University of Nevada, Reno

Experimental Benchmark of Computational Fluid Dynamics Models
to Predict Used Nuclear Fuel Cladding Temperatures during
Vacuum Drying Conditions

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by

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Abstract

Vacuum drying of a used nuclear fuel (UNF) canister, in which helium pressure is considerably reduced, is an important process the UNF undergo after it is removed from water and the canister is filled with helium. During this process, the temperature of the fuel claddings may considerably increase because it is the first time the fuel is transferred from a water cooled environment to a lower thermal conductivity helium environment while its heat generation is still relatively high. The low pressures associated with vacuum drying also contribute to the increase of temperature due to rarefaction effect. It is essential to keep the temperature of the fuel claddings below certain limits (roughly 400°C) to avoid temperature-dependent phenomena, such as corrosion and radial hydride formation, which has the potential to decrease the ductility of the claddings and make them unsafe for transportation and long-term storage.

This dissertation aims to develop a computational fluid dynamics (CFD) model that can be used to predict the temperature of UNF canisters during vacuum drying process by including the effect of gas rarefaction. The CFD model is first compared to two kinetic models that solve the Boltzmann equation (Direct simulation Monte Carlo, DSMC, and Shakhov S-model) in simple geometries. The model is then validated against measurements from an experimental setup that consists of a 7×7 array of heater rods enclosed in a stainless steel square cross section pressure vessel and maintained between two spacer plates. The CFD model was able to predict the temperature of the heater rods in all rarefaction regimes.
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<thead>
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<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>B</td>
<td>Coefficient of thermal expansion of gas</td>
</tr>
<tr>
<td>b</td>
<td>Intercept of best-fit line</td>
</tr>
<tr>
<td>$c_r$</td>
<td>Relative speed of simulated particle</td>
</tr>
<tr>
<td>$D$</td>
<td>Sample standard deviation for 95% confidence interval</td>
</tr>
<tr>
<td>$E_{95}$</td>
<td>Standard estimate of error for 95% confidence interval</td>
</tr>
<tr>
<td>$F_N$</td>
<td>No. of real molecule indicated by a single simulation particle</td>
</tr>
<tr>
<td>$f$</td>
<td>Velocity distribution function</td>
</tr>
<tr>
<td>$Gr$</td>
<td>Grashof number</td>
</tr>
<tr>
<td>$I$</td>
<td>Insulation thickness</td>
</tr>
<tr>
<td>$Kn$</td>
<td>Knudsen number</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann’s constant</td>
</tr>
<tr>
<td>$M$</td>
<td>Mass of a molecule of gas</td>
</tr>
<tr>
<td>$m$</td>
<td>Slope of best fit line</td>
</tr>
<tr>
<td>$n$</td>
<td>Number density of molecules</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$p$</td>
<td>Non-dimensional pressure</td>
</tr>
<tr>
<td>$p'$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$p_0$</td>
<td>Reference pressure</td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat generation rate</td>
</tr>
<tr>
<td>$q$</td>
<td>Non-dimensional heat flux</td>
</tr>
<tr>
<td>$q'$</td>
<td>Heat flux</td>
</tr>
<tr>
<td>$R$</td>
<td>Radius ratio</td>
</tr>
<tr>
<td>$R'$</td>
<td>Dimensional radius of wall</td>
</tr>
<tr>
<td>$r$</td>
<td>Non-dimensional radius</td>
</tr>
<tr>
<td>$S$</td>
<td>Standard estimate of error</td>
</tr>
<tr>
<td>$T$</td>
<td>Non-dimensional temperature</td>
</tr>
<tr>
<td>$T_{w}'$</td>
<td>Dimensional temperature of wall</td>
</tr>
<tr>
<td>$\bar{T}$</td>
<td>Average temperature</td>
</tr>
</tbody>
</table>
\( T \) - Temperature ratio
\( T_0 \) - Reference temperature
\( x, y, z \) - Three axes in Cartesian coordinate
\( \alpha \) - Thermal accommodation coefficient
\( \delta \) - Gas rarefaction parameter
\( \kappa \) - Conductivity
\( \lambda \) - Mean free path
\( \mu \) - Viscosity
\( \nu \) - Molecular velocity
\( \rho \) - Density
\( \sigma \) - Collision cross section
\( \omega \) - Viscosity index
\( \xi_T \) - Temperature jump coefficient
\( \vartheta' \) - Molecular collision frequency

**Subscript**

0 - reference
amb - ambient
B - bottom spacer plate
b - bottom
HR - heater rod
m - measured
max - maximum
min - minimum
r - radial distance from center
SP - spacer plate
s - simulated
T - top spacer plate
t - top
W - wall
CHAPTER I

INTRODUCTION

Nuclear fuel assemblies consist of Zircaloy cladding rods that contain highly radioactive uranium dioxide (UO$_2$) fuel pellets and high-pressure fission products and fill gases. The fuel rods are held in a square array of 7×7 to 18×18 by headers, footers and periodic spacer plates to form a fuel assembly.

Following removal from a nuclear reactor, used nuclear fuel (UNF) assemblies are stored underwater, in a water pool, to reduce their radioactivity and heat generation rate [1, 2]. After few years, a canister with an internal basket is placed in a transfer cask and both are lowered into the water pool. The canister is then loaded with the fuel assemblies, sealed, lifted out of the pool and drained. Small amount of water may remain at the bottom of the canister, crevices of the canister and cladding surfaces after draining. All the remaining moisture must be removed to avoid any corrosion or formation of combustible mixture of hydrogen and oxygen before the canister is filled with helium (or nitrogen) and transported to long-term storage facility.

Federal regulations (10CFR72) require that during long-term storage, the fuel configuration remains subcritical, confined and contained, and retrievable. The cladding is the primary barrier for the used fuel pellets and fission gas. Its integrity must be protected to assure that, after decades in storage, the assemblies can be safely transferred to other packages, and/or transported to other locations. The requirement of Federal regulations for
drop and hypothetical accidental condition tests, that include 0.3 m and 9 m drop, require adequate ductility of the cladding.

During reactor time, hydrogen resulting from water radiolysis precipitates into the cladding, forming zirconium hydride precipitates. The coolant pressure in the reactor is relatively high and the pressure difference across the cladding and the hoop stress within the cladding are low. Because of this, the zirconium hydrides are preferentially oriented in the circumferential direction. This orientation does not significantly affect the cladding ductility. During transfer and early dry storage, the pressure difference across the cladding, and the resulting hoop stresses within it, are relatively high due to the high temperature of the contained gases and relatively low external pressure. In long-term dry storage, the fuel heat generation rate decreases, causing the temperature of the UNF to slowly decline. This causes the hoop stress and hydrogen solubility within the cladding to simultaneously decrease. However, if the initial hoop stress and temperature of the cladding (during drying, loading and transferring operations) are sufficiently high, the circumferential hydrides that in the cladding may dissolve and form radial hydrides. The cycles of increasing and decreasing cladding temperature, which may occur during the drying process, can also increase the amount of dissolved hydrogen available for precipitation into radial hydrides. This orientation may affect the cladding ductility and cause them to become brittle.

Nuclear Regulatory Commission Interim Staff Guidance-11, Revision 3 (ISG-11) [3] specifies criteria that are intended to prevent radial hydride formation. For example, the maximum calculated fuel cladding temperature must remain below 400 °C for normal conditions of storage and short term loading operations like drying, backfilling with inert gas and transferring to storage pad. For low burnup fuel, a higher short term temperature
limit may be used, provided that the best estimate cladding hoop stress is limited to 90 MPa for the proposed temperature limit. During loading operations, repeated temperature cycling is allowed; but should be limited to less than 10 cycles if cladding temperature variations are higher than 65 °C. For off-normal conditions, the maximum cladding temperature should not exceed 570 °C, based on creep (stress) rupture consideration.

The UNF assemblies may experience their highest temperature during drying process because it is the first operation when the fuel assemblies are removed from water cooled environment to a relatively lower thermal conductivity helium environment while their heat generation rates are still relatively high. Vacuum drying is widely used to remove moisture from the fuel canisters [4]. During this process, helium pressure is reduced to as low as 67 Pa to promote evaporation and removal of water [5, 6]. At these low pressure, the temperature of the fuel claddings may considerably increase because of the rarefaction effect, which induces a temperature-jump thermal resistance at the solid-gas interfaces [7, 8]. It is important to accurately predict the peak cladding temperatures during vacuum drying operation to determine the maximum allowable heat generation rate of the fuel assemblies that can be safely stored in a canister, and their required underwater storage time. Over-conservatism in these calculations can lead to overly long storage times, especially for high-burnup fuel.

Package vendors typically use whole-canister simulations to calculate the peak cladding temperatures during drying and storage operations. These simulations use computational domains in which the fuel assemblies are replaced by smeared regions with effective thermal conductivities and effective flow porosities [5, 9]. The effective conductivity is determined to give the same peak fuel temperatures as simulations that use
more geometrically-accurate meshes, and model conduction though the fuel rods and basket walls, and conduction and surface-to-surface radiation across the gas-filled regions. However, the effective porosity is used to model buoyancy induced gas motion and the resulting natural convection heat transfer. These models have been validated [10] against temperature measurements performed in actual vertical and horizontal storage packages pressurized to 158 kPa with helium or nitrogen, and under vacuum conditions (as low as 110 Pa) [11, 12]. However, they do not include the effect of gas rarefaction (temperature-jump) during vacuum drying [10]. While the cladding temperature calculations have been validated, the fuel heat generation rate in the tested package was lower than that expected for high-burnup fuel.

In recent works [13, 14], the authors attempted to model a used nuclear fuel canister subjected to vacuum drying conditions and they included the effect of gas rarefaction. The modeled canister was a TN-24 loaded with 24 Westinghouse 15×15 used nuclear fuel assemblies. The results showed that the peak cladding temperature (PCT) increased as the pressure inside the canister is decreased from atmospheric pressure to 100 Pa. The increase was due to the effect of gas rarefaction and was as high as 73°C.

1.1 Gas Rarefaction

Gas rarefaction occurs when the average distance travelled by gas molecules between two successive collisions (also known as the mean free path, \( \lambda \)) is comparable or larger than the characteristic length \( (L_c) \) of a system. In this condition, the continuum fluid approximation breaks down and the particle nature of fluid must be taken into account. Using the hard sphere intermolecular collision model, the mean free path can be written as
\[
\lambda = \mu \frac{\sqrt{2k_B T}}{P} \sqrt{M}
\]  

(1.1)

where \( \mu \) is the temperature dependent gas viscosity, \( P \) is the pressure, \( k_B \) is the Boltzmann constant, \( M \) is the molecular mass and \( T \) is the temperature.

The ratio of the mean free path to the characteristic length of the system is defined as the Knudsen number

\[
Kn = \frac{\lambda}{L_C}
\]  

(1.2)

The Knudsen number is used to characterize the rarefaction level of a gas. Using this parameter, four regimes of rarefaction may be distinguished:

i. Continuum regime \( (Kn \leq 10^{-3}) \): The number of molecules are high enough and the flow and heat transfer can be accurately modeled using Navier-Stokes and conductive energy equation.

ii. Slip regime \( (10^{-3} \leq Kn \leq 10^{-1}) \): The Navier-Stokes and Fourier equations are still valid but conditions of velocity-slip and temperature-jump at the wall must be used. The number of collision between wall and molecules are reduced.

iii. Transitional regime \( (10^{-1} \leq Kn \leq 10) \): The flow needs to be modeled using the collisional Boltzmann equation as the collision between the molecules are highly reduced. The continuum methods like Navier-Stokes equation are not valid.

iv. Free molecular regime \( (10 \leq Kn) \): The gas is rarefied to the extent that the collision between molecules is negligible compared to collision with wall. The flow can be modeled using the collisionless kinetic Boltzmann equation.
Figure 1.1 shows the regimes of rarefaction categorized by the Knudsen number. Because of the low pressures associated with vacuum drying and the inner dimensions of the used nuclear fuel canisters, helium is in the slip regime. Under this regime, there is a temperature-jump between the solid surfaces and gas in contact with them. This jump acts like a thermal-resistance for heat conduction [7, 15-17]. As a result, the temperature inside the canister is higher during low-pressure condition than at normal or atmospheric pressure (continuum regime) condition.

### Table 1.1: Flow regimes categorized by Knudsen number

<table>
<thead>
<tr>
<th>Hydrodynamic Regime</th>
<th>Slip Regime</th>
<th>Transitional Regime</th>
<th>Free Molecular Regime</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>0.1</td>
<td>10</td>
<td>100</td>
</tr>
<tr>
<td>Kn</td>
<td></td>
<td></td>
<td>Free Mol. Limit</td>
</tr>
</tbody>
</table>

**Boltzmann Equation**
- Navier-Stokes Equation
- NS -extended bc

**Collisionless B.E.**

1.2 **Temperature Jump Boundary Condition**

In the slip regime, the collisions between the gas molecules are sufficiently high to model the gas in the bulk of the system as a continuum. However, the number of collisions between gas molecules and the walls is not enough for the gas molecules to reach equilibrium with the wall. Therefore, an abrupt change of temperature from surface to the gas occurs. This phenomenon is known as temperature-jump. As a result, the Navier Stokes equation can accurately model the momentum and energy transport away from the wall but temperature jump boundary condition must be used at the gas-wall interfaces [7, 18].
The temperature jump boundary condition can be expressed as [19]

\[ T_g = T_w + \xi_T \lambda \frac{dT}{dr}
\]

where, \( T_g \) is temperature of the gas at wall interface, \( T_w \) is wall temperature and \( \xi_T \) is temperature jump coefficient. Different expressions for the temperature jump coefficient \( \xi_T \) are proposed in the literature [20, 21]. In this study, the expression proposed by Welander [22] for monatomic gas, which was later generalized for polyatomic gases by Lin and Willis [23] is used. This expression reads

\[ \xi_T = \left( \frac{2 - \alpha}{\alpha} + 0.17 \right) \sqrt{\frac{\pi}{Pr}} \frac{\gamma}{\gamma + 1} \]

where, \( Pr \) is the Prandtl number, \( \gamma \) is the specific heat ratio of gas and \( \alpha \) is the thermal accommodation coefficient.

1.3 Thermal Accommodation Coefficient

At low-pressure condition, the collision that occurs between gas molecules and surfaces dominate the molecules-molecules collision. Under these conditions the local thermodynamic equilibrium and the continuity of temperature at the wall is not achieved, which is known as the temperature-jump conditions. The effect of temperature-jump was experimentally investigated by Smoluchowski but the concept of the accommodation coefficient was introduced by Maxwell [24]. He postulated that when the molecules collide with the surface, a range of possible interactions can take place depending upon the temperature of incident \( T_i \) and reflected \( T_r \) molecules as

\[ \alpha = \frac{T_i - T_r}{T_i - T_W} \]
where, \( T_W \) is temperature of the wall. The value of \( \alpha \) varies from 0 to 1. In case of \( \alpha \) equal to 1, the molecules are reflected diffusely i.e. the reflected molecule accommodates to the condition of the wall, whereas, in case of \( \alpha \) equal to 0, the molecules are reflected specularly without transferring any thermal energy to the wall. As the value of \( \alpha \) decreases, there is a larger temperature-jump at the solid-gas interface (see Eqn. 1.4). The value of \( \alpha \) depends on the type of gas molecule and surface it is interacting with. The value of \( \alpha \) for different gas molecules on different surfaces have been determined by experimental methods [25-28]. For helium and stainless steel \( \alpha \) is reported between 0.4 and 0.2, for temperature ranging from 0 to 700°C. Its value decreases with increase in temperature [28].

1.4 Objective of the Dissertation

The goal of this dissertation is to validate computational fluid dynamics (CFD) models that can be used to accurately predict the temperature of UNF canisters during vacuum drying process by including the effect of gas rarefaction. The working gas considered in this dissertation is dry helium and the effect of water vapor present in the canister during vacuum drying is not taken into account.

To achieve the goal mentioned above, a comparison between results from CFD simulations and two kinetic models that solve the Boltzmann equation (Direct simulation Monte Carlo, DSMC, and Shakhov S-model) in simple geometries (concentric cylinders and parallel plates) that contain rarefied gas in the slip regime is conducted. This comparison is carried out to check the validity of the CFD simulations in simple 1-D and 2-D geometries. The next step is to validate the CFD simulations against measurements in the continuum regime. Results from experiments conducted by Chalasani et al. [29] are
used for validation purpose. A different experimental setup that consists of a 7×7 array of heater rods enclosed in a stainless steel square cross section pressure vessel and maintained between two spacer plates is constructed. Experiments are conducted for pressures and heat generation rates relevant to vacuum drying conditions of a UNF canister. The results from these experiments are used to validate the CFD simulations in the slip regime.
CHAPTER 2

CFD VALIDATION IN SLIP REGIME IN SIMPLE GEOMETRIES

In this chapter, the CFD simulation for heat transfer across simple 1-D geometries (concentric cylinder and parallel plates) are validated against highly accurate numerical methods solving simplified Boltzmann equation. Shakhov (S-) model kinetic equation using discrete velocity method and Direct Simulation Monte Carlo (DSMC) method are used as methods with high accuracy. The results are compared for variation in parameters like rarefaction, thermal accommodation coefficient, temperature ratio and radius ratio. The results of this comparison provides an idea on limitation of use of CFD simulations. The accuracy of CFD simulation is highly dependent on all the parameters, varied for this study. The result of 1-D geometry presented in this chapter has been published [30]. Similar study for a simple two-dimensional geometry is also conducted and compared with CFD simulation. The chapter starts with brief description of numerical methods solving Boltzmann equation.

2.1 Boltzmann Equation

The Boltzmann equation describes the flow in all regimes from continuum to free molecular. Limiting case of this equation at extremely small mean free path gives the continuum description provided by the Navier-Stokes equation and at large mean free path gives the collisionless Boltzmann equation.

The Boltzmann equation for simple dilute gas is [31, 32]
\[
\frac{\partial}{\partial t} (nf) + \mathbf{v} \cdot \frac{\partial}{\partial r} (nf) + F \cdot \frac{\partial}{\partial \mathbf{v}} (nf) = \int_{-\infty}^{\infty} \int_{0}^{4\pi} n^2 (f^* f_1 - f f_1) \nu r \sigma d \Omega d c_1
\] (2.1)

where \( n \) is number density, \( f \) is velocity distribution function, \( \mathbf{v} \) is molecular velocity, \( \nu r \) is relative molecular speed, \( F \) is external force per unit mass, (*) indicates post collision values, \( f \) and \( f_1 \) represent the distribution function of two different types of molecules of class \( c \) and \( c_1 \), \( \sigma \) is collision cross section of molecule, \( t \) represents time, \( r \) represents physical space and \( \Omega \) represents solid angle.

The term on the right is collision term and is represented as \( Q(f, f^*) \). The difficulty associated with solving Boltzmann equation is in this term. To reduce this difficulty the collision integral is replaced by a relaxation term as:

\[
Q(f, f^*) = I(f, f_{mod}) = \frac{f_{mod} - f}{\tau}
\] (2.2)

where, \( f_{mod} \) is a model distribution function [33]. This distribution function depends on the type of kinetic model used. Different models have been proposed like BGK, S-model and Ellipsoidal (ES) model [34-36]. A brief description of S-model is given below.

### 2.1.1 S-Model Kinetic Equation

In steady state, and without any external force on the fluid, the S-model kinetic equation is

\[
\mathbf{v} \frac{\partial f'}{\partial r'} = \vartheta'(f^{s'} - f')
\] (2.3)

where, \( f'(r', \mathbf{v}) \) is one particle molecular velocity distribution function, \( \vartheta' \) is the molecular collision frequency. The equilibrium distribution function \( f^{s'} \) is
\[ f^{S'} = f^{M'} \left[ 1 + \frac{2mVq'}{15n'(k_BT')^2} \left( \frac{MV^2}{2k_BT'} - \frac{5}{2} \right) \right] \quad (2.4) \]

\[ f^{M'}(n', T') = n' \left( \frac{M}{2\pi k_BT'} \right)^{3/2} \exp \left[ -\frac{M(v - u')^2}{2k_BT'} \right] \quad (2.5) \]

where, \( f^{M'} \) is the local Maxwellian distribution function, \( u' \) is the bulk velocity vector, \( V = v - u' \) is the peculiar velocity vector and \( q' \) is the heat flux vector.

In the frame of this model, the molecular collision frequency is assumed to be independent of the molecular velocities and may be found as follows [35]

\[ \theta' = \frac{p'}{\mu'} \quad (2.6) \]

where, \( p' \) is pressure and \( \mu' \) is viscosity of the fluid. The macroscopic parameters are then calculated from the solution of the molecular distribution function \( f' \) obtained by solving eqn (2.4) as

\[ T'(r') = \frac{M}{3n' k_B} \int \int V^2 f'(r', \nu) d\nu \quad (2.7) \]

\[ q'(r') = \frac{M}{2} \int \int VV^2 f'(r', \nu) d\nu \quad (2.8) \]

The Discrete Velocity Method (DVM) is used to divide the continuum-molecular velocity space in the system of kinetic equations into a discrete velocity set.

### 2.1.2 Direct Simulation Monte Carlo Method

The traditional DSMC technique proposed by Bird [31] is employed in this dissertation. This technique enables gas flows to be modeled on a molecular level by simulating the motion of individual particles according to their physical properties. It can
be viewed as a Monte Carlo method for solving the time-dependent nonlinear Boltzmann equation.

A dilute gas is considered for DSMC, where dilute gas refers to gas that cover only a small portion of the space i.e. $\delta >> d$, where $\delta = n^{-1/3}$ is the mean molecular spacing and $d$ is the diameter of the molecules. In such gas, each molecule will move outside the range of influence of other molecule. This consideration is important because it allows collision process to be realized between only two molecules at a time. The other assumption is molecular chaos i.e. the probability of finding a pair of molecules in a two-particle configuration is simply the product of probabilities of finding each molecule in the corresponding one particle configuration.

DSMC comprises of deterministic modeling of particle motion with statistical approach for computing collisions between particles. The standard DSMC [31] makes use of time splitting scheme. The real process is divided into two steps that are decoupled:

- Motion of particle is applied for certain time $\Delta t$ where velocities are unchanged but position is changed.
- Collision between particles, where molecular velocities are changed but the position is unchanged.

The basic DSMC technique is discretization of space and time domain. The gas is represented by discrete number of particles that are combination of a huge number of real molecules in terms of size and mass. In summary, the process can be divided into following:

1. *Initialization*
The time interval is divided into $n_t$ with $\Delta t$ time steps. Similarly, the space is also divided into $n_x$ cells with $\Delta x$ size. The gas molecules are simulated in the gap stochastically with $x_i$ position and $z_i$ velocity. Each particle represents a certain number of real molecules. The main computational approximations associated is to select the proper ratio of real to simulated molecules, time step ($\Delta t$) which is smaller than mean collision time and cell size ($\Delta x$) which is smaller than mean free path ($\lambda$). In general, the rule of thumb for the step sizes are:

$$\Delta t < t/3, \Delta x < \lambda/3; \text{number of particles in cell} > 30$$

2. **Collision**

The collision between molecules is binary which is computed without moving the molecules. This step is the most complex one and is crucial to the consistency of the simulation. If $V_c$ is considered volume of a cell and number density be $n$, the cell contains $nV_c$ real molecules and the average number of simulated particles is given by $N = nV_c/F_N$. The probability of a collision between two particles is proportional to the product of their relative speed ($c_r$) and collision cross-section ($\sigma_T$). The total number of collisions per unit time per unit volume of gas is expressed as

$$N_c = \frac{1}{2} n^2 c_r \sigma_T$$

(2.9)

Many efforts have been made to improve the original time counter scheme. No time counter (NTC) scheme proposed by Bird [31] is used widely. The probability of collision between two simulated molecules over the time interval, $\Delta t$ is equal to the ratio of volume swept by the total cross section of the colliding molecules at the relative speed, $c_r$ to the volume of the cell.
\[
p = \frac{F_N \sigma_T c_r \Delta t}{V_c} \quad (2.10)
\]

The probability can be calculated for a set of all \(N(N-1)/2\) potential collision pairs. However, it is inefficient because \(p\) is generally a very small number and computational time is proportional to the square of the number of molecules in the cell. In NTC method, only a fraction of all possible collision pairs is considered and the resultant probability is increased by dividing eqn. (2.10) by the fraction

\[
p_{max} = \frac{F_N (\sigma_T c_r)_{max} \Delta t}{V_c} \quad (2.11)
\]

As \(N\) is not constant, \(N(N-1)\) is replaced by the product of instantaneous value and a time or ensemble averaged value. Therefore, the number of molecule pair considered for collision per time step in NTC method is equal to

\[
N_c = \frac{1}{2} N \bar{N} F_N (\sigma_T c_r)_{max} \Delta t \quad (2.12)
\]

The collision for selected pairs over time \(\Delta t\) is computed with probability of

\[
p = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}} \quad (2.13)
\]

The parameter \((\sigma_T c_r)_{max}\) should be updated immediately if a larger value is obtained and updated for each cell.

3. **Motion of the particles**

All the particles are moved inside the computational domain without colliding for time step of \(\Delta t\). For boundary condition or interaction at gas-surface, Maxwell’s specular and diffuse reflection models are used.
2.2 One-Dimensional (1-D) Problem

2.2.1 Problem Formulation

Simple one dimensional geometries (concentric cylinders and parallel plates) as shown in Fig. 2.1 are chosen to compare conduction heat transfer across annular gaps filled with helium in slip regime between two kinetic methods (S-model and DSMC, briefly described earlier) and continuum approaches (ANSYS/Fluent and Analytical). The radii and temperatures of the inner and outer cylinders are \((R_1', T_{w1}')\) and \((R_2', T_{w2}')\), respectively, with \(R_1' < R_2'\) and \(T_{w1}' > T_{w2}'\). For simplicity, the same notation is used for parallel plates: the \(r'\) axis is normal to both plate’s surfaces. The bottom and upper plates have the locations and temperatures \((R_1', T_{w1}')\) and \((R_2', T_{w2}')\), respectively, with \(R_2' = -R_1'\). The cylinders and plates are assumed to have infinite length in the direction perpendicular to the figure.

Both problems are similar; however, the coaxial cylinder problem is governed by three physical parameters, which are temperature ratio, radius ratio and rarefaction. The

Figure 2.1: Concentric Cylinder and Parallel Plate geometry used for DSMC and Fluent result comparison
parallel plate problem is governed by two parameters, which are temperature ratio and rarefaction. These parameters are defined as:

- Temperature ratio between two cylinders or plates \( \mathcal{T} = \frac{T'_{w_1}}{T'_{w_2}} \),
- The aspect ratio for cylinders \( \mathcal{R} = \frac{R_1'}{R_2'} \),
- The rarefaction parameter is defined as \( \delta = \frac{R_0}{\lambda} \).  

For convenience, the distance between two walls is taken as the reference (characteristic) length, \( R_0 \). The temperature of external cylinder or upper plate is used as the reference temperature. The problem considered is 1-D, hence, there is only one component for heat flux. Following non-dimensional variables are introduced

\[
 r = \frac{r'}{R_0}, \quad p = \frac{p'}{p_0}, \quad T = \frac{T'}{T_0}, \quad q = \frac{q'}{p_0 v_0} \tag{2.15}
\]

The influence of the gas-surface interaction is taken into account by the thermal accommodation coefficient \( \alpha \), Eqn 1.5).

### 2.1.1 Analytical Expression for Continuum approach

The analytical expression for heat flux and temperature can be obtained by energy balance. The hypothesis of zero macroscopic velocity and constant pressure between the plates or cylinders are used to derive the analytical expressions. The Fourier law can be applied to calculate heat flux

\[
 q' = -\kappa \frac{dT'}{dr'} \tag{2.16}
\]

For monoatomic gases, the gas thermal conductivity \( \kappa \) is related to gas viscosity \( \mu' \) as follows [31]
\[
\mu' = \mu_0 \left( \frac{T'}{T_0} \right)^\omega \tag{2.17}
\]

where, \(\omega\) is the viscosity index, which is equal to 0.5 for Hard Sphere (HS) model and 1 for Maxwell model. For this study, HS model was used.

In continuum regime, the temperature continuity condition may be assumed on the surfaces. However, in the slip regime, the temperature-jump conditions [37] must be used as boundary conditions given by Eqn. 1.3. The dimensionless form of the temperature jump boundary condition at the cylinders and plates walls can be written as:

\[
T = \begin{cases} 
T_{w1} + \frac{\xi_{T1}}{\delta} T_{w1}^{\omega+\frac{1}{2}} \frac{dT}{dr}, & r = R_1 \\
T_{w2} - \frac{\xi_{T2}}{\delta} T_{w2}^{\omega+\frac{1}{2}} \frac{dT}{dr}, & r = R_2
\end{cases} \tag{2.18}
\]

Here, \(\xi_{T1}\) and \(\xi_{T2}\) are the temperature jump coefficients of the hotter and colder surfaces respectively. The assumption of the constant pressure between the cylinders and plates is used to obtain eqn. 2.18. The expression proposed by Lin and Willis for temperature jump coefficient is used (Eqn. 1.4). The analytical expression is obtained by linearization of temperature using \(\varepsilon = \frac{T_w - T_g}{T_w}\) and neglecting the order of \(\varepsilon^2\). The expressions used for dimensionless temperature profile and heat flux profile for parallel plates are [38]

\[
T(r) = \frac{1}{2} \left[ (T_{g1}^{\omega+1} + T_{g2}^{\omega+1}) + C(\omega + 1)(R_1 + R_2 - 2r) \right]^{1/(\omega+1)} \tag{2.19}
\]

\[
q(r) = \frac{15}{8\delta} C \tag{2.20}
\]

where

\[
C = \frac{(T_{w1}^{\omega+1} - T_{w2}^{\omega+1})/(\omega + 1)}{R_2 - R_1 + \frac{\xi_{T1}}{\delta} T_{w1}^{\omega+\frac{1}{2}} + \frac{\xi_{T2}}{\delta} T_{w2}^{\omega+\frac{1}{2}}} \tag{2.21}
\]
The gas temperatures near the walls are

\[ T_{g1}^{\omega+1} = T_{w1}^{\omega+1} [1 - \eta_1 (\omega + 1)] \]

\[ T_{g2}^{\omega+1} = T_{w2}^{\omega+1} [1 - \eta_2 (\omega + 1)] \]  \hspace{1cm} (2.22)

where

\[ \eta_1 = \frac{\xi T_1}{\delta} C \frac{1}{T_{w1}^{1/2}}, \quad \eta_2 = -\frac{\xi T_2}{\delta} C \frac{1}{T_{w2}^{1/2}} \]  \hspace{1cm} (2.23)

The dimensionless coordinates \( R_1 \) and \( R_2 \) for parallel plates are \( R_1 = -0.5 \) and \( R_2 = 0.5 \).

Similarly, the expressions for temperature profile and heat flux profiles for coaxial cylinders are

\[ T(r) = \left\{ \frac{1}{2} \left[ (T_{g1}^{\omega+1} + T_{g2}^{\omega+1}) + C (\omega + 1) \left( \ln \left( \frac{R_1}{r} \right) + \ln \left( \frac{R_2}{r} \right) \right) \right] \right\}^{1/\omega+1} \]  \hspace{1cm} (2.24)

\[ q(r) = \frac{15 C}{8 \delta r} \]  \hspace{1cm} (2.25)

where

\[ C = \frac{(T_{w1}^{\omega+1} - T_{w2}^{\omega+1})/(\omega + 1)}{\ln \frac{R_2}{R_1} \xi T_1 T_{w1}^{1/2} + \xi T_2 T_{w2}^{1/2}} \]  \hspace{1cm} (2.26)

Two values of aspect ratio are considered for this study, \( \mathcal{R} = 0.5 \) and 0.1. The corresponding dimensionless coordinate \([R_1, R_2]\) for each case are: \([1, 2]\) and \([0.11, 1.11]\), respectively. The temperature of gas at wall interface is calculated by using the same expression as for parallel plate (2.22) whereas \( \eta_1 \) and \( \eta_2 \) are calculated as

\[ \eta_1 = \frac{\xi T_1}{\delta} C \frac{1}{R_1 T_{w1}^{1/2}}, \quad \eta_2 = -\frac{\xi T_2}{\delta} C \frac{1}{R_2 T_{w2}^{1/2}} \]  \hspace{1cm} (2.27)
2.2 Results

The results of steady state heat transfer between two parallel plates and coaxial cylinders in the slip regime are obtained from DSMC simulations. For comparison, the results from S-Model kinetic approach are also used [39]. These results are compared with continuum approaches using ANSYS/Fluent and analytical expressions mentioned above. The results are obtained for parallel plates and coaxial cylinders ($R = 0.5$ and $0.1$) and temperature ratio $T = 1.1$ and $2$. The rarefaction parameters are varied from $3$ to $100$ which covers near transitional regimes to continuum regimes.

Figure 2.2 shows the non-dimensional temperature profile for $T = 1.1$ and $R = 0.5$ (left) and $0.1$ (right) for $\delta = 3, 10, 50$ and $100$. The results for each $\alpha$ are shown separately. For $R = 0.5$, the temperature profiles are almost linear while for $R = 0.1$, the profile are logarithmic. The temperature jump increases with decrease in $\delta$ and $\alpha$ for all methods. For $\delta$ of $50$ and $100$, all methods show similar temperature profile and close temperature jump at both walls. However, for $\delta$ of $10$ and $3$, the profiles from ANSYS/Fluent and analytical expression differ from S-model and DSMC. As $\delta < 10$ is in transitional regime, the methods using continuum approach show some variation from kinetic approach.

Similarly, Fig 2.3 shows the temperature profile for $T = 2$. The temperature profiles from S-model and DSMC are close for all $\delta$ and $\alpha$ both radius ratios. But the difference with continuum approach is clear even for higher $\delta$ and for all $\alpha$. There is huge variation between kinetic and continuum approach. For smaller $\delta$, there is difference between profiles from ANSYS/Fluent and analytical expression. Figure 2.4 shows the temperature profile for parallel plates for $T = 1.1$ (left) and $2$ (right). The results are very similar to the
concentric cylinders where, the results from continuum approach shows good agreement with kinetic approach for $T = 1.1$. Similar to concentric cylinder, $T = 2$, there is huge discrepancy between the results from continuum approach and kinetic approach.
Figure 2.2: Non-dimensional temperature profile along radial direction for $R = 0.5$ and 0.1 and $T = 1.1$ for different $\alpha$
Figure 2.3: Non-dimensional temperature profile along radial direction for $R = 0.5$ and 0.1 and $\tau = 2$ for different $\alpha$. 

\( \alpha = 1 \) 
\( \alpha = 0.6 \) 
\( \alpha = 0.2 \)
Figure 2.4: Non-dimensional temperature profile across parallel plates for $\mathcal{T}=1.1$ and 2 for different $\alpha$
Figure 2.5 shows non-dimensional heat flux profile along radial direction for $T=1.1$ and $R=0.1$ and 0.5 for different $\delta$. The heat flux decreases along radial direction. The non-dimensional heat flux decreases with increase in $\delta$. As the value of $\alpha$ decreases, the non-dimensional heat flux also decreases. The profiles are nearly linear for higher $R$ whereas logarithmic for lower $R$. The heat flux profile from all four methods are almost identical for $\delta > 10$, whereas for $\delta < 10$, some discrepancy can be seen. The discrepancy between kinetic and continuum approach is higher for $R=0.1$ compared to 0.5 and increases as the value of $\alpha$ decreases. Figure 2.6 shows similar results as Fig. 2.5 for $T=2$. Similar to temperature profile, for larger temperature ratio, the difference between kinetic and continuum approach are observed clearly. At $\alpha = 0.2$, there is discrepancy between kinetic and continuum approach for highest values of $\delta$ as well. For parallel plates, as shown in Fig. 2.7, the comparison are very similar to concentric cylinder. It is obvious that the heat flux value is constant across the gap. These results show that the use of continuum approach for higher temperature ratios are not highly accurate even in slip regime, and specially for lower values of $\alpha$, the difference is significant.
Figure 2.5: Non-dimensional heat flux profile along radial direction for $\mathcal{T} = 1.1$ and $\mathcal{R} = 0.1$ and 0.5 for different $\alpha$. 
Figure 2.6: Non-dimensional heat flux profile along radial direction for $T = 2$ and $R = 0.1$ and 0.5 for different $\alpha$. 
Figure 2.7: Non-dimensional heat flux profile across parallel plates for $\mathcal{T} = 1.1$ and 2 for different $\alpha$
Figure 2.8 shows the dimensionless heat flux $q$, plotted as a function of rarefaction parameter $\delta$ for all combinations of $T$ and $R$ considered for this study and for $\alpha=1$, 0.6 and 0.2. Results from kinetic (S-model and DSMC) and continuum (numerical and analysis) approaches are included. It is clear from the figure that the value of $q$ increases as $\delta$ decreases and $\alpha$ and $T$ increase. The values of $q$ obtained from both continuum models are in a good agreement for case $T=1.1$ regardless of $R$ and $\alpha$. For $T=2$, the discrepancy between the two models increases as $\delta$, $\alpha$ and $R$ decrease. The value of $q$ for the continuum numerical model is systematically larger than the continuum-analytical model. At $T=1.1$, the continuum and kinetic results are in good agreement for all values of $\delta$, except for cases $R=0.1$ and $\alpha=1$.

The reason of this discrepancy is not clear and could be a good problem for future research. For $T=2$, the agreement is good for $R=0.1$ and $\alpha=1$, but not as good as $\alpha$ decreases and $R$ increases. The disagreement between the continuum and kinetic models, especially at large $T$, may be explained from the profiles of dimensionless pressure along radial direction. The reason of this discrepancy is not clear and could be a good problem for future research. For $T=2$, the agreement is good for $R=0.1$ and $\alpha=1$, but not as good as $\alpha$ decreases and $R$ increases. The disagreement between the continuum and kinetic models, especially at large $T$, may be explained from the profiles of dimensionless pressure along radial direction.
Figure 2.9 shows these profiles between the cylinders and plates obtained from the S-model kinetic equation in the case of full accommodation of the molecules at the walls. The results are plotted for $T = 1.1$ and 2, $R = 1, 0.5$ and 0.1 and $\delta = 100, 50, 10$ and 3. The radial axis is scaled from 1 to 2 for convenience of comparison. From this figure, it can be seen that, in all cases, the pressure varies long the $r$-axis between the cylinders and plates and this variation is larger as $\delta$ and $R$ decrease, and $T$ increases.
Figure 2.8: Non-dimensional heat flux as a function of the rarefaction parameter, \( \delta \), for all combination of \( R \) (a, b and c) and \( T \), and different values of thermal accommodation coefficient, \( \alpha \)
As mentioned earlier, the continuum models assume that the pressure is constant along the \( r \)-axis. Figure 2.9 shows that the pressure variations is very small for \( T=1.1 \), which explains the good agreement obtained between the continuum and kinetic approaches. However, for \( T=2 \), the pressure variation is significant for \( \delta < 10 \), therefore, the assumption of the constant pressure is not valid. This may explain the disagreement obtained in these cases. Figure 2.10 gives the percentage difference of non-dimensional heat flux \( q \) between DSMC and S-model (shown in black symbols) and the continuum-numerical and S-model (shown in red symbols) for both temperature and aspect ratios, and for three values of the thermal accommodation coefficient considered in this study. It can be seen from the figure that the heat fluxes obtained from the DSMC and S-model are within 3% of each other in all configurations. This difference decreases as \( \delta \) increases and
the gas approaches the continuum regime. It is also clear that, for the case $\mathcal{T}=1.1$, the percentage difference between the continuum-numerical and S-model is smaller than 4% for all values of $R$, $\alpha$, and $\delta$, which is of the order of the difference between the DSMC and S-model approaches. However, in case $\mathcal{T}=2$, the percentage difference between the continuum-numerical and S-models is significantly larger than the corresponding difference between DSMC and S-model and of the order of 50% at small $\delta$. This quantitative comparison between the continuum and kinetic approaches clearly demonstrates that the continuum models are appropriate for simulating heat transfer for small temperature ratio, however, for large ratio their ability is largely reduced even at large value of $\delta \geq 50$. In general, it can be concluded that the continuum models are accurate for $\delta \geq 10$ and $\mathcal{T}=1.1$, and for $\delta \geq 50$ and $\mathcal{T}=2$, regardless of the aspect ratio.
Figure 2.10: Percent difference of the dimensionless heat flux between S-model and DSMC (black), and numerical-continuum (red) models as function of the rarefaction parameter $\delta$ obtained for all $R$, $T$ and $\alpha$. 
2.3 Two-Dimensional (2-D) Problem

2.3.1 Geometry

A 2-D geometry with a heater rod centered inside a square enclosure filled with rarefied helium was used for the comparison between DSMC and CFD simulations. The heater rod consists of magnesium oxide cement covered by stainless steel cladding, see Fig. 2.11. The outer diameter of heater rod is 10.5 mm and thickness is 0.71 mm. The size of square enclosure is 18.4 mm. Heat is generated uniformly in the cement portion. The heater is placed in an enclosure filled with helium gas and the enclosure walls are maintained at constant temperature. As for the 1-D comparison, the CFD simulations were conducted in ANSYS/Fluent.

2.3.2 Cases

Three heat generations of 100 kW/m$^3$, 550 kW/m$^3$ and 5000 kW/m$^3$ are applied. For cement and stainless steel, constant values of thermal conductivity were used. The thermal accommodation coefficient ($\alpha$) of the cladding-helium wall was kept constant, $\alpha = 1$, for all cases, whereas three different values of $\alpha$ (1, 0.6 and 0.2) were applied on the four
enclosure walls, which are set at isothermal temperature of 300 K. Four pressure values were applied equivalent to rarefaction parameters ($\delta$, Eqn. 2.14) of 5, 10, 20 and 50 that cover near transitional regime and slip regime. In total, 36 different cases were simulated.

<table>
<thead>
<tr>
<th>Table 2.1 Different parameters varied for comparison</th>
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<tbody>
<tr>
<td>Heat generation, $q$ [kW/m$^3$]</td>
</tr>
<tr>
<td>Thermal Accommodation Coefficient ($\alpha$)</td>
</tr>
<tr>
<td>Pressure [Pa]</td>
</tr>
<tr>
<td>Rarefaction parameter ($\delta$)</td>
</tr>
</tbody>
</table>

2.3.3 Results

The temperature contour from DSMC and Fluent simulation for $q = 550$ kW/m$^3$, $P = 42$ Pa and $\alpha$-1 case is shown in Fig. 2.12. Maximum temperature is at the center of the heater rod. However, the temperature of heater rod is almost uniform. The temperature decreases gradually in helium-filled region. For further comparison of the results from DSMC and CFD simulation, the temperature profile along the diagonal line from center of the heater rod to one of the corners is plotted for all the cases. Figure 2.13, 2.14 and 2.15 show the temperature profiles along diagonal OD for $q = 100$ kW/m$^3$, 550 kW/m$^3$ and 5000 kW/m$^3$ respectively.

Figure 2.12: Temperature Contour for $q = 550$ kW/m$^3$, $P = 42$ Pa, $\alpha$-1 (a) DSMC (b) CFD (Fluent)
Figure 2.13: Temperature profile comparison of DSMC and CFD for $q = 100 \text{ kW/m}^3$ (a) heat generation in heater rod in CFD and DSMC (b) cladding temperature in CFD set to DSMC result
Figure 2.14: Temperature profile comparison of DSMC and CFD for $q=550 \text{ kW/m}^3$ (a) heat generation in heater rod in CFD and DSMC (b) cladding temperature in CFD set to DSMC result
Figure 2.15: Temperature profile comparison of DSMC and CFD for $q = 5000 \text{ kW/m}^3$ 
(a) heat generation in heater rod in CFD and DSMC (b) cladding temperature in CFD set to DSMC result
The left plots in Figs. 2.13, 2.14, and 2.15 show the temperature profiles from DSMC and CFD simulations along the diagonal line OD, shown in Fig 2.12, for \( q = 100, \ 550 \) and 5000 kW/m\(^3\), respectively, for three values of the thermal accommodation coefficient, \( \alpha = 1, \ 0.6 \) and 0.2 at the enclosure wall. In all these plots, the temperature increases as the pressure and thermal accommodation coefficient decrease and heat generation increases. The difference of maximum temperature of heater rod predicted between DSMC and CFD simulations is small (less than 0.5°C) for small heat generation rate (\( q = 100 \) kW/m\(^3\)) and increases as the heat generation rate increases, especially for low pressure cases (\( P = 21 \) and 42 Pa). This difference is very large for the case \( q = 5000 \) kW/m\(^3\) and \( P = 21 \) and 42 Pa for all \( \alpha \) (see Fig. 2.15a). In all cases, as the pressure decreases, the temperature-jump at the interfaces increases. The temperature-jump at both cladding and enclosure wall interfaces predicted by CFD simulations is higher than DSMC. The maximum temperature predicted by the CFD simulations are mostly lower than those from DSMC, except in few cases at low pressure and high heat generation rates. This behavior is not well understood and hard to explain.

In order to quantify the temperature jump at the interfaces and to conduct a direct comparison between CFD and DSMC simulations, the temperature of the heater rod obtained from DSMC simulations is used a boundary condition in the CFD simulations. This allows eliminating the comparison of maximum temperatures of the heater rod. Only meaningful comparisons are the temperature jump at each wall and temperature profile in the helium region. These results are presented in the right plots of Figs. 2.13, 2.14 and 2.15 for all conditions. These figures show the temperature profile along the same diagonal line shown in fig. 2.12. The temperature profiles in the bulk of the helium filled region are
different between CFD and DSMC simulations, especially for low pressure cases. Therefore, there is also a difference in the temperature jumps predicted at each wall for all cases. In general, the temperature jump predicted by CFD simulations is larger than those of DSMC simulations, except for the case $q = 100$ kW/m$^3$, $P = 208$ Pa, and $\alpha = 1$, where the opposite behavior is observed.

To better illustrate these differences, Fig. 2.16 shows the temperature-jump difference between the two models (CFD-DSMC) for both wall and all conditions of heat generation, $\alpha$, and rarefaction parameter ($\delta$). The left plots show the results for the enclosure wall ($\Delta T_{TJ,\text{wall, F-DSMC}}$), however, the right plots show the results for the cladding wall ($\Delta T_{TJ,\text{clad, F-DSMC}}$). For the enclosure wall, the results are consistent between all heat generations, except in one case ($q = 100$ kW/m$^3$, $\delta = 5$, and $\alpha = 0.6$). The difference in temperature jump increases with the decrease of $\delta$ and $\alpha$ and increase in heat generation rate, $q$. For the cladding wall, the results are not consistent. It should be reminded here that the value of the thermal accommodation $\alpha$ was kept constant, equal to 1, for the cladding wall. The values of $\alpha$ shown in the right plots of Fig. 2.16 are for the enclosure walls. As a result, the difference of temperature jump at this wall does not vary a lot with variation in the value of $\alpha$ for the enclosure wall. However, its variation as the rarefaction parameter $\delta$ and heat generation $q$ vary is clear. As $\delta$ decrease and $q$ increase, there larger differences.

From the above comparison between the DSMC and CFD simulations in the 2-D geometry, it shows that the CFD simulations are able to predict the temperature jump at the wall only for small heat generation rates.
Figure 2.16: Difference in temperature jump predicted from two methods (a) at enclosure wall (b) heater rod wall with same heater rod and enclosure wall temperatures
CHAPTER 3

EXPERIMENTAL VALIDATION OF CFD SIMULATIONS UNDER PRESSURIZED CONDITION

The primary objective of this research is to validate the CFD simulations in the slip regime for conditions relevant to vacuum drying process. The CFD simulations were validated in simple one and two-dimensional geometries by comparing them to the accurate kinetic models in previous chapter. The next step would be to validate them in complex three-dimensional geometry. However, without sufficient knowledge of accuracy and reliability of the CFD simulations for complex geometry in the continuum regime, it is not possible to obtain reliable results in the slip regime. Therefore, an “intermediate step” is taken, where a validation of the CFD simulations is conducted for a complex three-dimensional geometry in the continuum regime (atmospheric or higher pressures). The objective is to understand the effect of factors such as geometric tolerances, temperature measurement uncertainties, etc., which are inevitable in any experiment, on the results of CFD simulations of a complex three-dimensional geometry. The findings presented in this chapter has already been published [40].

In this chapter, the results from experiments conducted by Chalasani [29] for three different pressures and heat generation rates are used to validate CFD simulations conducted in this dissertation in the continuum regime. The experiment resembles to a portion of an array of 8×8 nuclear fuel assembly inside a canister. The description of the
experimental apparatus, numerical model used for the simulations and the comparison of the experimental and CFD simulation results are given in details in the following sections.

3.1 Experimental Apparatus

The experimental apparatus is designed to represent a section of a fuel assembly between consecutive spacer plates, within a helium-filled basket opening [23, 24]. A disassembled view is shown in Fig. 3.1. It consists of (a) an 8×8 array of heater rods, (b) two stainless steel spacer plates, and (c) a square anodized-aluminum enclosure. Each heater rod is 1.1 cm in diameter and 67.3 cm long. The sheath of each rod is made of 0.7-mm-thick Incoloy with compressed Magnesium Oxide (MgO) inside. Most of the rods are mildly bowed, such that the center of some rods are as much as 3 mm away from a line connecting the rod ends. Each rod contains a Nichrome heater coil. The coil ends are anchored to metal pins in both rod ends, which are connected to external power leads. The manufacturer specifies that heat generation is uniform along the length of the heater rods to within ±6%, except for 3.2 cm sections on both ends, which are unheated. For the 64 rods, the average and standard deviation of the heater resistances are, respectively 4 Ω and 0.12 Ω. Sets of eight heater rods are connected in series. The resulting eight sets are connected in parallel to a 0-1000W regulated DC power supply.

The stainless steel spacer plates are 0.635-cm-thick and 11.9 cm on each side. Both contain sixty-four 1.15-cm-diameter holes that hold the heater rods in position. The hole center-to-center pitch is 1.44 cm. A small threaded hole is centered between each set of four rod holes. To hold the heater rods in position, a bolt with an expansion ring is tightened in the threaded holes. The expansion ring pushes the rods to make them contact
the far sides of the rod holes. This eccentricity and the rod bowing lead to small but random (uncontrolled) variations of the rod locations.

To make the enclosure reasonably isothermal, it is constructed by tungsten inert gas-welding four 2.54-cm thick aluminum plates. The surfaces are black anodized. Its interior forms a 12 cm by 12 cm square, and its total length is 91.5 cm. Figure 3.2a shows an axial section of the assembled experiment. The heater rod array is centered axially within the enclosure, so there are 12-cm voids on each end to house power and thermocouple wires. The $z$-axis is shown, with its origin at the axial mid-plane. When in operation the heater rods are vertical, and the gravity vector $\mathbf{g}$ is oriented in the negative $z$-direction. The inner surfaces of the spacer plates are at $z = \pm 30.5$ cm, and are coplanar with the ends of the heated regions of the rods.

Forty-seven of the 64 heater rods contain Type-K (chromel/alumel) thermocouples, at one of four axial locations, $z = -17.3, 0, 17.3$ and 29.2 cm. These locations are known
to tolerances of ±1.3 cm, and are indicated in Fig. 3.2a. In each instrumented rod, a chromel wire exits one end while an alumel wire exits the other. Stainless steel endplates with O-rings are bolted to both ends to seal the enclosure. The top endplate has extension tubes with feedthroughs at their ends for thermocouple leads. The bottom endplate has a thermocouple/power feedthrough and another tube that is used to evacuate and backfill the enclosure. That tube is connected to a tree with an atmospheric valve, an evacuation valve connected to an oil filter attached to an oil-based vacuum pump, and high and low pressure gauges. To increase the enclosure temperature, fiberfrax insulation blankets, with thickness of either $l = 2.5$ or $5$ cm, are used on the enclosure and endplates. Figure 3.2b is a picture of the assembled apparatus wrapped in insulation.
In this sealed enclosure, buoyancy is expected to cause helium to flow upward in the warm center of the rod array, and downward near the relatively cool enclosure walls. This is somewhat different from the thermal syphoning pattern that exists in vertical storage canisters. Thermal syphoning is governed by the ratio of buoyancy to viscous forces, which is characterized by the Grashof number [5].

\[
Gr = \frac{gB(T_M - \bar{T}_W)\rho^2L^3}{\mu^2}.
\]  \quad (3.1)

In this expression \( g \) is the gravitational acceleration, \( B \) is the gas coefficient of thermal expansion, \( T_M \) is the maximum cladding temperature, \( \rho \) and \( \mu \) are, respectively the average gas density and dynamic viscosity, and \( L \) is the height of the heated fuel rods. Based on simulations for a canister that contains 24 fuel assemblies [6], the Grashof number is of the order \( Gr \sim 10^9 \).

Figure 3.3 is a schematic of the experimental apparatus cross section. The \( x \) and \( y \) coordinate system is also shown. The circles represent heater rods. Each is named according to its row (A to H) and column (1 to 8) location. The number inside certain rods represents the \( z \)-location of the thermocouple within that rod. The 17 rods without numbers do not contain a thermocouple. Twelve thermocouples are installed in the enclosure walls to measure its temperature. Figure 3.3 shows wells in the middle of each walls whose ends are 0.25 cm from the inner surface. Each wall has wells at \( z = -29, 0, \) and 29 cm. In Fig. 3.3 the four black-filled \( X \)'s near the center, top and upper corners of the rod array show the \( x, y \)-locations of thermocouples that are on both the top and bottom spacer plates. The open \( X \) near the bottom right corner indicates the position of a thermocouple that is only on the top spacer plate.
Table 3.1 Heater rods within each symmetry group

<table>
<thead>
<tr>
<th>Group Name</th>
<th>Group Heater Rods</th>
<th>Locations of Thermocouples</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>D4, D5, E4, E5</td>
<td>All z</td>
</tr>
<tr>
<td>β</td>
<td>C4, C5, D3, D6, E3 E6, F4, F5</td>
<td>All z</td>
</tr>
<tr>
<td>γ</td>
<td>B4, B5, D2, D7, G4, G5</td>
<td>z = 0</td>
</tr>
<tr>
<td>δ</td>
<td>A4, A5, D1, D8, E1, H4, H5</td>
<td>z = 0</td>
</tr>
<tr>
<td>ε</td>
<td>A3, A6, C1, F1, F8, H3</td>
<td>z = 0</td>
</tr>
<tr>
<td>ζ</td>
<td>A2, A7, B1, B8, G1, H2, H7</td>
<td>z = 0</td>
</tr>
<tr>
<td>η</td>
<td>A1, A8, H1, H8</td>
<td>All z</td>
</tr>
</tbody>
</table>

Figure 3.3: Experimental apparatus cross section showing heater rods, enclosure walls, coordinate system and row and column names. Numbers in rods indicate z-location of thermocouples, and Greek letters indicate symmetry group (Table 3.1)
The section of the experiment in Fig. 3.3 is symmetric about the x and y axes, and diagonal lines connecting heater rods A1-H8 and rods H1-A8. Due to the nearly isothermal enclosure walls, symmetry of the experiment geometry and the expected natural convection flow pattern, rods that are symmetrically located on either side of the symmetry planes are expected to have nearly the same temperatures. Greek letters \( \alpha, \beta, \gamma, \delta, \epsilon, \zeta \) and \( \eta \) in Fig. 3.3 identify rods in seven symmetry groups that contain thermocouples. Table 3.1 lists the rods in each groups, and the \( z \)-locations of the thermocouples within them. The \( \alpha \) group is the one that is closest to the array center, and the \( \beta, \gamma, \delta, \epsilon, \zeta \) and \( \eta \) groups are located increasing further away.

Table 3.1 and Fig. 3.3 show that symmetry groups \( \alpha, \beta \) and \( \eta \) have thermocouples at all four elevations, \( z = -17, 0, 17 \) and 29 cm. In this work, measurements from each group are assembled to construct an axial profile for a typical rod in that group. Based on distances of each group from the center of the array, groups \( \alpha, \beta \) and \( \eta \) are expected to contain, respectively, the hottest, second hottest and coolest rods in the array.

All the thermocouples in symmetry groups \( \gamma, \delta, \epsilon \) and \( \zeta \) are at \( z = 0 \). Based on symmetry, the temperature of the \( N = 6 \) or 7 thermocouples within each of these groups will be nearly identical. However, within each group the indicated temperature may differ by normally-distributed random amounts due to measurement and configuration errors. Configuration errors are caused by small but uncontrolled variations in the heater resistances, rod bowing, thermocouple placement in a rod, small variations in the enclosure temperature and other factors. While measurement errors are expected to be roughly the same for all symmetry groups, configuration errors are not the same. In this work the
variation in temperatures within each of these groups is used to determine the variation of configuration errors with group location.

3.2 Temperature Measurements

Table 3.2 describes the conditions of twelve experiments that are presented in this study. Experiments are performed for two insulation thicknesses \( I = 2.5 \) or \( 5 \) cm, three nominal helium pressures \( P_N = 1, 2, \) and \( 3 \) atm (which are measured when the apparatus is at room temperature), and three rod heat generation rates \( Q = 100, 300, \) and \( 500 \) W. For each experiment, Table 3.2 gives its Roman numeral experiment number, \( \text{Exp#} \), the measured pressure \( P \) when the experiment reached steady state conditions (which is higher than \( P_N \) due to the higher steady state temperature), and Grashof number (eqn. 3.1). For the Grashof calculation, \( T_M \) and \( \bar{T}_W \) are the maximum-rod and average-wall temperatures, and \( L \) is the heater rod length. The experiment Grashof numbers range from \( Gr \sim 10^7 \) to \( 10^8 \), which are one to two order of magnitude smaller than a nominal value for a vertical used fuel canister, \( Gr \sim 10^9 \). As described earlier, the flow pattern in the current experiment is also somewhat different from that of canisters. All twelve experiments were performed in a laboratory where the temperature was controlled to be approximately \( 23^\circ C \). The enclosure, spacer plate and rod temperatures were measured using a data acquisition system at a sampling rate of one sample/minute. When the heaters were off and the apparatus reached steady state, all the thermocouples indicated approximately the same temperature, within a standard deviation of \( 0.5^\circ C \). After the heater rods are powered, approximately 25 hours were required for the temperatures to reach steady-state conditions. After steady state was reached, all temperatures were sampled for at least 30 minutes,
Table 3.2 Conditions for all 12 experiments presented in this work.

<table>
<thead>
<tr>
<th>Insulation Thickness, ( I ) [cm]</th>
<th>Nominal Pressure, ( P_N ) [atm]</th>
<th>Total Rod Heat Generation, ( Q )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100 W</td>
<td>300 W</td>
</tr>
<tr>
<td></td>
<td>Exp#</td>
<td>( P ) [Atm]</td>
</tr>
<tr>
<td>2.5</td>
<td>1</td>
<td>1.38</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.53</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.66</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>1.16</td>
</tr>
</tbody>
</table>
and then averaged. The uncertainty of each thermocouple measurement was ±1.1°C.

The symbols in Fig. 3.4 show measured enclosure, spacer plate and heater rod temperatures versus axial (z) location for Experiments III (\(I = 2.5\) cm, \(P_N = 3\) atm, \(Q = 100\) W, \(Gr = 8 \times 10^7\)) and VII (\(I = 2.5\) cm, \(P_N = 1\) atm, \(Q = 500\) W, \(Gr = 1 \times 10^7\)). The temperature profile shapes in the two plots are similar, but their temperature scales are different. The
solid circles at the bottom of each plot show the temperatures on all four enclosure walls at the three axial locations. At each elevation, the temperatures are not the same on the four walls, but the average temperature increases with elevation due to natural convection. For each experiment the four triangles at \( z = -29 \) cm and five triangles at \( z = 29 \) cm show the temperatures of, respectively, the bottom and top spacer plates. Both plates are warmer than the enclosure, and the top plate temperature is higher than the bottom plate, again due to the natural convection inside the apparatus. As expected, on both spacer plates, the plate centers are hotter than locations near the enclosure walls. For both experiments, the open squares, diamonds and circles show temperatures measured at four different axial locations within, respectively, the \( \alpha \) (hottest), \( \beta \) (second hottest) and \( \eta \) (coolest) rod symmetry groups. The \( \alpha \) and \( \eta \) temperatures are measured in four different rods, as described in Table 3.1. The \( \beta \) temperatures (diamonds) are measured in eight different rods, and have two measurements at all four elevations. For the \( \beta \) temperatures, the two temperature measurements at locations \( z = -17, 0 \) and 17 cm are approximately the same, whereas at \( z = 29 \) cm the temperatures differ by 1°C to 3°C. This was observed in all twelve experiments. As described earlier, these differences are caused by configuration and measurements errors.

The Grashof number for Experiment III is eight times larger than that for Experiment VII. For Experiment III, in rod groups \( \alpha \) and \( \beta \), the temperatures at \( z = -17 \) cm are lower than they are at \( z = 17 \) cm. However, the temperatures at these locations are closer to each other in Experiment VII, in which the effect of natural convection is less
significant. The solid and dotted lines in Fig. 3.4 are simulated temperatures for the $\alpha$, $\beta$ and $\eta$ group rods, which are described in a later section. The boundary conditions for those simulations are the measured enclosure wall and spacer plate temperatures, which are described in the next section.
3.2.1 Boundary Temperatures

In this work the average measured enclosure wall temperature, \( \bar{T}_W \), is used to characterize each experiment. The horizontal lines in Figs. 3.4a and 3.4b shows averages in Experiments III and VII which are, respectively, \( \bar{T}_W = 67^\circ C \), and \( 218^\circ C \). In Fig. 3.5a the symbols connected by solid lines shows \( \bar{T}_W \) versus the total rod heat generation rate \( Q \), for all twelve experiments. As expected the average enclosure temperature increases with heat generation rate and insulation thickness. The data for \( I = 2.5 \text{ cm} \) indicate that the average enclosure temperature is essentially independent of the gas pressure.

Figure 3.5a also shows the average temperature differences between the spacer plates and the enclosure walls. The symbols connected by dotted lines show data for the top spacer plate, \( \bar{T}_T - \bar{T}_W \), while dashed lines are used for the bottom spacer plate, \( \bar{T}_B - \bar{T}_W \). For all experiments, the upper spacer plate is warmer than the bottom. For \( I = 2.5 \text{ cm} \), the temperature differences are more strongly affected by the heat generation rate than the pressures considered in this work. As the pressure increases, the top spacer plate gets slightly hotter and the bottom spacer gets slightly cooler, but the change for these pressures is less than \( 2^\circ C \). Increasing the pressure increases the gas density, Grashof number, and the effect of natural convection. This causes the hottest locations on the rods to move to higher \( z \)-elevations, and explains why the top spacer plate temperature increases and the lower one decreases as pressure increases. Figure 3.5a also shows that the temperature difference between the spacer plates and the wall is significantly smaller for \( I = 5 \text{ cm} \) than for \( I = 2.5 \text{ cm} \). As already noted, the thicker insulation makes the apparatus hotter, which increases radiation heat transfer. This decreases the temperature difference between the enclosure walls and spacer plates.
To quantify the temperature variations within the enclosure wall, we define the temperature range that statistically contains 95% of the measure values, assuming they are normally distributed. This deviation temperature is twice as large as the sample standard deviation, and is calculated as [26]:

$$D_W = 2 \sqrt{\frac{\sum (\bar{T}_W - T_{W,i})^2}{N_W - 1}}. \quad (3.2)$$

In this expression, $T_{W,i}$ is each individual measured wall temperature, and $N_W = 12$ is the number of wall measurements. The non-isothermality of the walls, and measurement errors, cause $D_W$ to be non-zero. The top and bottom spacer plate deviations, $D_T$ and $D_B$, which are calculated using Eqn. 3.2 but employing the top ($T$) and bottom ($B$) plate temperature measurements, assess measured temperature variations within those objects.

Figure 3.5b presents the measured temperature deviation versus heat generation rate for the three objects: the enclosure wall (symbols connected with solid lines), and the bottom (dashed lines) and top (dotted lines) spacer plates. The temperature deviation increases as the heat generation (and consequently object temperature) increases. For $I = 2.5$ cm the enclosure wall deviations increase marginally with gas pressure. The wall temperature deviation increases with insulation thickness because the insulation increases the wall temperature. For the top and bottom spacer plates, the deviations are nearly the same at $P_N = 2$ atm. However, as the pressure increases, the deviations on the top spacer plate increase (as its average temperature increases), while those of the bottom spacer plate decrease (as its average decreases). The temperature deviations on the spacer plates are smaller for $I = 5$ cm than they are for $I = 2.5$ cm. This is because as the insulation thickness
increases the experiment temperature and the radiation heat transfer increase, which makes the experiment temperatures more uniform. Even though the enclosure is physically larger than the spacer plates, its deviations are smaller. This is due to higher thermal conductivity of aluminum compared to that of stainless steel. Comparing Figs. 3.5a and 3.5b shows that the temperature deviation in the spacer plates is not negligible compared to the average temperature difference between those plates and the enclosure.

3.2.2 Configuration Errors

As described earlier, all rods in symmetry groups $\gamma$, $\delta$, $\epsilon$ and $\zeta$ have thermocouples at $z = 0$. The variations within each of these groups are used to quantify each group’s configuration errors, which are caused by uncontrolled experimental geometric and boundary conditions. To do this, the average and deviation (Eqn. 3.2) temperatures of each of these four symmetry group was calculated for each of the 12 experiment. The Modified
Thompson Tau test was used to determine if any samples within these 48 populations was a statistically unlikely members of its population. As a result, measurements from rod H5 were removed for all 12 experiments, and those from rod A7 were removed from experiments I to IX. After these 21 thermocouple measurements were eliminated, the average ($\bar{T}_\gamma, \bar{T}_\delta, \bar{T}_\epsilon$, and $\bar{T}_\zeta$) and deviation ($D_\gamma, D_\delta, D_\epsilon$, and $D_\zeta$) temperatures were determined for all four symmetry groups and all twelve experiments.

Figure 3.6 is a plot of the temperature deviation for each group $D_j$ (for $j = \gamma, \delta, \epsilon$ and $\zeta$) versus the average temperature difference between the group and the wall $\bar{T}_j - \bar{T}_w$. Data from all twelve experiments are presented. Dotted lines that are fit to the results of each group are included to better show trends in the data. For each group the deviation in temperature increases roughly linearly with the temperature difference.

The deviations in Fig. 3.6 are caused by both measurement and configuration errors. We expect the measurement errors from each group to be roughly the same, so the differences between groups is caused by the difference in configuration errors in each symmetry group. The configuration error is smallest for the $\gamma$ group, which is the one that is closest to the array center. The error for the $\delta$ and $\epsilon$ groups, which are the second and third closest groups, are larger than those for the $\gamma$ group. The $\zeta$ group, which is the furthest from the array center, has a lower error than those of the $\delta$ and $\epsilon$ groups.

To understand this behavior, we consider the temperature profiles along lines that radiate from the array axis ($x = y = 0$). These temperature profiles pass through the gas and rods. They are fairly flat near the array center, but exhibits steeper gradients near the walls. Bowing of the heater rods causes the thermocouples at $z = 0$ to be shifted in the $x$- and $y$-
directions by small but random amounts. The rods in the $\gamma$ group are relatively close to the array center, so small shifts in their location will not cause a large change in their temperatures. However, rods in the $\delta$, $\varepsilon$ and $\zeta$ groups are close to the walls where the radial temperature gradient is steep. As a result, their temperatures are relatively sensitive to small location variations. Interestingly, the temperature deviations within the $\zeta$ group are relatively small. It is possible that the rods in that group are relatively straight compared to that of the other groups. Unfortunately, it is not possible to test that hypothesis because the bowing of those rods were not observed before the experiment was disassembled.

Figure 3.6 shows that the configuration error within a symmetry group is larger for groups that are nearer the array periphery, because their temperatures are more sensitive to random location variation than those in groups near the array axis. We conclude that measurements made near the array axis are more valuable for assessing the accuracy of simulations than ones near the periphery.

3.3 Numerical Simulations

3.3.1 Computational Domain

Two and three-dimensional computational meshes representing the experimental apparatus were generated using ANSYS Meshing. Figure 3.7a shows an $x,y$-plane of a computational mesh. The outer portion of the plane consists of a 0.25-cm-thick aluminum region, which represents the portion of the enclosure that is inside the locations where temperatures are measured. It also contains regions for the 64 heater rods (magnesium
oxide core and Incoloy sheath), and the helium between the rods and enclosure. This mesh was extruded in the $z$-direction (normal to the plane of the mesh) to form the three-dimensional mesh.

At the ends of the extrusion, the properties of 0.635-cm-long regions are modified to represent the two stainless steel spacer plates. Figure 3.7b is an expanded view of Section 1 from Fig. 3.7a, showing the solid and gas regions near the spacer plates. Darker
shaded regions show the helium-filled gaps. These gaps are between the spacer plate and enclosure wall (except at the corners where the spacer plates are supported), and between the rods and plate holes. As described earlier, expansion rings between each set of four rods press the rods against the portions of the spacer holes that are away from the rings. The resulting eccentricity of the rods and holes are represented in the mesh as a 45°-arc contact surface. The total number of mesh elements in the three-dimensional domain is 1,834,880. For comparison, another mesh was constructed with the rods symmetrically centered within the holes.

Temperature dependent material properties were assigned to all of the magnesium oxide, Incoloy, stainless steel, aluminum and helium regions. The emissivities of the anodized aluminum enclosure walls, Incoloy heater rod sheaths, and stainless steel spacer plates were measured. However, after the experiments were completed and the enclosure was reopened, all interior surfaces were found to be coated with a film of vacuum pump oil. The emissivity of the coated surfaces were not measured, but were approximated to be very near unity [25].

In the model, heat is generated uniformly throughout the magnesium oxide, except in the z-locations within the spacer plates. For the simulation of each experiment, the total heat generation rate is equal to that of the experiment. The outer surfaces of the aluminum region is set uniformly to the average measured temperature of the enclosure walls.

At the top and bottom of the domain (outer surfaces of the spacer plates), the end surfaces of the heater rods and the helium gaps are insulated. Three different types of boundary conditions are applied to the stainless spacer plates. The first is the Regional Temperature condition, in which the spacer plates are divided into nine regions, which are
shown in Fig. 3.7a separated by the vertical and horizontal lines. The temperature in
Middle region of the top and bottom plates (marked M in Fig. 3.7a) is set to the temperature
measured at the center thermocouple for each plate (center X in Fig. 3.3). The temperature
of all four Side regions (marked S) is the value measured by the thermocouple at the side
of each plate (X near the top of Fig. 3.3). The Corner region temperature (marked C) is set
to a value that is the average of the measured two or three corner regions for that plate,
which was then averaged with the measured enclosure temperature. This second average
was used because simulation results show that significant portions of the corner regions
are cooler than the location where the temperature is measured. The second type of spacer
plate boundary condition is a Uniform Temperature, in which the area-weighted-average
temperature for each plate is applied to that plate’s entire outer surface. In the third type
of boundary conditions, the outer surfaces of the spacer plates were simply insulated.

Conduction, natural convection, and radiation heat transfer within the domain were
simulated using ANSYS/Fluent. The steady-state momentum and energy equations were
solved using a pressure-based solver where the pressure-velocity coupling was achieved
using the SIMPLE scheme and discretization was achieved using a second order upwind
scheme [27]. The discrete ordinate model was used to calculate radiation heat transfer.
For natural convection, buoyancy induced flow was generated using gravitational
acceleration in negative $z$-direction. Temperature-based density was applied to helium for
the steady-state pressure measured for each experiment.

To check the sensitivity of the mesh, two finer meshes were constructed with
2,111,992 and 4,730,080 elements. Simulations representing Experiments I and IX (see
Table 3.2) were performed using all three meshes. The difference between the maximum
temperatures for each mesh was less than 0.3°C. Hence, the coarse mesh shown in Fig. 3.7 was used for all presented simulations.

3.4 Simulations Results

Figure 3.8 shows simulation results for the rod heat generation rate, gas pressure and enclosure wall and spacer plate temperatures measured for Experiment VII. These simulations employed the Regional Temperature spacer plate boundary conditions. Figure 3.8a shows rod surface temperature contours. Half of the rods are removed to expose the center of the array. The hottest region is slightly above the array mid-height, at \( z = 4.4 \text{ cm} \). Much of the central rod surface temperatures are fairly uniform, but the temperature exhibits rapid drop offs at the rod tops and bottoms, and on rods close to the walls. Figure 3.8b shows the vertical component of gas velocity at the mid-height (\( z = 0 \)). The surface is colored according to the gas temperature. It shows that natural convection causes the warm gas near the center to move upward with a maximum speed of around 4 cm/s, and downward along the walls with a peak of around -3 cm/sec. The gas moves in rounded-cross-section up-flowing and down-flowing jets in between the heater rods.

For Experiment VII, the average measured enclosure wall temperature and the maximum measured rod temperature are, respectively, 217.5°C and 288.8°C, corresponding to a maximum rod-to-wall temperature difference of 71.3°C. The simulation shown in Fig. 3.8 used the measured enclosure temperatures as boundary conditions, and predicted a temperature difference of 71.9°C. A simulation performed with no fluid motion gave a temperature difference that was only 0.01% larger. Another simulation was performed with surface emissivity of 0.75 (reduced from unity), and gave a temperature difference of 88.5°C. These results indicates that natural convection
contributes little to heat transfer in this system, but radiation and conduction are both important.

The solid lines in Fig. 3.4 show the temperatures within the $\alpha$, $\beta$ and $\eta$ rods from simulations that use the Regional Temperature spacer plate boundary conditions. Even though there are multiple rods in each of these groups, only one line is needed since, due to the precise symmetry of the simulation domain and boundary conditions, the temperatures in all the rods are identical. For both Experiment III and VII, the rod temperatures are fairly uniform in the middle 20 cm of the rods and drop off near the top and bottom spacer plates, and the $\alpha$ and $\beta$ rods are significantly warmer than the $\eta$ rods. The simulations show that the heat loss through the outer surfaces of the spacer plates is
less than 8% of the total rod heat generation rate. In the $\alpha$ and $\beta$ rods, the location of the maximum temperature is at a larger value of $z$ for Experiment III than for Experiment VII. This is caused by natural convection, and is similar to the trend exhibited by the measurements.

Temperature profiles from simulations that use the Uniform Temperature spacer plate condition are nearly the same as those from the Regional Temperature boundaries, and so are not included. The dotted lines in Fig. 3.4 show rod temperatures results assuming the spacer plate outer surfaces are insulated. While insulation increases the temperatures of the rod ends, it has little effect on the middle 10 cm of the rods, where the highest temperatures reside. From this, we conclude that the majority of the heat generated within the center region of the rods is transferred radially to the enclosure walls, and not axially to the endplates. To confirm this, simple two-dimensional simulations were performed using the mesh shown in Fig. 3.7a. The $\times$, $+$ and $*$ symbols at $z = 0$ of Fig. 3.4 show temperatures within the $\alpha$, $\beta$ and $\eta$ rods groups, respectively. The good agreement between the two-dimensional and three-dimensional simulations for both Experiment III and VII indicate that the spacer plate thermal boundary conditions have very little effect on maximum rod temperatures, which are located near the rod mid-height.

### 3.5 Comparison between Simulated and Measured Rod Temperatures

In Fig. 3.4, the simulated temperature for all three rods ($\alpha$, $\beta$, and $\eta$) in both Experiment III and VII are within 3°C of the measured values at all four elevations where they are measured, $z = -17$, 0, 17 and 29 cm. For the $\eta$ rods, which are near the array corners, the simulated temperature is below the measured value at $z = 17$ cm, but above it
at $z = -17$ cm. An additional simulation was performed using an axially varying enclosure temperature that was hotter at the top than at the bottom, based on the measured enclosure temperatures. The resulting simulated temperatures for the $\eta$ rod is in better agreement with the measurements than curves in Fig. 3.4, and had little effect on the $\alpha$ and $\beta$ rods. This suggests that temperatures of rods in the periphery of the array are more affected by the wall temperature than those near the center. This supports the assessment that rods near the array periphery may exhibit larger configuration errors than ones near the array center, since they are more sensitive to the enclosure temperature profile.

Since the measured enclosure wall and spacer plate temperatures are used as boundary conditions, the simulations essentially calculate the temperature difference between the rods and the enclosure. To compare the simulated and measured temperatures,
for all 47 thermocouples in each of the 12 experiments, we calculate the measured rod
temperature minus the average wall temperature, $\Delta T_m = T_m - \bar{T}_W$, and the simulated rod
temperatures minus the wall temperature, $\Delta T_s = T_s - \bar{T}_W$. Since 21 measurements were
excluded based on the Modified Thompson Tau test, there are 543 measurements and
simulation results. Figure 3.9 is a plot of the simulated versus measured temperature
differences. These temperature differences are as large as $72^\circ C$. As expected, the
simulated temperature difference increases as the measured difference increases, and the
correlation appears to be linear.

If the simulations perfectly recreated the measured data, then all of the data would
lie along $\Delta T_s = \Delta T_m$, which is shown in Fig. 3.9 using a thin solid line. The simulated
results are scattered in a fairly narrow band above and below that line. The dotted line in
Fig. 3.9 shows the best linear fit to the data, $\Delta T_{s,fit} = m \Delta T_m + b$, where $m$ and $b$ are
respectively the slope and intercept found from the least-squares technique. For the results
in Fig. 3.9, $m = 1.02$ and $b = -1.2$ °C. The difference between the best-fit line and the
ideal line $\Delta T_s = \Delta T_m$ is an indication of the systematic differences between the simulated
and measured temperatures. The solid and dotted lines in Fig. 3.9 show that this difference
is small compared to the random differences.

The scatter of the results above and below the best-fit line is an indication of the
random differences between the simulations and measurements. The estimate of the best-
fit line’s random error, with a 95%-confidence level [26], is calculated as:

$$E_{95} = 2 \sqrt{\frac{\sum (m\Delta T_m + b - \Delta T_s)^2}{N-2}}.$$

Eqn. 3.3
The summation is carried out for the \( N = 543 \) pairs of \( \Delta T_m \) and \( \Delta T_S \). In terms of Fig. 3.9, this is the vertical distance above and below the best-fit line that statistically contains 95% of the data. For the results in Fig. 3.9, \( E_{95} = 5.7 \, ^\circ\text{C} \), and dashed lines are placed 5.7 °C above and below the best-fit line. The region between these two lines contain roughly 95% of the results.

**Table 3.3** Slope and Intercept values of regression line for difference boundary conditions and models tested

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Slope ( m ) [-]</th>
<th>Intercept ( b ) [°C]</th>
<th>Random Error ( E_{95} ) [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>1.02</td>
<td>-1.2</td>
<td>5.7</td>
</tr>
<tr>
<td>Concentric Heater Rods</td>
<td>1.02</td>
<td>-1.1</td>
<td>5.6</td>
</tr>
<tr>
<td>Area-Weighted Average Spacer Plate Temperature</td>
<td>1.02</td>
<td>-1.5</td>
<td>6.2</td>
</tr>
<tr>
<td>Baseline (without Outermost Heater Rods)</td>
<td>1.02</td>
<td>-0.1</td>
<td>4.4</td>
</tr>
<tr>
<td>Baseline (Maximum Temperature Only)</td>
<td>0.99</td>
<td>1.4</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Table 3.3 reports the best-fit slope, intercept and random error for several simulations and comparisons. The baseline comparison, which is presented in Fig. 3.9, uses (a) the simulation mesh with rods placed eccentrically within the spacer plate holes, (b) the Regional Temperature spacer plate boundary condition, and (c) all 543 qualified measurements. The best-fit slope, intercept and random error for the baseline are given in the first line of Table 3.3. Under ideal conditions, \( m = 1, b = 0 \) and \( E_{95} = 0 \), and simulations that give parameters that approach those values are judged to be superior to ones whose values are further away. Table 3.3 shows that simulations using the computational domain
with rods placed concentrically (rather than eccentrically) in the spacer holes gave parameters that are slightly more favorable than the baseline. Simulations that use the Uniform Temperature (Area-Weighted Average) spacer plate boundary condition gave larger random errors than the baseline.

The random differences between the measured and simulated temperatures are affected by inaccuracies of the simulations, configuration errors, and thermocouple measurement errors. The objective of this work is to assess the inaccuracies of the simulations. As discussed earlier, the configuration errors are larger in the array periphery than they are near its center. Table 3.3 shows that if the outermost rods (all rods in rows A and H, and column 1 and 8 of Fig. 3.3) are eliminated from the comparison between the simulations and measurements, then the random differences between the measured and simulation results is reduced to 4.4°C. If only the maximum measured and simulated temperatures are compared, the random error is only 2.0°C, a 63% reduction compared to the baseline comparison. This is not substantially larger than the thermocouple measurement uncertainty of 1.1°C. However, the simulations systematically overpredicted the maximum temperature. We view these latter comparisons to be a better assessment of the uncertainties of the simulation methods than the ones that include all of the rods, because the outer rods are more affected by configuration errors.
CHAPTER 4

RAREFIED GAS EXPERIMENT

In this chapter, the design and construction of an experimental apparatus consisting of a 7×7 array of electrically-heated-rods maintained between two spacer plates and enclosed inside a square cross-section stainless steel pressure vessel is presented. The experiment is used to evaluate the temperature of the rods in a geometry relevant to a nuclear fuel assembly within a dry storage canister subjected to vacuum drying conditions. Thermocouples are installed in all the heater rods, spacer plates and enclosure walls to provide a complete temperature profile of the experiment. Various pressures, ranging from ~ 50 to 10^5 Pa of dry helium and heat generation rates Q = 50, 100 and 150 W relevant to vacuum drying conditions are tested. The results from this experiment will be used in the following chapter to validate CFD simulations for vacuum drying condition (low pressure).

4.1 Experimental Apparatus

The experiment was designed to represent a central portion of a 7×7 fuel assembly surrounded by stainless steel basket between two consecutive spacer plates inside a nuclear canister oriented vertically. The experimental apparatus consists of a stainless steel enclosure containing heater rods bundled in a 7×7 configuration and held by two spacer plates. Figure 4.1 shows the model of the experiment. The enclosure is made transparent to show the inner parts of the experiment. The most important components of the experiment are described below.
4.1.1 Heater Rods

Electrically powered heater rods are used to simulate fuel rods of a nuclear assembly between two consecutive spacer grids. Each rod consists of a Nichrome heating coil surrounded by compressed magnesium oxide (MgO) cement and covered with a stainless steel sheath of 0.72 mm thickness. They have a diameter of $1.25 \pm 0.003$ cm and a total length of $65 \pm 0.5$ cm long. Each heater rod is rated to be $20 \pm 1$ W. Heat is generated
throughout the length of the rod except for unheated sections at both ends. The unheated length was designed by the manufacturer to be 2.2 cm long. However, by taking X-rays of 10 random heater rods, the unheated length was found to be 3 cm on average. As the rods are bundled together in a 7×7 array, seven rods in each of the seven rows are connected in series. These seven groups are then connected in parallel.

All the heater rods have one type-K thermocouple installed at one of five different axial locations. The uncertainty of these thermocouples is ±2.2°C. There are 21 heater rods with thermocouple at their axial center (z = 0 cm, Plane 0), 13 rods with thermocouple at z = 25 cm (above the axial center, Plane 25), 11 rods with thermocouple at z = -25 cm (below the axial center, Plane -25), 2 rods with thermocouple at z = 10 cm and two others with thermocouples at z = -10 cm. The above cited axial locations of the thermocouples were provided by the manufacturer. A test was conducted to check their locations, and it was found that their actual location varied within ±5 cm from the value stated by the manufacturer. The new location of the thermocouples was determined with an uncertainty of ± 3 mm.

4.1.2 Spacer Plate

Two square stainless steel plates with a thickness of 1.5 mm and a length of 11.5 cm, are used to maintain the heater rods in the 7×7 configuration. Each plate has 49 holes with a diameter of 1.17 cm and a center-to-center pitch of 1.625 cm. The corners of spacer plates were rounded to accommodate the inner shape of the enclosure and to leave a constant circumferential gap between the plates and enclosure inner walls. Small slots on four edges of the spacer plate are created to bolt the plates to the support rods, which are
used to secure the spacer plates and heater rods in place, see Fig. 4.1b and 4.1c. Fourteen (14) type-K thermocouples, with an uncertainty of ±1.1°C, are welded to small holes of 1 mm diameter and 0.5 mm depth, drilled in specific locations of the spacer plates, see Fig 1c. These thermocouples are used to obtain a complete temperature profile of the spacer plates.

4.1.3 Support Rods

Support rods are used to secure the spacer plates and heater rods in place. Figure 4.1b shows two support rods bolted to the top spacer plate and enclosure. The length, width and thickness of each rod is 21.5 cm, 0.65 cm and 0.6 cm. The top of each rod has a threaded hole to bolt the spacer plate to the rod as shown in enlarged view of section B in Fig. 4.1d. A step is machined on the same end with a depth equal to thickness of the spacer plate. The thickness of the step is equal to the gap between the spacer plate and enclosure wall as shown in Fig. 4.1d. On the other end, a slot was machined to bolt the supporting rod to the enclosure wall. The slot facilitates ease in assembly small amount of movement of the support rods relative to the enclosure wall. This ensures the change in length of the heater rods without bending when temperature changes. Eight support rods are used, four on each spacer plate.

4.1.4 Enclosure

The enclosure consists of a square stainless steel tube with 12.7 cm outside dimension and a wall thickness of 4.75 mm. The total length of the tube is 122 cm. The dimension of two sides is slightly different (12.76 cm and 12.90 cm). Since the tube is constructed by folding a stainless steel plate, the corners are round. On the outer walls of the enclosure, grooves of 1.2 mm depth and 1 mm wide were machined to host 13
thermocouples on each wall as shown in Fig. 4.2a. These thermocouples are calibrated and their uncertainty is ±1.1 °C. The thermocouple locations are shown as small circles at the beginning of these grooves. On each wall, there are three thermocouples located at $z = 0$ cm (axial center), $z = 30$ cm and $z = -30$ cm (spacer plate axial locations), and a thermocouple each at $z = -15$ and $15$ cm. Two thermocouples are placed beyond spacer plate level. These thermocouples provide complete axial and longitudinal temperature profiles of the four outer walls of the enclosure.

The enclosure is covered with 2.5 cm thick insulation board on all four walls. 2.5 cm thick insulation blanket is used to cover other parts where flat board cannot be used. Additional 2.5 cm thick insulation was also used on top of insulation board for experiments with 5 cm thick insulation.

4.1.5 Vacuum System

Ultra-high vacuum flanges were welded to both ends of the enclosure to hold vacuum inside the chamber. The top flange hosts four thermocouple feedthroughs and one power feedthrough, which are used to connect the heater rod and the top spacer plate thermocouples. The bottom flange houses a thermocouple/power feedthrough and a vacuum tree. The vacuum tree consists a stainless steel tube attached to which are a vacuum pump (HiCube 80 Eco), pressure gages (MKS 626 C 1000 and MKS 622B 20), and a helium tank through an open/close and a leaking valve. Both pressure gages have uncertainty of 0.25% of reading and the zero-temperature coefficient error is 0.005% of full scale. This induces the pressure reading error of 6.6 Pa and 0.13 Pa per °C of change in the ambient temperature for 1000 Torr and 20 Torr pressure gage respectively. For
pressure below ~ 2000 Pa, readings from MKS 622B 20 is used. Figure 4.3b shows a picture of the experimental apparatus fully assembled.

4.1.6 Symmetry groups

In order to obtain the complete temperature profile from the heater rods, the location of the thermocouple in each heater was strategically chosen by taking advantage of the geometrical symmetry of the experiment. If all the enclosure walls have the same temperature profile, then there is symmetry across \(xz\) and \(yz\) planes, and planes passing through \(d_1d_1'\) and \(d_2d_2'\) of the square enclosure, as shown in Fig. 3a. Therefore, only a one-eight (\(1/8\))th cross-section can represent the complete temperature profile of the experiment. The circles in Fig. 4.3a represent the heater rod and the numerical values inside these circles represent the distance in centimeters of the thermocouple location from the axial center in each rod. The Greek letters represent the group of rods that are in symmetric locations in all the one-eight sections. There are ten symmetric locations in each section and hence, ten symmetry groups. Since all the symmetry groups, except the centermost one that has just one heater rod, have rods with thermocouples at various axial locations, axial profiles of temperature can be generated for each group. For example, the group \(\delta\) has four heater rods, two of these rods have a thermocouple at \(Plane\ 0\) and the two others have a thermocouple at \(Plane\ -25\) and 25, respectively. Figure 4.3b shows the number of rods with thermocouples at the same axial location (or \(Plane\)) for each symmetry group. The left one-eight section gives the Greek letter names of the symmetry groups, however the next three sections give the number of thermocouples in \(Plane\ -25\), \(0\), and 25, respectively. All groups have at least one thermocouple in all planes, except for group \(v\), which has no thermocouple
The thermocouples that are in the same symmetry group and the same plane should ideally measure the same temperature. Therefore, they are used to verify the symmetricity assumption of the experiment.

The row position of the heater rods are represented by alphabets from A to G, whereas the columns are represented by numbers from 1 to 7, as shown in Fig. 4.3a. The combination of alphabets and numbers can be used to name the heater rods in any position if needed.
4.2 Experimental Conditions

Experiments are carried out for heat generation rates of \( Q = 50, 100 \) and \( 150 \) W, nine nominal pressure, \( P_N \) ranging from \( 58 \) to \( 10^5 \) Pa and two insulation thicknesses \( I = 2.5 \) cm and \( 5 \) cm. The pressure values are selected according to Knudsen number (Eqn 1.1 and 1.2). Based on the dimensions of the experiment, helium is in continuum and slip regime for the pressures applied during the experiment.

Table 4.1 Nominal pressure, heat generation and insulation thickness for different experimental cases and final pressure for each experimental case

<table>
<thead>
<tr>
<th></th>
<th>( Kn )</th>
<th>10</th>
<th>20</th>
<th>50</th>
<th>100</th>
<th>300</th>
<th>1000</th>
<th>3000</th>
<th>10000</th>
<th>20000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Pressure, ( P_N ) [Pa]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>58</td>
<td>116</td>
<td>290</td>
<td>580</td>
<td>1745</td>
<td>5820</td>
<td>17460</td>
<td>58190</td>
<td>116380</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5 cm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( Q )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50 W</td>
<td>65</td>
<td>129</td>
<td>284</td>
<td>590</td>
<td>1746</td>
<td>5816</td>
<td>17850</td>
<td>57938</td>
<td>101788</td>
<td></td>
</tr>
<tr>
<td>100 W</td>
<td>65</td>
<td>126</td>
<td>276</td>
<td>575</td>
<td>1771</td>
<td>5762</td>
<td>17484</td>
<td>58095</td>
<td>112715</td>
<td></td>
</tr>
<tr>
<td>150 W</td>
<td>72</td>
<td>135</td>
<td>299</td>
<td>576</td>
<td>1721</td>
<td>5749</td>
<td>17548</td>
<td>58243</td>
<td>108045</td>
<td></td>
</tr>
<tr>
<td>5 cm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50 W</td>
<td>65</td>
<td>135</td>
<td>302</td>
<td>593</td>
<td>1750</td>
<td>5793</td>
<td>17400</td>
<td>55741</td>
<td>103535</td>
<td></td>
</tr>
<tr>
<td>100 W</td>
<td>85</td>
<td>139</td>
<td>285</td>
<td>580</td>
<td>1749</td>
<td>5774</td>
<td>17440</td>
<td>58077</td>
<td>103267</td>
<td></td>
</tr>
</tbody>
</table>

Initially, the experimental apparatus was outgassed for few days with an applied heat generation rate of \( 50 \) W to assist in the outgassing process. The experiments are conducted for one value of \( Q \) for all nine nominal pressures before moving on to next \( Q \) value. Between each experiment, the apparatus is vacuumed for approximately 30 min. As the pressure inside the apparatus is not precisely controlled, the final pressure varies slightly from nominal pressure. Table 4.1 shows nine Knudsen number and corresponding nominal pressures that are varied for different experiments for two different insulation thickness. The insulation is indicated by \( I = 2.5 \) cm and \( I = 5 \) cm for \( 1 \) and \( 5 \) cm insulation
thickness respectively. The final pressure for each experiment is also shown. The ambient 
temperature in lab varies within 21 to 23 °C. Each experiment takes about 36 hours to get 
to steady state. The experiments are run for few additional hours past steady state to collect 
data.

4.3 Experimental Results

4.3.1 Temperature profile of the enclosure walls

As mentioned earlier, 13 thermocouples are installed in each of the four walls to 
measure the temperature. Figure 4.4 shows the temperature variation along z-axis of the 
four walls for lowest nominal pressure, $P_N = 58 \text{ Pa}$ for $I = 2.5 \text{ cm}$ respectively. The 
temperature profile is plotted for thermocouple installed along center of enclosure wall. 
The temperature measured by thermocouples beyond the spacer plate location is not 
presented, as they are not of particular interest for this study. The temperature of the wall 
varies significantly along the axial direction ($z$-axis). The axial wall temperature profiles 
are slightly asymmetric across the mid-plane. The temperatures measured above the mid-
plane ($z > 0$) are slightly larger than the ones below it ($z < 0$). The maximum temperature 
measured is at axial center and the minimum temperature measured is at the lowest $z$ in 
Fig. 4.4. The difference of temperature for all four walls at same $z$-location is less than 2 
°C. Furthermore, the temperature variation on each enclosure wall along the longitudinal 
direction ($x$ or $y$ axes) is less than 2 °C in all cases. Hence, the average of all measured 
temperatures of four walls at same $z$-location is used to represent temperature profiles of 
the walls. The solid line in Fig. 4.4 shows the fit curve for average wall temperature along 
axial direction.
4.3.2 Temperature Profile of Spacer Plate

The temperature profiles of the spacer plates along $x$-$y$ directions are expected to form a dome shape with the highest temperature at the center of the plates. The six thermocouples along the diagonal of the spacer plates (see Fig. 4.1c) are used to generate their temperature profiles as a function of radial distance from the center. Figure 4.5 shows the temperature profiles for the top and bottom spacer plates for the case, $P = 65$ Pa, $Q = 50$ W, and $I = 2.5$ cm. The temperature of the top spacer plate is higher than the bottom spacer plate in the central region but is lower in the peripheral region. This behavior is observed for all cases with insulation thickness of 2.5 cm, which suggests that more heat is being conducted through the lower part of the experiment through the central region of the spacer plate and more from the top in the peripheral region. This is due to the presence
of vacuum tree connected to the bottom of the experimental apparatus. Moreover, the experiment rests on a table creating an additional path for heat conduction. However, for $I = 5 \text{ cm}$ insulation thickness cases, the temperature profile of top spacer plate is higher than bottom spacer across the whole radial distance for the same reason explained above. The spacer plate temperatures are averaged using a second-order polynomial equation as shown in Fig. 4.5.

### 4.3.3 Temperature variation with pressure

Figure 4.6 and 4.7 shows the maximum and minimum wall temperature and average temperatures of two spacer plates for all heat generation rates as a function of pressure for

$$T_{SP, t} = -0.1353r^2 + 3E-05r + 84.07$$

$$T_{SP, b} = -0.0453r^2 + 1E-05r + 82.76$$
Figure 4.6: Average top and bottom spacer, maximum and minimum wall temperature for nine pressures for $Q = 50, 100$ and 150 W for $I = 2.5$ cm
I = 2.5 and 5 cm respectively. The maximum wall temperature is the average of all measured temperatures at z = 0 plane from four walls. Similarly, the minimum wall temperature is the average of all measured temperatures at z = -30 cm. The variation in maximum and minimum enclosure wall temperatures is less than 1.5 °C as pressure varies and seems to be mainly affected by the variation in room temperature, as their profiles look
very similar for all heat generations. The average spacer plate temperatures are between the maximum and minimum wall temperatures. The average temperature of top spacer plate is higher than bottom spacer plate for all cases. This difference is higher in the cases with \( I = 5 \text{ cm} \). As the pressure decreases from \( \sim 10^5 \) to 5000 Pa (continuum regime), the average spacer plate temperature is almost constant. As the pressure decreases below 5000 Pa (slip regime), a noticeable increase in the spacer plate temperature can be observed. This is due to the effect of gas rarefaction (temperature jump).

4.3.4 Consistency Check of Heater Rod Temperature

As shown in Fig. 4.3, there are ten symmetry groups of heater rods. Among them, there are nine groups at Plane 0, four groups at Plane 25, and three groups at Plane -25 with at least two thermocouples at those planes. Comparing the temperatures at these symmetric locations, the symmetricity and/or consistency of measurements can be checked. Symmetricity is checked if the maximum difference between the thermocouples at the same axial location and symmetry group is smaller than the uncertainty on thermocouples, \( \pm 2.2^\circ\text{C} \). However, consistency is verified if the calculated temperature difference between thermocouples at the same axial location and symmetry group is nearly constant as the pressure changes.

It was mentioned in the **Heater Rods** section that the thermocouple location in some of the heater rods was found to vary by as much as \( \pm 5 \text{ cm} \) from the pre-determined location. These heater rods are not included in the symmetricity/consistency check as their temperature may vary considerably.
Figure 4.8: Maximum temperature difference between heater rods at the same symmetric location for three different planes and for all $Q$, with insulation thickness, $I = 2.5$ cm.

Figure 4.9: Maximum temperature difference between heater rods at the same symmetric location for three different planes and for all $Q$, with insulation thickness, $I = 5$ cm.
Figures 4.8 and 4.9 show the maximum temperatures difference between thermocouples that are at the same symmetric location and symmetry group for three different planes, for all heat generations rates and all nine pressures, and the two insulation thicknesses, respectively. The symmetric locations are plotted as the radial distance from the origin of the xy-plane. The circular markers indicate Plane 0, square markers indicate Plane 25, and diamond markers indicate Plane -25. If the experiment is perfectly symmetric and thermocouple uncertainty is zero, then the temperature difference between thermocouples at the same axial location and symmetry group will be equal to zero. These figures show that there are some differences between the symmetric thermocouples, which are due to geometrical and thermocouple axial location uncertainties, and error related to temperature measurements. From these plots, it can be observed that the maximum difference increases as heat generation increases for all thermocouples in symmetric locations. Most of these differences are less than the uncertainty on the temperature measurement. The obtained maximum differences for the 2.5 cm insulation thickness are as high as 1.7, 2.5 and 3.0 °C for \( Q = 50, 100 \) and 150 W, respectively. For the 5 cm insulation thickness, the maximum differences are as high as 2.1 and 3.0 °C for \( Q = 50 \) and 100 W, respectively.

As the pressure changes, it seems that there is no or a negligible variation in the maximum temperature difference for the symmetric thermocouples. This demonstrates that the experimental results are very consistent with regard to the pressure variation. Since the variation in temperature difference is negligible, this suggests that these differences are due to systematic error caused by the variation of the axial location of the thermocouples in the heated rods.
4.3.5 Maximum Temperature of Heater Rod

Figure 4.10 shows the maximum heater rod temperature minus maximum wall temperature as a function of pressure for all heat generation rates and two insulation thicknesses. The maximum heater rod temperature is measured at the central rod (D4, see Fig. 4.3a), which has a thermocouple installed at the axial center ($z = 0$ cm). The maximum wall temperature is the average of all measured temperatures at $z = 0$ plane from four enclosure walls as mentioned earlier. The error bar indicates the uncertainty of the thermocouples used for measurement, and is equal to 2.2°C. The dotted vertical lines indicates the limits of the continuum and slip regimes. However, the dashed horizontal lines show the average of the continuum regime temperatures.

It is clear from Fig. 4.10 that the temperature difference in the continuum regime is nearly constant for all heat generation rates and insulation thicknesses. However, in the slip regime, the temperature difference increases as the pressure decreases below 2000 Pa. This increase in temperature is due to temperature-jump caused by rarefaction effect at low pressures, which acts as thermal resistance at the gas-solid interfaces. It can also be noticed that, for a given insulation thickness, the increase in temperature difference is larger as heat generation rate, $Q$, increases. However, for the same heat generation rate, the increase in temperature difference is lower for thicker insulation. Furthermore, temperature differences obtained for the 5 cm insulation are lower than those obtained for the 2.5 cm thick insulation. As more insulation is added to the experiment, the temperatures of the experiment, including heater rods and enclosure wall, increase considerably. This causes heat transfer by radiation to relatively increase compared to conduction heat transfer through helium, which decreases the temperature difference between the heater rods and
Table 4.2 Temperature increase due to rarefaction effect

|  | Temperature increase due to rarefaction [°C] |
|---|---|---|---|
|  | $I = 50$ W | $Q = 100$ W | $Q = 150$ W |
| 2.5 cm | 9.8 | 17.7 | 25.7 |
| 5 cm | 8.8 | 16.0 | - |
enclosure walls. The total temperature increase caused by rarefaction effect for each heat generation and insulation thickness is given in Table 4.2. This increase is as high as 25.7 °C for $Q = 150$ W and for insulation thickness of 2.5 cm.

4.4 Conclusion

An experimental setup representing a central portion of a 7×7 fuel assembly between two consecutive spacer plates within a square basket and inside a canister is designed and constructed. The experiment was used to study the effect of gas rarefaction during vacuum drying process applied to nuclear fuel assemblies. The experiment consists of a stainless steel enclosure containing heater rods bundled in a 7×7 configuration and held by two spacer plates. Dry helium was used as the working gas. The experiments were conducted for nine different pressures ranging from 65 to $10^5$ Pa and for three heat generation rates of 50, 100 and 150 W, and two insulation thicknesses of 2.5 and 5 cm. Thermocouples were installed on the enclosure outer walls and spacer plates to obtain their profiles. For the same heat generation rate and insulation thickness, the enclosure wall temperature profile was not affected by pressure change. However, the temperature of the spacer plates slightly increased when the pressure was decreased.

Furthermore, as the pressure was decreased, the temperature of the heater rods increased considerably. The increase was as high as 25.7 °C for heat generation rate of 150 W, and insulation thickness of 2.5 cm. This increase in temperature was due to the effect of temperature-jump caused by gas rarefaction at the gas-solid interfaces. Quantification of the temperature-jump at all the walls cannot be done using this experiment. However, comparison to numerical simulations may allow its quantification. The experimental results obtained will be compared to the CFD simulations in next chapter.
CHAPTER 5

VALIDATION OF THE NUMERICAL SIMULATIONS

In the previous chapter, the results from experiments performed for different pressures (continuum to slip regimes), heat generation rates and insulation thicknesses were presented. The complete temperature profiles of the enclosure walls and the two spacer plates, and pressure measurements provide all the information necessary for conducting CFD simulations. The temperature of the heater rods measured at different axial locations are used as the parameters to compare with the CFD simulation results.

In this chapter, the model used for the CFD simulations is described. A sensitivity study on the effect of various parameters on the CFD simulation results is conducted to assure that the uncertainties on those parameters do not significantly affect the CFD results. Finally, the CFD simulation results for different cases are compared with the experimental results. From this comparison, the differences between the experimental results and CFD simulation results are quantified and the use of the CFD simulations in complex three-dimensional (3-D) geometry under rarefied gas conditions is validated.

5.1 Numerical Model

A three-dimensional (3D) geometrically-accurate numerical model of the 7×7 array of heated rod experimental apparatus described in the previous chapter is generated using ANSYS package. The domain consists of a bundle of heater rods surrounded by helium between two spacer plates and within a stainless steel enclosure. Figure 5.1 shows a cross section view of the computational mesh. The outer square represents the stainless steel
Figure 5.1: Computational domain in $x$-$y$ plane

Figure 5.2: 3-D Computational domain, enclosure is cut by $yz$ plane
enclosure. It contains the regions for 49 heater rods, which are composed of magnesium oxide (MgO) core within stainless steel sheaths (black rings). The heater rods are named according to position in the array by letters A to H (rows) and numbers 1 to 7 (columns). The name of five heater rods are shown inside the heater rod circle. The space between the rods and enclosure is modeled as helium gas. This mesh is extruded in the $z$-direction (normal to the plane of the mesh) to form the 3-D domain (see Fig. 5.2). At both ends of the extrusion, the properties of 1.5 mm thick regions are modified to represent two stainless steel spacer plates. The rectangular black regions in Fig. 5.1, on four sides, are small part of the support rods that maintain equal gap between spacer plate and enclosure, and exist only in 1.5 mm thick regions representing spacer plates on both ends of the domain as shown by gray colored plates in Fig. 5.2. The square enclosure is cut by $yz$-plane to show heater rod cladding (red) which are filled with MgO cement (cyan blue). The regions between the two spacer plates and the enclosure are modeled as helium (colorless). The center of the 3-D domain is the origin and $z = 0$ plane is termed as the mid-plane. A mesh sensitivity study was conducted to determine the optimum mesh in terms of accuracy and computational resources. The maximum temperature of the rods was used as a parameter for this study. Table 5.1 shows that increasing the number of mesh elements did not affect the maximum rod temperature. Therefore, the mesh # 1 with 2,180,416 elements was selected. This mesh has a high orthogonal mesh elements quality.

<table>
<thead>
<tr>
<th></th>
<th>Mesh 1</th>
<th>Mesh 2</th>
<th>Mesh 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of elements</td>
<td>2,180,416</td>
<td>3,694,704</td>
<td>10,188,024</td>
</tr>
<tr>
<td>$T_{max}$ [°C]</td>
<td>170.58</td>
<td>170.59</td>
<td>170.64</td>
</tr>
</tbody>
</table>
Conduction, natural convection and radiation heat transfer within the domain are simulated using ANSYS/Fluent. Heat is generated uniformly along the heater rods modeled as MgO cement. Temperature-dependent material properties for stainless steel and helium are used. For density of helium, ideal compressible gas law is employed. The emissivity of stainless steel used in the heater rods, the enclosure tube and the spacer plates was measured and found to be 0.21, 0.25 and 0.23, respectively, and was used in the simulations. The discrete-ordinate radiation model is used to consider radiation heat transfer. The steady-state momentum and energy equations are solved using pressure-based solver. The pressure-velocity coupling is achieved by using the SIMPLE scheme and a second-order upwind scheme is used for discretization [41].

Temperature boundary conditions from the experimental results are applied on the outer walls of the enclosure and the spacer plates. For enclosure walls, an average axial temperature profile of the four walls is used in the simulations. A temperature as a function of distance from the center of the spacer plate is used as temperature boundary condition on the outer walls of the spacer plates. The example of these profiles are presented and discussed in Chapter 4. The temperature-jump boundary conditions, as described by Eqs. 1.3 and 1.4, are applied to the gas/solid interfaces in ANSYS/Fluent. A constant value of the thermal accommodation coefficient (\( \alpha \), Eq. 1.5) was applied in all nine simulations for each heat generation rate, \( Q \). Hence, \( \alpha \) was different for each \( Q \), and was determined using the average temperature from nine experiments.

**Conductivity of Heater Rod Core**

The thermal conductivity of the heater rod core, which includes MgO cement, thermocouple and Nichrome heater coil, was not provided by the manufacturer. It was
reported in the literature that the thermal conductivity of MgO cement ranges from 4 to 30 W/mK for polycrystalline sintered disk of MgO [42], depending on the fabrication process, resulting density and temperature, which makes the actual thermal conductivity of cement used in heater rod difficult to be determined. The thermal conductivity of MgO insulation cement used in wire by commercial manufacturer mentions that the conductivity varies from 0.8 to 2.4 W/mK [43] depending upon density. A thermal conductivity of 2.07 W/mK was reported by Canan and Klein [44] for MgO used in the electrical heater rods used for similar experiment. The conductivity value of 2.07 W/mK was also used by Chalasani [29] in his study and was used in validation in Chapter 3 [40]. However, the geometry and fabrication process of the heater rods used in this study are different from the ones used in above mentioned studies. Hence, it was necessary to predict the effective thermal conductivity of heater rod core to use in this study.

In order to determine the effective thermal conductivity of the heater rod core, a comparison between CFD simulations and experimental results were performed at atmospheric pressure (~ 10^5 Pa, continuum regime) for six heat generation rates, Q, varying from 25 to 150 W. The different heat generation rates were applied to get the comparison results in different temperatures. CFD simulation predictions are satisfactorily accurate in the continuum regime. This validation has been conducted in Chapter 3 for a similar setup filled with helium at high pressures [40]. The comparison of the temperatures of all 49 heater rods from the experiment was made with the simulation results, with different thermal conductivity of the heater rod core. The conductivity value that makes the simulation results closest to the experimental data was chosen as the thermal conductivity of the heater rod core that will be applied in all simulations.
From this comparison, the effective conductivity was determined to be 4 W/mK.

The comparison results from the six heat generation rates with 4 W/mK is shown in the Fig. 5.3. The direct comparison of the measured and the simulated temperature shows good agreement for all heat generation rates indicated by different markers. The slope (1.0) and the intercept (0.29 °C) of the best linear fit equation also indicates a good agreement between the measured and the simulated results. All the data are distributed within a narrow band of 1.72 °C for 95% of confidence interval calculated by Eqn. 3.3 in Chapter 3.

5.2 Sensitivity Study on the Parameters Affecting Simulation Results

A sensitivity study on the effect of the experimental uncertainties on the simulation results was conducted. These uncertainties are mainly related to the temperature measurements. The uncertainty of the thermocouples used to measure the enclosure wall
and spacer plate temperature is ± 1.1 °C. The uncertainty in the pressure measurement is small (< 0.5% of reading) to make any significant difference. Another parameter that can affect the simulation results is the value of thermal accommodation coefficient, \( \alpha \). As mentioned earlier, a constant value of \( \alpha \) corresponding to the average temperature of nine experiments for a heat generation rate, \( Q \), is used for simulation. As \( \alpha \) is temperature dependent, and different surfaces in the experiment have different temperatures, there is uncertainty related to the use of constant value of \( \alpha \) in the simulation. If these uncertainties are taken into account in the simulations, they may affect the results considerably.

To quantify the effect of the uncertainties mentioned, the sensitivity tests were conducted for three nominal pressures \( (P_N = 116380, 1745 \text{ and } 54 \text{ Pa}) \) at three heat generation rates. The three pressures are chosen to represent the continuum regime \( (P_N = 116380 \text{ Pa}) \), the continuum/slip regimes limit \( (P_N = 1745 \text{ Pa}) \), and the slip/transitional regimes limit \( (P_N = 54 \text{ Pa}) \). The first sensitivity test is conducted for different temperature boundary condition at the enclosure wall and the spacer plates \( (T_W \text{ and } T_{SP}) \). The uncertainty of thermocouple, ±1.1 °C, is added to and subtracted from the maximum and minimum temperature profile among four enclosure walls (Fig. 4.4) respectively, measured for each experiment. Similarly, for the spacer plates, 1.1 °C is added to and subtracted from the temperature profile shown in Fig. 4.5. The obtained highest and lowest possible temperature boundary condition for the enclosure wall and the spacer plates are applied in the CFD simulation. Similarly, two different values of \( \alpha \) corresponding to the maximum heater rod temperature and minimum enclosure wall temperature measured in the experiment are applied in the simulation. The maximum temperature of centermost heater rod predicted from simulation is used as the sensitivity analysis parameter.
Table 5.2 shows the results of the sensitivity study. The second row of the table gives the three nominal pressure considered, and the first column gives the total heat generations tested. For each case \((Q, P_N)\), the maximum rod temperature obtained without varying any of the parameters (called: “Reference Case”) is given which serves as a reference. For each case, two parameters (temperature - \(T_W\), \(T_{SP}\), and \(\alpha\)) are varied separately as explained in previous paragraph, to estimate their effects on the maximum rod temperature. The results of parameter variation are given as the difference with the result of “Reference Case”. The positive values are increase in the temperature whereas negative values means decrease in temperature.

<table>
<thead>
<tr>
<th>Nominal Pressure, (P_N)</th>
<th>(Q = 50) W</th>
<th>(Q = 100) W</th>
<th>(Q = 150) W</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>54 Pa</td>
<td>1745 Pa</td>
<td>116380 Pa</td>
</tr>
<tr>
<td>Reference Case</td>
<td>107.65</td>
<td>98.24</td>
<td>97.39</td>
</tr>
<tr>
<td>(T_W, T_{SP})</td>
<td>1.7</td>
<td>-1.33</td>
<td>1.86</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>0.17</td>
<td>-0.32</td>
<td>0.00</td>
</tr>
<tr>
<td>Reference Case</td>
<td>181.22</td>
<td>163.91</td>
<td>162.02</td>
</tr>
<tr>
<td>(T_W, T_{SP})</td>
<td>1.95</td>
<td>-1.16</td>
<td>2.53</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>0.89</td>
<td>-0.61</td>
<td>0.04</td>
</tr>
<tr>
<td>Reference Case</td>
<td>242.64</td>
<td>221.35</td>
<td>218.57</td>
</tr>
<tr>
<td>(T_W, T_{SP})</td>
<td>2.12</td>
<td>-0.96</td>
<td>2.47</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>1.63</td>
<td>-0.87</td>
<td>0.11</td>
</tr>
</tbody>
</table>

From Table 5.2, it can be observed that the effect of the enclosure (\(T_W\)) and the spacer plate (\(T_{SP}\)) temperature is within the maximum difference of 2.59 °C. The behavior of variation of the maximum heater rod temperature for different pressures and the heat
generation rates do not hold significant meaning. This behavior may just be the effect of high/low deviation in temperature measurement of the four walls for particular case, because the average of all four walls is used in “Reference Case”. On the other hand, the effect of $\alpha$ is significant only at the lowest nominal pressure, $P_N$. This is expected as pressure of 1745 Pa is in slip-continuum regime where temperature jump effect is not as significant. The effect of $\alpha$ variation increases as $Q_T$ increases. The maximum temperature increase of 1.63 °C is observed for the case $Q = 150$ W and $P_N = 54$ Pa, which is caused by the decrease of $\alpha$. This variation in $\alpha$ may be reduced if a temperature-dependent thermal accommodation coefficient is used in the simulations. Currently, the implementation of temperature dependent $\alpha$ is not possible in ANSYS/Fluent.

5.3 Results and Discussion

Figure 5.4a shows the temperature contour of the computational domain, cut by $yz$-plane to show the array temperature at middle, for the case $P = 64$ Pa and $Q = 100$ W. The central heater rod experiences the highest temperature of 181°C at $z = 0$ cm (mid-plane). The outer temperature gradient in the enclosure wall shows the measured temperature profile used as boundary condition for the simulation. Figure 5.4b shows the temperature profile at the mid-plane. The temperature is highest at the central region and decreases rapidly towards the enclosure wall. The contour of temperature for other heat generations and pressures are very similar to Fig. 5.4 with different temperature range.
To observe the profile of temperature change from central region to enclosure wall, the temperature profiles along the horizontal line drawn in Fig. 5.4b are plotted in Fig. 5.5 and Fig. 5.6. The profiles are plotted for the lowest and highest pressures considered for each heat generation, $Q$. The simulation results plotted as lines show that, for both pressures, the temperature gradient is larger near the enclosure wall compared to the center of the array. For all heat generations, the temperature at the enclosure wall ($x = 6.45$ cm) is nearly the same for both pressures. The temperature of the rods predicted at low pressures is always higher than at high pressures for all cases. The increase in maximum rod (central rod at $x = 0$ cm) temperature due to the decrease in pressure is 10.2, 18.1 and 24.4 °C for $Q = 50$, 100 and 150 W ($I = 2.5$ cm) respectively, and 9.3 and 15.1 °C for $Q = 50$ and 100 W ($I = 5$ cm) respectively. At the lowest pressures, helium is in the slip regime, which causes a temperature-jump at the gas/solid interfaces. This jump can be observed as vertical lines in Fig. 5.5 and 5.6 for all $Q$. However, at highest pressures, helium is in the continuum

Figure 5.4: Computational results for $P = 64$ Pa and $Q = 100$ W (a) Temperature contour of half domain (b) Temperature contour at mid-plane.
Figure 5.5: Comparison of temperature along horizontal line in Fig. 5.4b from simulation and experiment for two pressures, three $Q$ and $I = 2.5$ cm
regime, where no temperature-jump conditions are observed. The circular markers show the experimental results for the heater rods that lie in symmetry group along the horizontal line shown in Fig. 5.4b. The temperatures obtained from the simulation results are close to the experimental results at both pressures, all heat generation rates and for two insulation thicknesses.

Figure 5.6: Comparison of temperature along horizontal line in Fig. 5.4b from simulation and experiment for two pressures and $Q$ for $l = 5$ cm
The comparison of the maximum rod temperatures for all pressures for each heat generation rate is shown in Fig. 5.7 and 5.8 for \( I = 2.5 \) cm and 5 cm respectively. The plotted data shows the average temperature of five heater rods at the central region (C3, C4, C5, D3 and D4, see Fig. 5.1), which have thermocouples at mid-plane, minus the maximum enclosure wall temperature for both experiment and simulation results. The average temperature of the five heater rods is used to minimize the uncertainty on thermocouple measurements, whereas, the enclosure wall temperature is subtracted to minimize the effect of change in ambient condition during each experiment. The solid lines with filled markers represent the experimental results and the dashed lines with open marker represent the simulation results. The dotted vertical lines in each plot represent the limits of the slip and continuum regimes. The band gap between the two regimes represents the range where the two regimes overlap due to the choice of the characteristic length of the experiment used to calculate the Knudsen number. The error bars are shown for thermocouple uncertainty for experimental results. The solid and dashed horizontal line shows the average of measured and simulated temperatures in the continuum regime \((P_N=5820\) to \(P_N=113680\) Pa) respectively. The difference of this average is 0.33, 0.21 and 0.14 °C for \( Q = 50, 100, \) and 150 W respectively for \( I = 2.5 \) cm. For \( I = 5 \) cm, this difference is 0.46 and 0.22 °C for \( Q = 50 \) and 100 W respectively. It shows that in continuum regime, the simulations predict the maximum temperatures accurately within 0.5 °C.

Figure 5.7 and 5.8 shows that there is a slight increase in maximum rod temperature caused by pressure reduction in the continuum regime. As the pressure decreases further to slip regime, the increase in rod temperature is very significant. This is clearly due to the
Figure 5.7: Comparison of experimental and simulation results of the average temperature of five central heater rods as a function of final pressure for all $Q$.
temperature-jump effect in the slip regime caused by gas rarefaction, which creates a thermal-resistance at the gas/solid interfaces and causes the temperature of the rods to increase. The figures show that the CFD simulations slightly under-predicted the maximum rod temperature for most of the conditions. However, for some pressure values at $Q = 100$ and $150$ W for $I = 2.5$ cm, the simulations slightly over-predicted the temperature as well. The difference in measurement and simulation prediction is low compared to uncertainty in the thermocouple, with the maximum difference of $1.3$ °C, for $Q = 100$ W, $P_N = 580$ Pa.

Figure 5.8: Comparison of experimental and simulation results of the average temperature of five central heater rods as a function of final pressure for all $Q, I = 5$ cm.
and $I = 2.5$ cm. The total increase in temperature (temperature-jump) caused by the pressure reduction is 9.2, 16.9 and 22.8 °C for measured, and 9.2, 17.9 and 22.5 °C for simulated temperature for $Q = 50$, 100 and 150 W respectively. Similarly, this increase is 8.3 and 13.0 °C for measured, and 8.5 and 12.5 °C for simulated temperature for $Q = 50$ W and 100 W respectively for $I = 5$ cm.

Symmetricity of the experiment allows the use of rods at symmetric positions that have thermocouples at different axial locations to build axial profiles of temperature as mentioned in Chapter 4. Different symmetry groups are identified and named with Greek letters (Fig. 4.3). 10 symmetry groups with the heater rods in these groups are shown in Table 5.3. Each heater rod used in experiment has thermocouple at one of three different axial locations, $z = -25$, 0 and 25 cm from mid-plane. Figure 5.9 compares the measured and simulated axial temperature profiles of five symmetry groups ($\beta$, $\Phi$, $\Theta$, $\rho$, $\psi$) for two pressures (highest and lowest) and all $Q$ for $I = 2.5$ cm. The solid lines represent the simulation results, whereas the circular markers represent the experimental data. Error bars for the measured data are not included for the clarity of the plots. For high pressure cases ($P \sim 10^5$ Pa), the temperature predicted by simulations, for all axial location and all heat generations, seems to be very close to the measured values. For both pressures, the simulations seems to under-predict the measured temperatures around mid-plane ($z = 0$ cm) except for centermost heater rod, for which the simulation slightly over predicts the temperature. For the other two axial locations ($z = -25$ and 25 cm), simulations generally slightly under-predicts the measured temperatures. The maximum difference between measurement and simulation is observed for rods close to the central region of the array (group $\Phi$ at $z = 25$ cm) with difference as high as 7.3 °C. The high difference is observed
Figure 5.9: Comparison of the axial heater rod temperatures from simulations and experiments for five symmetry groups for all $Q, I = 2.5$ cm. Left plots are for highest pressure and right plots are for lowest pressure. Lines indicate simulation results and markers indicate experimental results.
for all pressure and heat generation rate for same heater rod temperature. However, the
difference becomes smaller as the rods are closer to the enclosure walls. Overall, the
measured axial temperatures of the heater rods correlate well with simulated temperatures
with difference less than 2°C for most of the heater rods.

<table>
<thead>
<tr>
<th>Symmetry Group</th>
<th>Heater Rods</th>
</tr>
</thead>
<tbody>
<tr>
<td>β</td>
<td>D4</td>
</tr>
<tr>
<td>δ</td>
<td>C4, D3, D5, E4</td>
</tr>
<tr>
<td>φ</td>
<td>C3, C5, E3, E5</td>
</tr>
<tr>
<td>θ</td>
<td>A4, A7, A1, A6</td>
</tr>
<tr>
<td>α</td>
<td>B4, D2, D6, F4</td>
</tr>
<tr>
<td>Ω</td>
<td>B3, B5, C2, C6, E2, E6, F3, F5</td>
</tr>
<tr>
<td>Θ</td>
<td>B2, B6, F2, F6</td>
</tr>
<tr>
<td>Ψ</td>
<td>A4, D1, D7, G4</td>
</tr>
<tr>
<td>τ</td>
<td>A3, A5, C1, C7, E1, E7, G3, G5</td>
</tr>
<tr>
<td>ω</td>
<td>A2, A6, B1, B7, F1, F7, G2, G6</td>
</tr>
</tbody>
</table>

To see how all the measured temperatures compare to simulated results, direct
comparison between simulated and measured temperatures is carried out and is presented
in Fig. 5.10 for \( Q = 50, 100 \) and 150 W. The measured temperatures of all 49 heater rods
and all nine pressures (441 points) are presented for each heat generation. The comparison
is made between the measured heater rod minus minimum measured wall temperature
(\( \Delta T_m \)) and the simulated heater rod temperature at same location minus minimum measured
wall temperature (\( \Delta T_s \)) for each case. The solid line represents the case when \( \Delta T_m = \Delta T_s \).
and if the simulations perfectly recreated the measured data, all the data points would lie on this solid line. From Fig. 5.10 and 5.11, it can be seen that most of the data points are below this line, for all heat generations, suggesting that most of the measured values are slightly larger than the simulated values. This behavior was observed in Fig. 5.9 as well. The results are scattered in narrow band for all $Q$ for both insulation thickness. The dotted lines represent the best linear fit of all the data. The slope ($m$) and intercept ($b$) of the best linear fit line for $Q = 50$ W are 0.96 and 0.02 °C, $Q = 100$ W are 1.02 and -1.97 °C and $Q = 150$ W are 1.02 and -2.34 °C, respectively, for $I = 2.5$ cm. For $I = 5$ cm, slope and intercept for $Q = 50$W are 1.00 and -0.98 °C, $Q = 100$ W are 1.02 and -2.35 °C respectively. In addition, the scatter of the results above and below the best-fit line can be used as an indication of random difference between the simulations and measurements. The estimation of best-fit line’s random error with 95% confidence level is given by Eqn. 3.3 which is

$$ E_{95} = 2 \sqrt{\frac{\sum(m\Delta T_m + b - \Delta T_s)^2}{N - 2}} $$

This summation is carried out for all $N = 441$ measured values. The value of $E_{95}$ represents the vertical distance from the best-fit line that statistically contains 95% of the data. In Fig. 5.10 and 5.11, two dashed lines above and below the best-fit line should contain 95% of the total data points. For $Q = 50$, 100 and 150 W with $I = 2.5$ cm, $E_{95} = 1.39$, 2.27 and 2.95 °C, respectively, whereas for $I = 5$ cm, $E_{95} = 1.34$ and 2.31 °C for $Q = 50$ and 100 W respectively. The random error appears to increase with increase in $Q$. The random difference between the measured and simulated temperatures are affected by inaccuracies
Figure 5.10: Comparison of simulated and measured temperatures for all pressures at each heat generation rate, $Q = 50, 100$ and $150$ W for insulation thickness, $I = 2.5$ cm
of the simulations, inaccuracies of the measurements, tolerance in size of different parts
and uncertainty in the location of thermocouple in the heater rods. Considering these
inaccuracies, the standard error of estimate for 95% confidence interval given by $E_{95}$ for
all $Q$ are fairly low.

Figure 5.11: Comparison of simulated and measured temperatures for all pressures
and both insulation thicknesses at each heat generation rate, $Q = 50$ and $100$ W for
insulation thickness $I = 5$ cm
Similar to the results presented in Fig. 5.10 and 5.11, Fig. 5.12 shows a comparison between measured and simulated temperatures for all three $Q$ and all pressures for both insulation thickness in the continuum regime (4 pressure) and slip regime (5 pressure). These figures are used to assess how accurate the CFD simulations are in the continuum and slip regimes, separately. The slope and intercept of best-fit line for continuum regime

![Graph showing comparison between measured and simulated temperatures for continuum and slip regimes.](image)

Figure 5.12: Comparison between the simulated and measured temperatures for all heat generation rates, $Q$. (a) Continuum regime ($P > 5000$ Pa) and (b) Slip regime ($P < 5000$ Pa) for both insulation thicknesses, $I = 2.5$ and 5 cm
are 1.00 and -0.86°C, respectively, and are 1.00 and -1.09°C, respectively for the slip regime. The estimate of random error given by $E_{95}$ for continuum and slip regimes are 1.85 °C and 2.35 °C, respectively. The separation of continuum regime and slip regime provides the estimate of systematic and random errors introduced in numerical simulation in slip regime compared to continuum regime. The comparison of slope and intercept of best-fit line for both regimes shows that there is no significant difference. Hence, the numerical simulation predicts the temperature in both regimes with similar accuracy. However, the random error is slightly high in slip regime compared to continuum regime.

5.4 Conclusion

The comparison between the simulation and experimental results showed that the simulations predicted the measured temperatures fairly well with simulations slightly under predicting the measurements. The maximum increase of temperature caused by the pressure decrease (rarefaction effect) is 22.5°C from simulation compared to 22.8°C from experiment for $Q = 150$ W. The direct comparison of all the data points showed that the random errors for 95% confidence interval for is as high as 2.95°C. This study demonstrated that CFD models could be used to predict the temperature of the fuel assemblies subjected to vacuum drying with good accuracy. It should be noted here that these results does not include the effect of vapor on the temperature of the rods, which is present during vacuum drying. Vapor may cause the temperature of the rods to increase further because of its low thermal conductivity, however, its effect on the temperature-jump is not known.
CHAPTER 6

CONCLUSION

During vacuum drying of a UNF canister, the temperature of the fuel cladding may increase considerably due to the effect of gas rarefaction. At low pressures associated with vacuum drying, there is a temperature-jump thermal resistance that develops at the gas-solid interfaces and causes the temperature of the fuel claddings to increase. It is important to limit the temperature of the fuel cladding to roughly 400°C, as specified by the NRC ISG-11 [3], to prevent temperature-dependent phenomena like corrosion and radial hydride formation that may cause the claddings to be unsafe for transportation and long-term storage.

In this dissertation, CFD simulations were developed and validated against an experiment subjected to conditions similar to vacuum drying. These simulations can be used later to predict the temperature of a UNF canister subjected to vacuum drying conditions. The working gas considered in this study is dry helium. The validation process is initially performed in simple 1-D and 2-D geometries by comparing the results from the CFD simulations to accurate kinetic models (S-model and DSMC) that solve the Boltzmann equation. The results showed a good agreement between the CFD and kinetic models, especially in the slip regime and for small temperature ratio. For a higher temperature ratio, the discrepancy between the kinetic and continuum approaches was large, especially for small rarefaction parameter ($\delta$). The study of simple geometries
provided an understanding on the limitation of the use of the CFD simulations in rarefied gas condition.

The validation of the CFD simulations for a three-dimensional geometry is not feasible by using the kinetic approach. Hence, the validation was conducted against experimental data, first in the continuum regime and then, in the slip regime. For validation in continuum regime, the data from previous research, which was conducted in a geometry resembling to a portion of a UNF assembly inside a canister, was available. The experiments were conducted for helium pressures of 1, 2 and 3 atm and heat generation rates of 100, 300 and 500 W. The comparison between the CFD simulations and experiment data showed that the simulations predicted the experimental temperatures with an uncertainty of 4.4 °C for 95% confidence interval. This uncertainty was much smaller if only the maximum temperature of the assembly was compared. This indicated that the maximum temperature (central heater rod) was not highly influenced by the uncertainties of the experiment. The comparison also suggested that the boundary condition applied on the spacer plates did not have significant effect on the temperatures at the axial center of the heater rods.

For the slip regime, an experimental setup similar to the one used in previous research was constructed. This experiment consisted of an electrically heated rod array held by two spacer plates inside an enclosure. The pressure of helium was varied from ~ 1 atm to 50 Pa and three heat generation rates of 50, 100 and 150W were applied. The results showed that the increase in the heater rod temperatures as the pressure was reduced from ~ 1 atm to 50 Pa was as high as 22.8 °C. The simulations predicted the maximum
temperatures within 1.3°C for all pressures. The direct comparison of all the measured temperatures for all cases with the simulation results showed that the systematic error was insignificant, and the random error increased with the increase in heat generation rate. The maximum random error was 2.95 °C for heat generation rate of 150 W. The separate comparison of results for the continuum and slip regimes showed that the simulation predicted the experiments with similar uncertainty in both regimes. This study concluded that the CFD simulations developed in this dissertation could be used to accurately predict temperature complex geometry, such as a UNF canister, subjected to low-pressure (vacuum drying) conditions.
CHAPTER 7

FUTURE WORKS

The thermal accommodation coefficient is a temperature dependent variable. In the current study, a constant value of $\alpha$ was used. Sensitivity study showed that the effect of $\alpha$ was not very significant. However, it is important to understand that the geometry used in this study resembles a small portion of a real nuclear fuel canister. The temperature difference observed was less than 100 °C across the experiment. The difference between maximum and minimum temperature in a real UNF canister will be significantly higher. Therefore, the use of a constant value of $\alpha$ for all the surfaces will not result in accurate temperature prediction. It is necessary to develop CFD simulation methods where $\alpha$ can be used as a temperature-dependent property.

The current work validated the CFD simulations for vacuum drying conditions for dry helium. However, during drying operation, the gas inside the canister is a mixture of helium and water vapor. The properties like conductivity, thermal accommodation coefficient ($\alpha$), molecular mass, viscosity, etc. of mixture of helium and water vapor are different compared to dry helium. These properties may affect the gas rarefaction condition and heat transfer significantly. However, there is not much information about $\alpha$ for a mixture of helium and water vapor at different ratios. Further research needs to be done to understand the effect of inclusion of water vapor on temperature of UNF canister during vacuum drying.
APPENDIX A

PUBLICATIONS

Journals


Journals (In Preparation)

- Maharjan D., Hadj-Nacer M., Greiner M., “Experimental Benchmark of Modified Computational Fluid Dynamics Simulations of an Array of Heated Rods within a Square-Cross-Section Enclosure Filled with Rarefied Helium”

Conferences (Publication and Talk)


Conference (Poster Presentation)

REFERENCES


