodynamic properties of the propane in state 1 are determined by tabulated data in EES, namely the pressure \( P_1 \), enthalpy \( h_1 \), and entropy \( s_1 \). The isentropic pressure drop to state 2 to results in an enthalpy of \( s_2 = s_1 \). Pressure was determined from the critical pressure ratio.

\[
P_{\text{crit}} = \frac{P_2}{P_1} = 0.835 \quad \text{(B.2)}
\]

\[
P_2 = 0.835P_1 \quad \text{(B.3)}
\]

Given the pressure and enthalpy of state 2, the remaining thermodynamic properties are found from tabulated data, including density \( \rho_2 \). Velocity at the nozzle outlet \( v_2 \) is determined based on constant stagnation enthalpy.

\[
h_1 = h_2 + \frac{v_2^2}{2000} \quad \text{(B.4)}
\]

Finally, the mass flow rate through the nozzle is determined.

\[
\dot{m} = \rho_2 v_2 A_t \quad \text{(B.5)}
\]

With this set of equations, and the tabulated data in EES, the script can be used to calculate mass flow rate for any given nozzle of diameter \( d_t \). Table B-1 shows the thermodynamic properties for both states for a 4mm diameter nozzle. Resulting flow rates for nozzle diameters between 3mm and 6mm are shown in Table B-2. Nozzles of this scale are realistic for large scale field tests.

---

**Table B-1: EES results for a 4mm nozzle diameter case.**

<table>
<thead>
<tr>
<th>State</th>
<th>Pressure [kPa]</th>
<th>Temperature [C]</th>
<th>Density [kg/m³]</th>
<th>Quality</th>
<th>Enthalpy [kJ/kg]</th>
<th>Entropy [kJ/kg-K]</th>
<th>Velocity [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>836.6</td>
<td>20</td>
<td>499.8</td>
<td>0</td>
<td>252</td>
<td>1.181</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>698.6</td>
<td>13.3</td>
<td>196.6</td>
<td>0.049</td>
<td>251.5</td>
<td>1.181</td>
<td>30.53</td>
</tr>
</tbody>
</table>
Table B-2: Calculated flow rates for various lab type nozzle diameters.

<table>
<thead>
<tr>
<th>Nozzle Diameter [mm]</th>
<th>Rate [kg/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.043</td>
</tr>
<tr>
<td>4</td>
<td>0.076</td>
</tr>
<tr>
<td>5</td>
<td>0.119</td>
</tr>
<tr>
<td>6</td>
<td>0.171</td>
</tr>
</tbody>
</table>

The EES code used for this model is provided below.

"Propane Flash Calculations"

\[
d = 0.004 \text{ [m]}
\]
\[
A = \pi \left(\frac{d}{2}\right)^2
\]

"State 1 - Tank"

\[
T[1] = 20 \text{ [C]}
\]
\[
X[1] = 0
\]
\[
h[1] = \text{enthalpy(Propane, T=T[1], x=x[1])}
\]
\[
s[1] = \text{entropy(Propane, T=T[1], x=x[1])}
\]
\[
P[1] = \text{pressure(Propane, T=T[1], x=X[1])}
\]

"State 2 - Nozzle"

\[
s[2] = s[1]
\]
\[
\text{ratio} = 0.835
\]
\[
P[2] = P[1]\times\text{ratio}
\]
\[
X[2] = \text{quality(Propane, s=s[1], P=p[2])}
\]
\[
rho[2] = \text{density(Propane, s=s[1], P=p[2])}
\]
\[
h[2] = \text{enthalpy(Propane, s=s[1], P=p[2])}
\]
\[
h[1] = h[2] + \left(\frac{v[2]^2}{2}\right)\times\text{convert(J/kg,kJ/kg)}
\]
\[
mdot = \rho[2]\times v[2]\times A
\]
\[
\text{rate} = \text{mdot}\times\text{convert(kg/s,kg/hr)}
\]

B.2. Swirling Boundary Condition

A MATLAB code was developed to calculate the swirling velocity boundary conditions for a set number of concentric rings. The swirling boundary was based on a combined free and forced vortex model. This model is a continuous distribution of two vortex velocity profiles. Inside a defined radius \( R \) often called ‘the core’, a forced vortex profile is defined, with tangential velocity \( V_\theta \) directly proportional to radial
distance \( r \) i.e. solid body rotation with angular velocity \( \omega \). Outside of the core, a free vortex profile is defined and tangential velocity is inversely proportional to radius, defined by strength \( K \left[ \frac{m^2}{s} \right] \) which is based on the circulation \( \Gamma \left[ \frac{m^2}{s} \right] \). The tangential velocity is continuous at the boundary \( r = R \).

\[
V_\theta = \begin{cases} 
\omega r & r \leq R \\
\frac{K}{r} & r > R 
\end{cases}
\]  
(B.6)

\[Figure \ B-3: \text{Normalized tangential velocity profile for the swirling boundary condition.}\]

This swirl condition is only tangential meaning there is no radial outflow. The whole profile can be determined from a set core radius and desired maximum velocity noting that at the extent of the core \( K = \omega R^2 \). The non-linear nature of the tangential velocity outside the core cannot be defined on a 2D plane in Fluent. To approximate this profile a discrete number of rings were used, each with constant cylindrical velocity components. The MATLAB code takes inputs for core radius, maximum tangential velocity, and number of rings outside the core and returns the approximated profile of \( N \) constant tangential velocity
bands, where $N$ is the number of prescribed rings. As the free vortex profile is asymptotic, the code truncates the profile when ideal tangential velocity becomes lower than 10% of the maximum value.

Figure B-4, Figure B-5, and Figure B-6 display the discretized profiles generated for $N = 3$, 5, and 7 respectively. Note that the inner forced vortex profile can be defined ideally in Fluent.
Figure B-6: Normalized tangential velocity profiles for \( N=7 \).

The code also returns the necessary parameters to define the geometry and boundary conditions of the rings in the form of each ring radius, and its accompanying tangential velocity. The MATLAB code is provided below.

```matlab
%% Swirl Velocity Distribution Calculator
clear all
close all
clc

%% Inputs
rmax = 0.18; % radius of maximum velocity [m]
vmax = 1; % tangential velocity at rmax [m/s]
steps = 5; % number of approximation steps

%% Calculations
w = vmax/rmax; % calculate angular velocity of solid body rotation [rad/s]
K = w*rmax^2; % calculate K

pos = 0:0.01:rmax*10; % only accounts for velocities 10% and greater

for i=1:length(pos)
    if pos(i)<rmax
        vel(i)=w*pos(i);
    else
        vel(i)=K/pos(i);
    end
end

figure(1) % plot ideal curves
plot(pos,vel)
ylim([0 vmax*1.2])
```

Normalized Radial Distance

Normalized Tangential Velocity

Ideal Profile

Discretized Profile

0 1 2 3 4 5 6 7 8 9 10

0

0.2

0.4

0.6

0.8

1

Normalized Radial Distance

Normalized Tangential Velocity
x = 1; % initialize counter
for i=vmax/steps:vmax/steps:vmax
    binhigh = i; % calculate step velocities
    binlow  = binhigh-vmax/steps;
    for j=1:length(vel)
        if (vel(j)<=binhigh) && (vel(j)>binlow) && pos(j)>=rmax
            vel(j) = i-0.5*vmax/steps;
            dimen(1,x) = pos(j); % report step dimensions (r)
            dimen(2,x) = vel(j); % report step velocity
        end
    end
x = x+1; % step counter
end
dimen = fliplr(dimen) % report ring dimensions and velocities
hold on % plot approximation
plot(pos,vel,'.
xlabel('Radial Distance')
ylabel('Tangential Velocity')
legend('Ideal Profile','Discretized Profile')

B.3. Solid Flame Model Code

Provided below is the code used to complete the solid flame analysis. This code is based on the B-32 view factor as described in the exhaustive online database produced by Howell [25]. The code first solves for the view factor using an loop structure based on user defined dimensions. The resulting incident radiation is plotted over the range of interested using the formulation provided in 2.5.

clear all
close all
clc

% Solid Flame Model Calculation
% This code calculates the view factor B-32 for the solid flame model
% Target 1 - Flame 2
s = 2:0.1:15; % distance to target from flame center axis
D = 0.94; % equivalent flame diameter
r = D/2; % flame (cylinder) radius
h = 11.62; % flame (cylinder) height
for j = 1:length(s); % view factor calculation loop
    F12 = 0;
    F21 = 0;
    diff = 0.01;
        for x = diff/2:diff:0.5-diff/2
            for y = diff/2:diff:1-diff/2
                S = s(j)/r;
                X = x/r;
                Y = y/r;
                H = h/r;
                
            end
        end
    end
end

\begin{align*}
A &= X^2 + Y^2 + S^2; \\
B &= S^2 + X^2; \\
C &= (H-Y)^2; \\

P_1 &= \arccos\left(\frac{Y^2 - B + 1}{A - 1}\right) + \arccos\left(\frac{C - B + 1}{C + B - 1}\right); \\
P_2 &= Y \cdot \left(\frac{(A + 1)}{\sqrt{(A - 1)^2 + 4 \cdot Y^2}}\right) \cdot \arccos\left(\frac{Y^2 + B + 1}{B^0.5 \cdot (A - 1)}\right); \\
P_3 &= C \cdot 0.5 \cdot \left(\frac{(C + B + 1)}{\sqrt{(C + B - 1)^2 + 4 \cdot C}}\right) \cdot \arccos\left(\frac{C - B + 1}{B^0.5 \cdot (C + B - 1)}\right); \\
P_4 &= H \cdot \arccos\left(\frac{1}{B^0.5}\right); \\

F_{12iter} &= \left(\frac{S}{B} - \frac{S}{2 \cdot B \cdot \pi \cdot (P_1 - P_2 - P_3 + P_4)}\right) \cdot \text{diff}^2 / 0.5; \\
F_{12} &= F_{12} + F_{12iter}; \\
endend
F_{12} &= F_{12} \cdot 2; \% symmetry \\
A2 &= \pi r h; \% exposed surface area \\
F_{21} &= F_{12} / A2; \% reciprocity \\

T &= 1400; \% temperature \\
emm &= 0.45; \% emissivity \\
sig &= 5.67 \cdot 10^{-8}; \% SB constant \\
H &= 60; \% rel humidity \\
\tau &= 0.79 \cdot (100. / H)^{(1/16)} \cdot (30.5 / (s(j) - r))^{(1/16)}; \% calculate \tau \\
E &= \text{emm} \cdot \text{sig} \cdot T^4; \% emissive power \\
I(j) &= F_{21} \cdot E \cdot \tau; \% resulting incident radiation \\
endend

plot(s, I / 1000) \% plot results \\
xlabel('Distance from Flare Axis [m]') \\
ylabel('Incident Thermal Flux [kW/m^2]')

\textbf{C. Additional CFD Material}

\textbf{C.1. Grid Independence Study}

A grid independence study is necessary to study the impact of changing the mesh density on variables of interest. In this work three meshes were used of increasing densities - roughly 0.9 million, 2.1 million, and 3.4 million cells. Key variables are evaluated and compared on each grid. The method used in this work is the \textit{Celik Grid Convergence Index} (GCI) method [26]. The GCI method is based on Richardson extrapolation and has been widely evaluated on a variety of CFD cases. A basic overview of the formulation for this method is provided here, but full details are provided in literature. To complete this analysis, a MATLAB script written and validated by Maverick Zawislak was used.
The first step involves selecting a representative cell size \( h \) for each mesh. In this work, the representative size was considered as the local cell size within the flare region, as this is where measurements are taken. With \( h_1 < h_2 < h_3 \), \( r_{xy} = \frac{h_y}{h_x} \), and \( \varepsilon_{xy} = \phi_x - \phi_y \) the apparent order of the fit \( p \) is determined as follows, where \( \phi_x \) is any measured value, say temperature or pressure, on the \( x^{th} \) mesh. Here, \( q(p) \) provides an offset, and \( s \) is a sign function to handle oscillations.

\[
\begin{align*}
    p &= \frac{1}{\ln(r_{21})} \left| \ln \left( \frac{\varepsilon_{32}}{\varepsilon_{21}} \right) \right| + q(p) \\
    q(p) &= \ln \left( \frac{r_{21}^p - s}{r_{32}^p - s} \right) \\
    s &= 1 \cdot sgn \left( \frac{\varepsilon_{32}}{\varepsilon_{21}} \right)
\end{align*}
\]

The extrapolated values for the metrics of interest \( \phi_{ext}^{xy} \) are then solved, that is the project value for an infinitely resolved mesh, along with an accompanying relative error \( e_{a}^{xy} \), an extrapolated error \( e_{ext}^{xy} \). Finally and the fine CGI is determined. The CGI is a percentage measure of how far the computed value is from the asymptotic value, or what percentage change would be seen in that value if the mesh was infinitely refined.

\[
\begin{align*}
    \phi_{ext}^{21} &= \frac{r_{21}^p \phi_1 - \phi_2}{r_{21}^p - 1} \quad (C.4) \\
    e_{a}^{21} &= \left| \frac{\phi_1 - \phi_2}{\phi_1} \right| \quad (C.5) \\
    e_{ext}^{21} &= \left| \frac{\phi_{ext}^{21} - \phi_1}{\phi_{ext}^{21}} \right| \quad (C.6) \\
    CGI_{fine}^{21} &= \frac{1.25e_{a}^{21}}{r_{21}^p - 1} \quad (C.7)
\end{align*}
\]
For this study, the metrics of interest selected include the flame surface area, incident radiation on the 6m target, temperature taken at the third monitor, and a measurement of soot volume fraction. Table C-1 displays these values for each grid used in the study. The results of the analysis are summarized in Table C-2.

<table>
<thead>
<tr>
<th>Grid Number</th>
<th>Cell Count (10^6)</th>
<th>(h)</th>
<th>Flame Area (m²)</th>
<th>Target Rad (kW/m²)</th>
<th>Temperature (K)</th>
<th>Soot Volume Fraction (10^-6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.4</td>
<td>0.02</td>
<td>34.6</td>
<td>2.41</td>
<td>1659.2</td>
<td>2.12</td>
</tr>
<tr>
<td>2</td>
<td>2.1</td>
<td>0.12</td>
<td>36.4</td>
<td>2.43</td>
<td>1586.9</td>
<td>2.10</td>
</tr>
<tr>
<td>3</td>
<td>0.9</td>
<td>0.30</td>
<td>36.0</td>
<td>2.56</td>
<td>1611.4</td>
<td>4.03</td>
</tr>
</tbody>
</table>

Table C-2: Results from the independence study.

<table>
<thead>
<tr>
<th>Value</th>
<th>Target Radiation</th>
<th>Temperature</th>
<th>Flame Area</th>
<th>Soot Volume Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>(p)</td>
<td>2.04</td>
<td>0.45</td>
<td>0.54</td>
<td>5.07</td>
</tr>
<tr>
<td>(\phi_{ext}^{21})</td>
<td>2.41</td>
<td>1716.7</td>
<td>33.5</td>
<td>2.12\times10^{-6}</td>
</tr>
<tr>
<td>(e_{a}^{21})</td>
<td>&lt; 1%</td>
<td>4.3%</td>
<td>5.2%</td>
<td>&lt; 1%</td>
</tr>
<tr>
<td>(e_{ext}^{21})</td>
<td>&lt; 1%</td>
<td>3.5%</td>
<td>3.2%</td>
<td>&lt; 1%</td>
</tr>
<tr>
<td>(GCI_{fine}^{21})</td>
<td>&lt; 1%</td>
<td>3.4%</td>
<td>3.9%</td>
<td>&lt; 1%</td>
</tr>
</tbody>
</table>
C.2. Sample Script

A sample script that was used to run the Fluent process on the CAC is provided below. The scripts first function is to open the Fluent case file which has all of the data for solution generation. The script is also responsible for setting up the monitors used during solution generation, and also setting the URFs. The URF values are lowered after a set number of iterations.

```
rc 3.4test.cas

/solve/set/under-relaxation pressure 0.2
/solve/set/under-relaxation density 0.2
/solve/set/under-relaxation body-force 0.2
/solve/set/under-relaxation mom 0.2
/solve/set/under-relaxation k 0.5
/solve/set/under-relaxation epsilon 0.5
/solve/set/under-relaxation turb-viscosity 0.5
/solve/set/under-relaxation enthalpy 0.5
/solve/set/under-relaxation temperature 0.9
/solve/set/under-relaxation fmean 0.9
/solve/set/under-relaxation fvar 0.9
/solve/set/under-relaxation dpm 0.2
/solve/set/under-relaxation pollutant-12 0.8
/solve/set/under-relaxation pollutant-13 0.8

/surface/point-surface/centerline-1m 0 0 2
/surface/point-surface/centerline-2m 0 0 3
/surface/point-surface/centerline-3m 0 0 4
/surface/point-surface/centerline-4m 0 0 5
/surface/point-surface/centerline-6m 0 0 7
/surface/point-surface/centerline-8m 0 0 9
/surface/plane-bounded/radtarget1 -2 -0.5 0.5 -2 0.5 0.5 -2 0.5 1.5 no
/surface/plane-bounded/radtarget2 -4 -0.5 0.5 -4 0.5 0.5 -4 0.5 1.5 no
/surface/plane-bounded/radtarget3 -6 -0.5 0.5 -6 0.5 0.5 -6 0.5 1.5 no
/surface/plane-bounded/radtarget4 -10 -0.5 0.5 -10 0.5 0.5 -10 0.5 1.5 no
/surface/plane-bounded/radtarget5 -15 -0.5 0.5 -15 0.5 0.5 -15 0.5 1.5 no

/solve/monitors/surface/set-monitor
mass-flux
"Mass Flow Rate"
wall1 wall2 wall3 wall4 roof ()
no yes yes massflux 1

/solve/monitors/surface/set-monitor
total-radiation
"Integral"
incident-radiation
wall1 wall2 wall3 wall4 roof floor solid one two three four five ()
no yes yes radtotal 1

/solve/monitors/surface/set-monitor
target-radiation1
"Integral"
incident-radiation
radtarget1 ()
```
no yes yes radtarget1 1
/solve/monitors/surface/set-monitor
target-radiation2
"Integral"
incident-radiation
radtarget2 ()
no yes yes radtarget2 1
/solve/monitors/surface/set-monitor
target-radiation3
"Integral"
incident-radiation
radtarget3 ()
no yes yes radtarget3 1
/solve/monitors/surface/set-monitor
target-radiation4
"Integral"
incident-radiation
radtarget4 ()
no yes yes radtarget4 1
/solve/monitors/surface/set-monitor
target-radiation5
"Integral"
incident-radiation
radtarget5 ()
no yes yes radtarget5 1
/solve/monitors/surface/set-monitor
point1-temp
"Vertex Average"
temperature
centerline-1m ()
no yes yes t1 1
/solve/monitors/surface/set-monitor
point2-temp
"Vertex Average"
temperature
centerline-2m ()
no yes yes t2 1
/solve/monitors/surface/set-monitor
point3-temp
"Vertex Average"
temperature
centerline-3m ()
no yes yes t3 1
/solve/monitors/surface/set-monitor
point4-temp
"Vertex Average"
temperature
centerline-4m ()
no yes yes t4 1
/solve/monitors/surface/set-monitor
point6-temp
"Vertex Average"
temperature
centerline-6m ()
no yes yes t6 1

/solve/monitors/surface/set-monitor
point8-temp
"Vertex Average"
temperature
centerline-8m ()
no yes yes t8 1

/solve/monitors/volume/set-monitor
sootvol
"Volume Integral"
soot-volume-fraction
fluid ()
no yes yes sootvol 1

/solve/iterate 5000

/solve/set/under-relaxation pressure 0.2
/solve/set/under-relaxation density 0.2
/solve/set/under-relaxation body-force 0.2
/solve/set/under-relaxation mom 0.2
/solve/set/under-relaxation k 0.3
/solve/set/under-relaxation epsilon 0.3
/solve/set/under-relaxation turb-viscosity 0.3
/solve/set/under-relaxation enthalpy 0.3
/solve/set/under-relaxation temperature 0.6
/solve/set/under-relaxation fmean 0.6
/solve/set/under-relaxation fvar 0.6
/solve/set/under-relaxation dpm 0.2
/solve/set/under-relaxation p1 0.5
/solve/set/under-relaxation pollutant-12 0.4
/solve/set/under-relaxation pollutant-13 0.4

/solve/iterate 3000

/solve/set/under-relaxation pressure 0.2
/solve/set/under-relaxation density 0.2
/solve/set/under-relaxation body-force 0.2
/solve/set/under-relaxation mom 0.2
/solve/set/under-relaxation k 0.2
/solve/set/under-relaxation epsilon 0.2
/solve/set/under-relaxation turb-viscosity 0.2
/solve/set/under-relaxation enthalpy 0.2
/solve/set/under-relaxation temperature 0.4
/solve/set/under-relaxation fmean 0.4
/solve/set/under-relaxation fvar 0.4
/solve/set/under-relaxation dpm 0.2
/solve/set/under-relaxation p1 0.5
/solve/set/under-relaxation pollutant-12 0.3
/solve/set/under-relaxation pollutant-13 0.3

/solve/iterate 1000

/file/write-data 3.4test7
exit
yes