

University of Nevada, Reno

**ANSYS/Fluent Simulation Model Development for
Forced Helium Dehydration Process**

A thesis submitted in partial fulfillment
of the requirements for the degree of
Master of Science in Mechanical Engineering

by

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prepared under our supervision by

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**ANSYS/Fluent Simulation Model Development For Forced Helium Dehydration
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requirements for the degree of

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ABSTRACT

This thesis describes the development and design of simulation model in “ANSYS FLUENT” for Spent Nuclear Fuel dehydration process by “Forced Helium Dehydration” [13] method [28]. The simulation model was developed using the computational fluid dynamics software “FLUENT” [28]. After defueling a nuclear reactor, the fuel rods are kept underwater. Later they are put into a transfer cask. The fuel rods have to be stored in dry condition for long term storage. “Forced helium dehydration” [13] process uses dry helium gas flow to remove water content from the transfer cask. The mass transfer occurs due to diffusion-advection and evaporation-boiling. There are several evaporation and boiling methods available built in “FLUENT” [28]. So, an optimized method was chosen which was used for simulation of mass transfer in the “Forced Helium Dehydration” [13] process. The method was verified in a two dimensional model, then applied to a three dimensional model. The spent nuclear fuel rods can be arranged in different arrays inside the canister. For our simulation, we used a 7 x 7 array of spent nuclear fuel rods.

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CHAPTER I

INTRODUCTION

The USA is the largest producer of nuclear power in the world. Around 25% of worldwide nuclear generation of electricity is produced in the USA [1]. There are around 100 reactors operating in 31 states of the USA [2]. Among the reactors, 65 are pressurized water reactors (PWRs) and 35 are boiling water reactors (BWRs) [3]. They represent about 19% of total electrical output [1].

The PWR core uses normal water as moderator and also as primary coolant. The water in PWR is kept under considerable pressure (about 10 MPa) to prevent it from boiling. The temperature rises to about 550-600°F. [4]

In case of BWR, water is converted directly to steam in the reactor pressure vessel. The steam which is at about 290°C and 7 MPa is then used to drive a turbine to generate electricity. [4]

1. Nuclear Fuel Assembly

Nuclear Fuel assembly (see Fig. I.1) is consisted of cylindrical rods put into bundles. A uranium oxide ceramic is converted into pellets and then inserted into Zircaloy cladding tubes. The tubes are bundled together. The tubes are about 1 cm in diameter, and the fuel cladding tube is filled with helium gas to improve the heat conduction. In case of PWR, there are about 289 fuel rods per fuel assembly. About 121 to 193 fuel assemblies are used into the reactor core. [6] A fuel assembly can contain 200 to 500 kilograms of heavy metal [5]. The fuel bundles consist of fuel rods which are bundled as 14×14 to 17×17 array for PWR and 7×7 to 9×9 array for BWR [6].

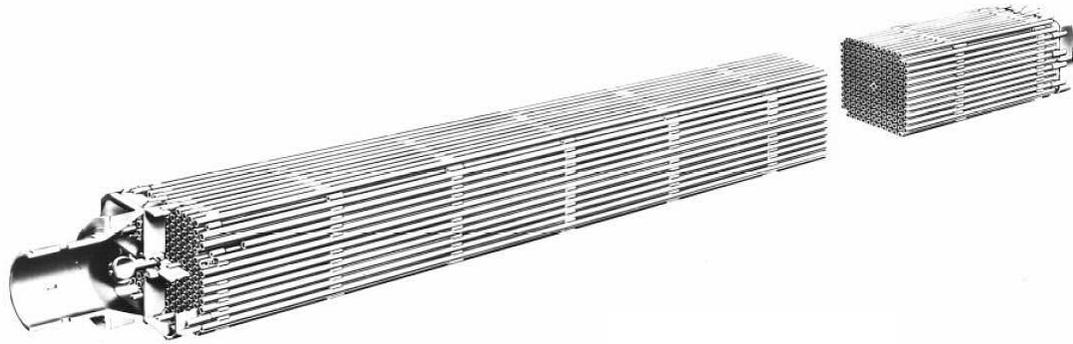


Figure I.1: Fuel Assembly [6].

2. Nuclear Fuel Cycle

The nuclear fuel cycle is the sequence of stages that nuclear fuel go through (see Fig. I.2). The cycle can be open or closed depending on the reprocessing of the spent nuclear fuel. In USA, the nuclear fuel cycle is open as the spent nuclear fuel is not reprocessed.

To extract the uranium ore, Uranium is recovered. The ore is then concentrated to produce "yellowcake (U_3O_8)". The "yellowcake" is then converted to uranium hexafluoride (UF_6). The concentration of uranium-235 (U^{235}) in UF_6 is increased by enrichment process. The enriched UF_6 is converted into fuel and used in the nuclear reactor. After usage in the reactor, the fuel is removed and stored in water pool. The fuel is then stored in the canister for interim storage. The fuel is transported for reprocessing (or recycling), long-term storage, or final disposal. [7]

A large 1000 MWe nuclear reactor usually produces 25–30 tons of spent fuel every year [4]. Currently, there is about 240,000 tons of used fuel. Around 90% of these assemblies are in storage pools or in dry storage [8]. As the USA does not reprocess the spent nuclear fuel, the pool storage spaces are becoming smaller. Long term storage or dry storage is becoming an important solution for spent nuclear fuel (SNF). [9]

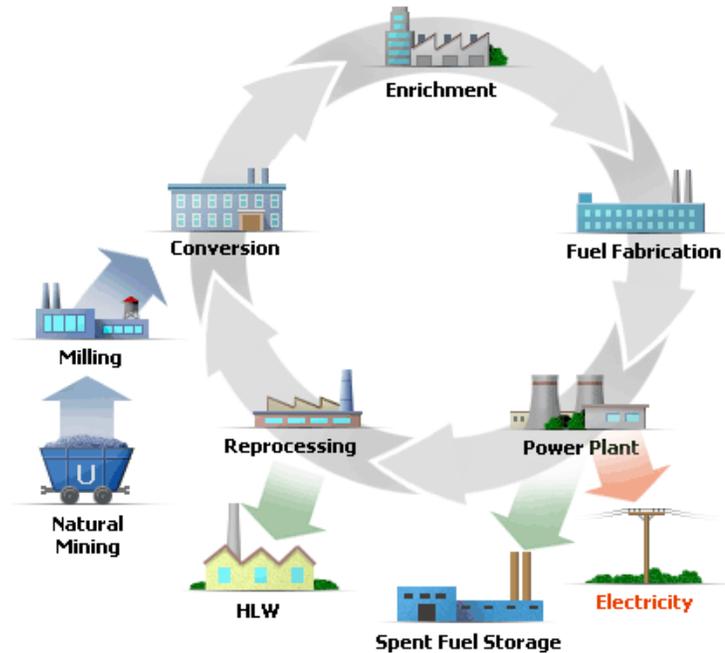


Figure I.2: The Nuclear Fuel Cycle [7]

3. Spent Nuclear Fuel Storage

The used fuel assemblies are radioactive because the products of fission are radioactive. After removing the fuel assemblies from the reactor core, they are kept under water in a spent fuel pool for years. The spent nuclear fuel still generates heat from the decay of radioactive elements. [10] After a certain period of time, the spent nuclear fuel assemblies are transferred from the storage pool into the cylindrical canisters. The cylindrical canisters are also known as “dry storage canister”. Then the water from inside the transfer cask is drained. There might be a very small amount of water remaining at the bottom of the canister or in crevices of the canister and cladding surfaces. To prevent corrosion, all the moisture has to be removed. [12] The dry storage units do not require power for cooling. Hence they are called “Passively Safe” [11]. To reduce the moisture content, vacuum drying or forced helium dehydration processes are used.

4. Objective

The objective of this work is to design and model a “Forced Helium Dehydration” [13] process using “FLUENT” [28]. This work will create a thermodynamic model in “FLUENT” [28] to simulate the moisture removal process. “FLUENT” [28] has in-built evaporation and boiling models. Those models are evaluated based on the boundary conditions. After results are verified in 2-D model, a 3-D model was generated and simulations were done based on boundary conditions. The model was generated to simulate “Forced Helium Dehydration” [13] process which can be applied to geometrically-accurate-three-dimensional model of spent fuel canister.

CHAPTER II

FORCED HELIUM DEHYDRATION

The spent nuclear fuel (“SNF”) assemblies are placed under water after they are discharged from the reactor. The water keeps the “SNF” cool and also provides shielding against radiation. The “wet storage” is done for long enough so that the decay of heat and radiation is reduced to a significantly low level. Then the SNF is transferred to dry casks for long term storage. Dry storage is done by storing in a dry inert gas atmosphere which is contained within a structure. For storing SNF for a long period of time, storage cask is a common structure. [13]

1. Transfer of Fuel Rods

As the used fuel assemblies are still radioactive, the transfer operation is done underwater to shield against the radiation. An open lid canister is placed into a transfer cask and both are then lowered into the nuclear fuel pool. The spent fuel assemblies are transferred to the canister which is done underwater. The canister is then sealed to contain the fuel assemblies. The transfer cask and the canister are taken out of the pool and the water inside the canister is drained by forcing helium through an inlet port which is located at the top of the lid. Small amount of water might remain at the bottom of canister and in the crevices. To remove the remaining water, a drying process is used. A time limit is set between transfer of fuel rods and the start of drying operations. The bounding heat-up rate for the transfer cask is 3.77° F per hour to avoid the boiling of water before the drying operation. [15]

2. Remaining Water inside Canister

When the water inside the canister is drained, the temperature increase (there is no water to keep the temperature low). Drying the canister is important to avoid the pressurization problem as the steam creates a possibility of container or cladding corrosion and fuel oxidation. [16]

From Peehs et al. (1986) report, the total amount of water which was collected from one waterlogged breached SNF rod was around 0.1 to 0.2 moles (1.9 to 3.8 ml (0.067 to 0.134 oz.)). If 1-percent cladding failure is considered and 0.23 moles (4.1 ml (0.144 oz.)) of water release is considered from one waterlogged breached rod, the amount of water that is present in a canister would be 11 moles (0.2 L). [17]

The residual water in dry storage can also be from chemisorbed water. The chemisorbed water can exist in hydroxides or hydrates. About 0.02 to 1.53 L chemisorbed water might remain on $ZrO(OH)_2$, assuming 1 to 100% decomposition at 10 mm thickness. [18]

The total amount of water remaining inside the storage cask depends on various factors (size of cask, backfill pressure etc.). The amount of remaining water can be calculated experimentally or analytically. In 1997, Westinghouse Savannah River Company calculated the amount of water remaining inside the canister. According to them, around 2-4 liters (0.5-1 gal) of residual water might remain within the cask after bulk water was drained. [14]

At INL (Idaho National Laboratory), an experiment was conducted where canisters were filled with water and stored onsite. The canisters contained 20 to 250 pounds of water which is trapped inside the lower head after the draining of water was done. There was

analytical approach to calculate the amount of water remaining inside the canister before drying. INL research team calculated the remaining water in a canister for a mock material test reactor (MTR). The calculation showed that the amount of free water on cropped assembly is 16.6 g, water of hydration is 42.576 g, and absorbed water is 0.015 g. So, the total amount of water on cropped assembly is 59.191 g before dehydration. [14]

In 2011, the Southwest Research Institute evaluated the adequacy of drying for spent fuel dry storage. Water sources and types for the drying process are: Unbound water (trapped water, thin wetted water), Physisorbed water (bound water on all surfaces) and chemisorbed water (hydroxide or hydrates). [18]

In 2012, calculation of remaining water was done on SNF of “HPCTR” (High Power Channel Type Reactors). The theoretical calculation showed that the calculated amount of moisture on the cluster of fuel elements just before charging into the ampoule would be 35 g. [19]

3. Forced Helium Cycle

The “FHD” or “Forced Helium dehydration” [13] cycle shown in Fig II.1 is a method of drying a cavity which is loaded with radioactive elements. The method consists of different stages. A desired degree of dryness is determined first. Then dry helium gas is inserted into the “cask” which removes moisture from the “cask” [13]. The wet gas is then goes through a chiller where the moisture is taken out as condensate. The helium gas is then flows through a heater to superheat the gas. The circulation continues until the desired dryness is achieved. As per N.R.C. regulations, the vapor pressure (“ v_p ”) within the canister has to be below 3 Torrs before the canister can be backfilled with an inert gas and sealed for long term storage. [20] Figure II.2 shows the thermodynamic cycle for “FHD”. After

wet helium gas comes out of the canister (state 1), it goes to a chiller where the gas is de-superheated (state 2) and condensed (state 3). The water comes out of the gas as condensation and removed. The dry gas (state 4) is then passed through a heater which ensures that there is no moisture in the gas (state 5). Then the gas is pumped to the reservoir and the cycle continues until the desired water vapor pressure is reached. [13]

3.1. Moisture Removal

During the “forced helium dehydration” [13] process, the moisture inside the cask is absorbed. Initially the heat and mass transfer occur due to the diffusion. Then the heat and mass transfer occur due to the bulk fluid flow over the water surface or by advection. In case of forced convection, the evaporation happen due to a combination of advection and diffusion. [20] The flow of helium through the inlet port creates bulk flow or advection inside the cask. Due to the SNF temperature inside the “cask” [13], boiling of water also happens. If the water is warmed up slowly due to the circulation of helium gas, evaporation starts eventually. After a short period, steady state or equilibrium state is reached. This is known as constant-rate period. The transport of heat and the evaporation from the body are at steady-state and this creates a constant evaporation rate. The surface of the water is at a uniform temperature or saturation temperature. [21]

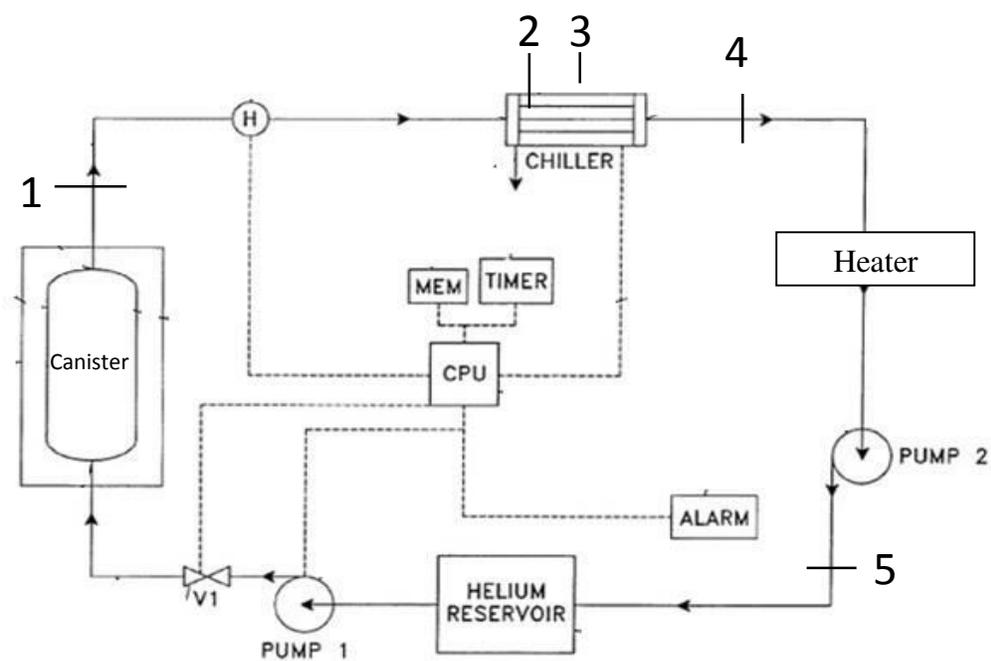


Figure II.1: "Forced Helium Dehydration Cycle" [13]

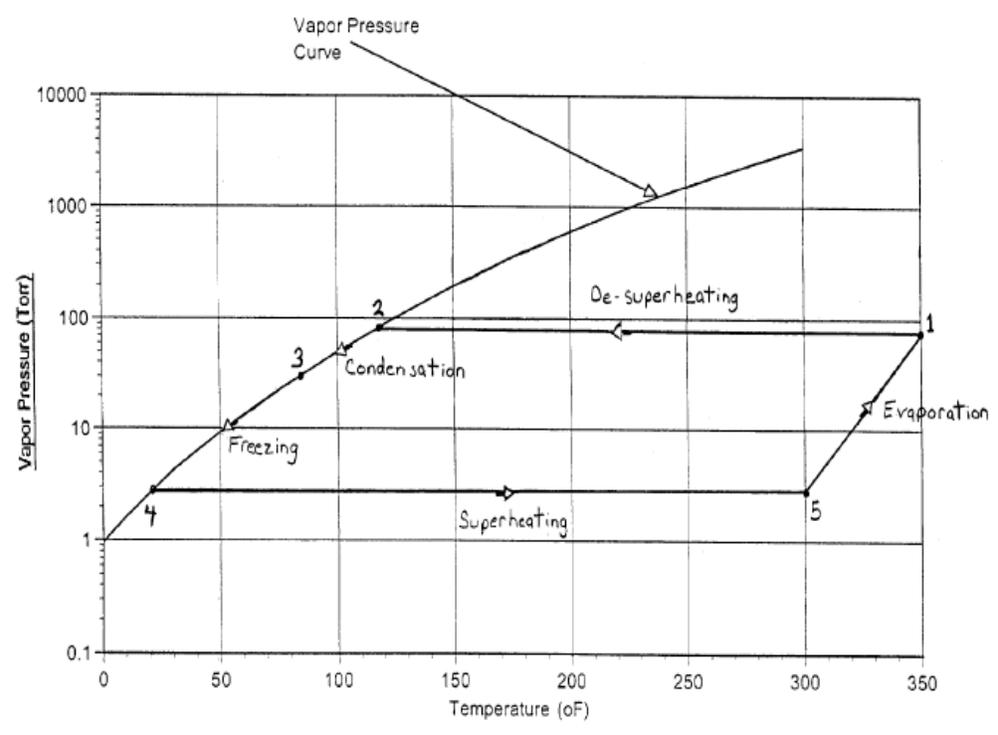


Figure II.2: Thermodynamic Cycle of "Forced Helium Dehydration" [13]

4. Modeling Forced Helium Dehydration

The moisture removal through “FHD” [13] occurs due to evaporation and advection-diffusion. To model “FHD” [13], mass transfer from water is to be considered for both evaporation-boiling model and advection-diffusion model.

4.1. Evaporation Model

There are very few analytical solution for boiling and evaporation mass transfer rate. To find empirical equation for boiling mass transfer for a particular problem, lots of experiments were conducted. Dalton determined the law of partial pressure and published the first empirical result. [22] An empirical equation can overestimate or underestimate the true value of mass transfer. As the evaporation mass transfer process is very complex, there very few working theoretical formulas available. So, there are lots of experimental formulas for particular problem. [23]

The empirical hydrodynamic approach was started by Dalton [22] to the evaporation problem. He stated that “evaporation is proportional to the difference in vapor pressure at the surface of the water and in the air and that the velocity of the wind affects this proportionality”. A lot of investigations were done based on Dalton’s proposal.

Most common form of evaporation rate is [22]:

$$E = \frac{(a+bV)(P_w-P_a)}{h_w} = \frac{h_e(P_w-P_a)}{h_w} \quad (1)$$

Where E is the evaporation rate [kg/m²s]

a, b are the coefficients of empirical equation

V is the wind velocity (velocity of air parallel to water surface) [m/s]

P_w is the saturated water vapor partial pressure at the water temperature [Pa]

P_a is the water vapor partial pressure at the air temperature and humidity [Pa]

h_e is the evaporative heat transfer coefficient [W/m²Pa]

h_w is the latent heat of vaporization of water [J/kg]

$(P_w - P_a)$ is the vapor pressure difference between saturated air at pool surface temperature and the room air [Pa]

a subscript, at room temperature and humidity

w subscript, saturated at water surface temperature

Willis H. Carrier published the following empirical formula in 1918. This is the most widely used expression till now [24]:

$$E = \frac{(0.0888 + 0.0783V)(P_w - P_a)}{h_w} \quad (2)$$

The formula was based on tests which were performed on an unoccupied pool with air flow. This equation has been used widely for calculating evaporation from pools without air flow by imputing $V=0$ in the formula. So, this formulae can be used for evaporation-boiling without any helium circulation. This formulae was also recommended by the 1999 ASHRAE Handbook [25] for HVAC applications.

4.2. Diffusion

When there is a difference in concentration, there is net movement of molecules or atoms. This motion is defined as “Diffusion” [27]. This movement is due to a concentration gradient [28]. A gradient is defined as the change in the value of concentration with the change in distance [27].

“Fick’s law” describes the diffusion rate of a non-reacting gas mixture with two molecular species: A and B . The mass transfer rate equation from Fick's law was applied

to the Stefan problem. So, diffusion mass transfer rate analytical solution can be found from the Stefan problem. In the Stefan problem (shown in Fig II.3) [26], Liquid form of species 'A' is maintained at a fixed height in a glass cylinder. A mixture of species 'A' and 'B' in gaseous form flow over the cylinder. If there is a concentration difference, then the species 'A' in liquid form will diffuse from the interface to the open end of the cylinder. Now from the Fick's Law, mass flux of 'A' [26],

$$\dot{m}_A'' = Y_A(\dot{m}_A'' + \dot{m}_B'') + \left(-\rho D_{AB} \frac{dY_A}{dx}\right) \quad (3)$$

Advection Diffusion

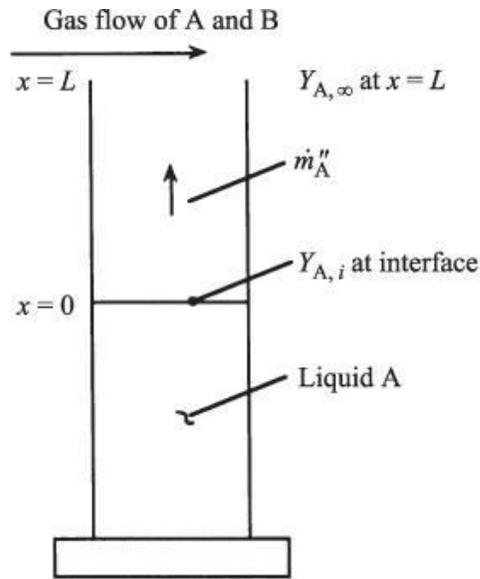


Figure II.3: Schematic of Stefan Problem [26]

Species 'B' is insoluble in liquid 'A'. So, mass flux of 'B' is zero: $\dot{m}_B'' = 0$ [26],

$$\dot{m}_A'' = Y_A(\dot{m}_A'') + \left(-\rho D_{AB} \frac{dY_A}{dx}\right) \quad (4)$$

Solving with boundary condition: $Y_A(x = 0) = Y_{A,i}$, [26]

$$Y_A(x) = 1 - (1 - Y_{A,i}) \left(\frac{1 - Y_{A,\infty}}{1 - Y_{A,i}} \right)^{\frac{x}{L}} \quad (5)$$

Now, if we ignore Advection term, the solution for only diffusion is [26]:

$$Y_A(x) = (Y_{A,i}) + \frac{x}{L} (Y_{A,\infty} - Y_{A,i}) \quad (6)$$

So, the Stefan diffusion problem gives the profile of mass fraction of water vapor due to diffusion.

CHAPTER III

Computational Fluid Dynamics

“Computational fluid dynamics” or “CFD” [28] can obtain flow and pressure profiles for flows of different types by numerical computation and analysis. The actual geometry is provided by the user in the form of a “mesh” [28], which divides the geometry into a large number of sub-cells for which the software is able to solve the fundamental equations for the flow. [27]

The “forced helium dehydration” [13] process can be modeled using the “CFD” [28] approach. The transfer cask is modeled using “ANSYS”, then using “FLUENT” the model can be solved for diffusion-advection and evaporation-boiling of water remaining inside the cask before drying [28]. The simulation can be done for steady state and also can be solved for transient condition. The different boundary conditions imposed can be analyzed to find the optimum condition. The mass transfer rate due to evaporation-boiling and advection-diffusion can be solved under different boundary conditions. Both two dimensional and three dimensional models can be simulated.

1. Governing Equations

The computational procedure is based on the solution of the governing equations for the dependent variables: velocity components, pressure, and temperature [20].

Continuity Equation [20]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho U_i) = 0 \quad (7)$$

- ρ is density of the fluid [kg/m³]
- t is time [s]

- U_i is mean velocity component corresponding to the i direction [m/s]
- x_i is coordinate in direction i [m]

Momentum Equation (Navier-Stokes Equation) [20]:

$$\frac{\partial}{\partial t}(\rho U_i) + \rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial U_i}{\partial x_j} - \rho \overline{u_i u_j} \right) + \rho g_i \quad (8)$$

- P is pressure [Pa]
- m is laminar dynamic viscosity [kg/ms]
- u_i is fluctuating velocity component in the i direction [m/s]
- g_i is gravitational acceleration in the i direction [m/s²]

Energy Equation [20]:

$$\frac{\partial}{\partial t}(\rho T) + \rho U_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\gamma \frac{\partial T}{\partial x_j} - \rho \overline{u_j T'} \right) + S_T \quad (9)$$

- T is time-mean temperature of the fluid [°C]
- γ is diffusion coefficient [m²/s]
- T' is fluctuation temperature [°C]
- S_T is source term [W/m³]

2. Steady State and Transient Simulation:

A system is in a steady state when it has numerous properties that are constant with time. For those properties (p) the partial derivative with respect to time will be zero [29]:

$$\frac{\partial p}{\partial t} = 0 \quad (10)$$

For our model, both steady and transient conditions are simulated. The closed cask reaches steady state where the vapor pressure is equal to the saturation pressure and the mass transfer rate becomes steady. During the drying process, the system is considered

transient. As helium circulation continues, the vapor pressure inside the cask reduces with time. The mass transfer rate is also time dependent [29].

3. Numerical Modeling:

The evaporation-boiling and the diffusion-advection inside the canister can be simulated in “FLUENT” [28] by using pre-defined models. The boiling and evaporation of water can be modeled using “Multiphase Flow models” [28] and Diffusion can be modeled by the “Species Transport model” which are available in “FLUENT” [28].

3.1. Modeling Evaporation - Multiphase Model

In “ANSYS Fluent”, different “multiphase models” are available. For complex multiphase flows, first the aspect of the flow that is of most interest is selected. Then the model that is most appropriate for that aspect of the flow is chosen. [28] For our simulation, the “Mixture model” [28] is used based on the type of application of the model.

“The mixture model is designed for two or more phases (fluid or particulate). The mixture model solves for the mixture momentum equation and prescribes relative velocities to describe the dispersed phases” [28]. As our simulation consists of more than two phases (helium gas, water liquid and water vapor), “the mixture model” [28] is appropriate for this case.

3.1.1. Phase Interaction

After selecting the appropriate model, the phase interaction mechanism between different phases was selected. Phase interaction is the way of mass transfer between different phases. In case of “FHD” (“Forced Helium Dehydration”) [13], phase interaction occurs between water liquid and water vapor in the form of evaporation and condensation. “ANSYS Fluent calculates interphase mass transfer through evaporation-condensation

depending on the multiphase model and interfacial heat transfer models being used. In most cases the Lee model is used” [28]. So, evaporation-condensation mass transfer can be calculated from Lee model.

“The Lee model is a mechanistic model with a physical basis. In the Lee model, the liquid-vapor mass transfer (evaporation and condensation) is governed by the vapor transport equation” [28]:

$$\frac{\partial}{\partial t} (\alpha_v \rho_v) + \nabla \cdot (\alpha_v \rho_v \vec{V}_v) = \dot{m}_{lv} - \dot{m}_{vl} \quad (11)$$

Where

v = vapor phase

α_v = vapor volume fraction

ρ_v = vapor density

\vec{V}_v = vapor phase velocity

\dot{m}_{lv} , \dot{m}_{vl} = the rates of mass transfer due to evaporation and condensation, respectively.

These rates use units of kg/s/m³

Based on the following temperature regimes, the mass transfer can be described as follows [28]:

If $T_l > T_{sat}$ (evaporation)

$$\dot{m}_{lv} = coeff \times \alpha_l \rho_l \times \frac{(T_l - T_{sat})}{T_{sat}} \quad (12)$$

If $T_l < T_{sat}$ (condensation)

$$\dot{m}_{vl} = coeff \times \alpha_v \rho_v \times \frac{(T_{sat} - T_l)}{T_{sat}} \quad (13)$$

“The coefficient that can be interpreted as a relaxation time. α and ρ are the phase volume fraction and density, respectively. The source term for the energy equation can be obtained by multiplying the rate of mass transfer by the latent heat” [28].

Using Hertz Knudsen equation and solving for parameters [28]:

$$\dot{m}_{lv} = \frac{6}{d_b} \beta \sqrt{\frac{M}{2\pi RT_{sat}}} L_h \left(\frac{\alpha_v \rho_v}{\rho_l - \rho_v} \right) \alpha_l \rho_l \frac{(T_l - T_{sat})}{T_{sat}} \quad (14)$$

$$\dot{m}_{vl} = \frac{6}{d_b} \beta \sqrt{\frac{M}{2\pi RT_{sat}}} L_h \left(\frac{\alpha_v \rho_v}{\rho_l - \rho_v} \right) \alpha_v \rho_v \frac{(T_{sat} - T_l)}{T_{sat}} \quad (15)$$

3.2. Modeling Diffusion - Species Transport Model

Diffusion of mass can be modeled in “ANSYS/Fluent” by a pre-defined mass transfer model. “ANSYS Fluent can model the mixing and transport of chemical species by solving conservation equations describing convection, diffusion, and reaction sources for each component species”. [28]

“ANSYS Fluent calculates the local mass fraction of each species, Y_i through the solution of a convection-diffusion equation for the i^{th} species. This conservation equation has the following general form” [28]:

$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (16)$$

“Where R_i is the net rate of production of species by chemical reaction and S_i is the rate of creation by addition from the dispersed phase. An equation of this form will be solved for $N - 1$ species where N is the total number of fluid phase. As the sum of mass fraction of the species must be unity, the N^{th} mass fraction is determined as one minus the sum of the $N - 1$ solved mass fractions” [28].

3.3. User Defined Function (UDF)

In the “FLUENT evaporation-condensation” [28] model, the bulk flow or advection term for boiling and evaporation process is not present. So, to model advection the user defined function is used to incorporate Carrier’s equation [24] (described in chapter II, section 4.1) into “FLUENT” [28] solver.

“A user-defined function, or UDF, is a C function that can be dynamically loaded with the ANSYS Fluent solver to enhance its standard features. It can be used to:

- Customize boundary conditions, material property definitions, surface and volume reaction rates, source terms in ANSYS Fluent transport equations, source terms in user-defined scalar (UDS) transport equations, diffusivity functions, and so on.

- Adjust computed values on a once-per-iteration basis.
- Initialize a solution.
- Perform asynchronous (on demand) execution of a UDF.
- Execute at the end of an iteration, upon exit from ANSYS Fluent, or upon loading of a compiled UDF library.

- Enhance post processing.
- Enhance existing ANSYS Fluent models (such as discrete phase model, multiphase mixture model, discrete ordinates radiation model)” [28].

UDFs are programmed using additional macros and functions that access ANSYS Fluent solver data and perform other tasks.

CHAPTER IV

Results and Discussion

The “FHD” (“Forced Helium Dehydration”) process is used to remove moisture from the canister [13]. The water inside the canister is evaporated and then the moisture is removed by diffusion and advection due to the flow of helium gas. So, both diffusion-advection and evaporation have to be modeled for the simulation of the process. Evaporation can be modeled in “ANSYS/FLUENT” using in-built pre-defined model (multiphase-mixture model) and diffusion-advection can be modeled using in-built Species transport model [28]. First, the “Species transport model” was used in “FLUENT” to solve the Stefan diffusion problem [28]. The mass fraction of water vapor was found from simulation results. These results were then compared with the analytical solution of Stefan problem. The “multiphase-mixture model” was used to model boiling and evaporation in “FLUENT” [28]. The vapor pressure was found from the simulation result, which was compared with analytical solution for vapor pressure. After comparison with the analytical model, the multiphase-mixture model and species transport model of “FLUENT” were verified. But there were some limitations of the “FLUENT” models which were overcome by using “UDF” (“User Defined Function”) [28]. As “FLUENT” [28] can model advection-diffusion and evaporation-boiling, these models were applied to simulate the “FHD” process [13]. The modeling of “FHD” [13] in “FLUENT” [28] was done for simple two dimensional geometry first. The verified models were then applied to 3D model. The 3D model was then used to find the optimum inlet velocity of helium gas.

1. Stefan Diffusion Model

The Stefan diffusion model described in section 4.2 of chapter 2, was modeled in “FLUENT” [28] with simple two dimensional geometry. The mass fraction of water in the tube depends on the mass fraction of water at the interface (between water and air) and the mass fraction of vapor at the end of tube. A constant mass fraction equal to 0.99 was assumed at the interface between air and water. The mass fraction of water inside the tube was calculated based on Stefan diffusion equation for different mass fraction of water vapor at the end of the tube. The analytical solution of Stefan equation was calculated and the same equation was modeled in “FLUENT” by using “user defined function” (“UDF”) (Appendix A.1) [28]. Figure IV.1 shows the results of analytical and simulation solutions of Stefan diffusion problem for constant interface mass fraction of water $\gamma_{A, I} = 0.99$ and mass fractions of water at the end of the tube, $\gamma_{A, \infty} = 0.2, 0.4, 0.6, 0.8, 0.9$. From the result, it can be seen that for particular value of $\gamma_{A, I}$ and $\gamma_{A, \infty}$, the mass fraction of water vapor inside the tube decreases non-linearly with increasing distance from the interface. When the difference between the interface mass fraction and end of tube mass fraction is highest ≈ 0.9 , the decrease in mass fraction is with highest gradient. As the difference between mass fractions decreases, the gradient also decreases. The error in simulation and analytical solution is very small and negligible.

Figure IV.2 shows the mass flow rate of water vapor from simulation compared with the analytical solution (based on equation 5). The mass flow rate decreases as the difference between the mass fraction of interface and end of tube decreases. From Stefan diffusion mass flux equation, the mass flux depends on the concentration gradient. So, as the concentration gradient decreases, the mass flux also decreases.

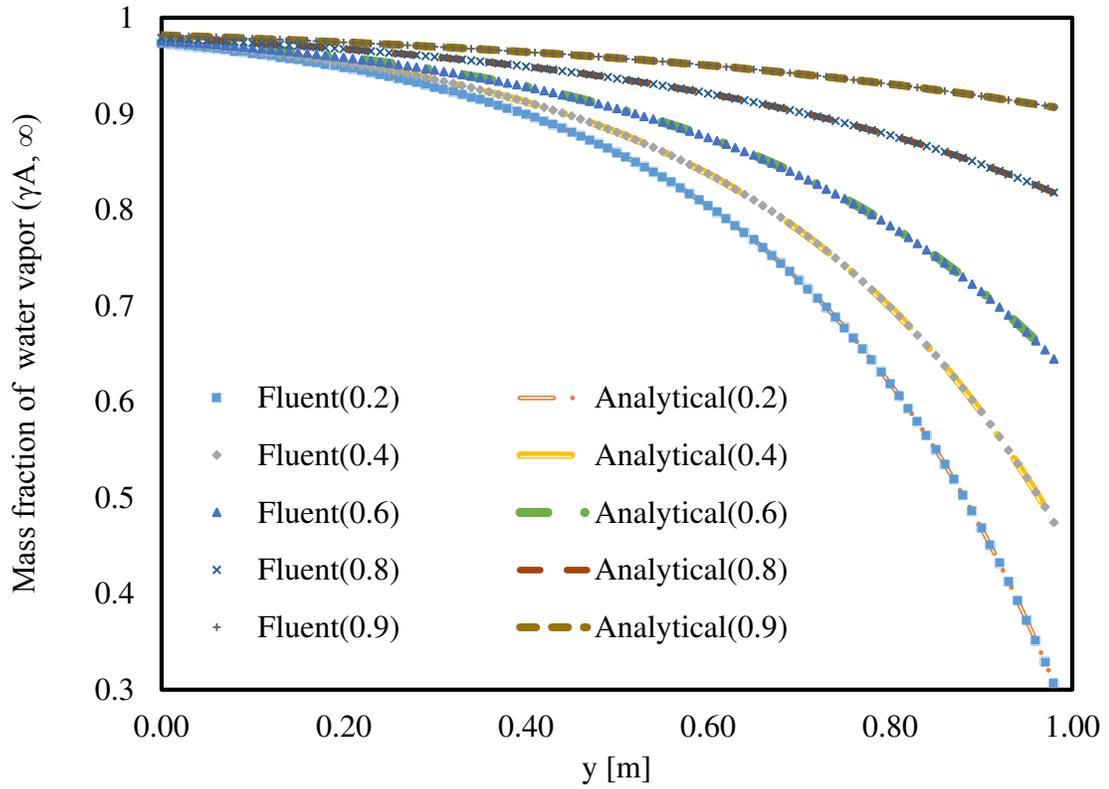


Figure IV.1: Vapor mass fraction as function of location (Analytical vs “FLUENT” [28])

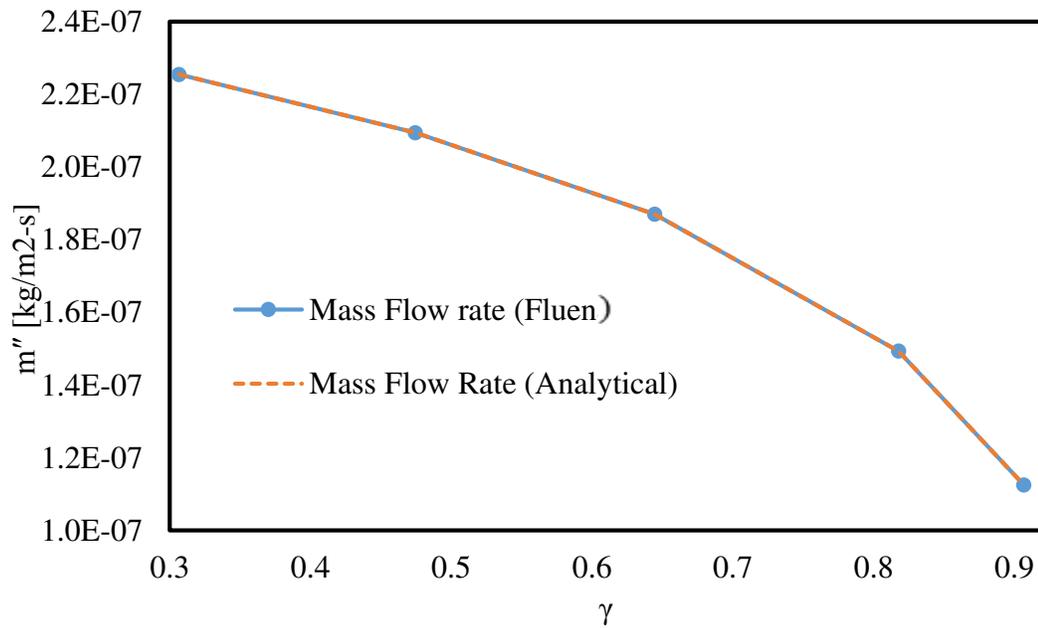


Figure IV.2: Mass flow rate versus mass fraction for fixed bottom wall mass fraction γ_i

Figure IV.2 shows a good agreement between the analytical solution and “FLUENT” [28] simulations. Figure IV.1 and IV.2 show that “FLUENT” [28] can be used for the simulation of Stefan diffusion problem. So, diffusion can be modeled in “FLUENT” [28] for the simulation of “Forced Helium Dehydration” [13].

2. Boiling Models

The analytical solution of simple two dimensional geometry boiling problem was compared with “FLUENT” “Multiphase mixture model” simulation solution [28]. Very small amount of water was boiled by applying boundary heat flux, as shown in Figure IV.3. The mass transfer rate from water to vapor was calculated analytically by using energy balance equation [30].

$$\Delta U = Q - W \quad (17)$$

where ΔU is the change in internal energy, Q is the net heat supplied to system, and W denotes the net work done by the system. Then, the vapor pressure was calculated from ideal gas law [31] $PV = nRT$ (where P is the pressure of gas, V is the volume, n is the number of moles, R is the universal gas constant, T is the temperature of the gas).

Heat was applied on the bottom wall, $Q = 1000 \text{ W}$, all the other walls were at temperature of 353 K . The equations were modeled in “FLUENT” using “UDF” (Appendix A.2) [28].

Figure IV.4 shows the comparison of vapor pressure between analytical and simulation. As the amount of vapor increases, vapor pressure increases and reaches the saturation pressure.

The analytical and simulation gives the same trend for vapor pressure. As the difference is very small, “FLUENT” [28] can be used for boiling modeling.

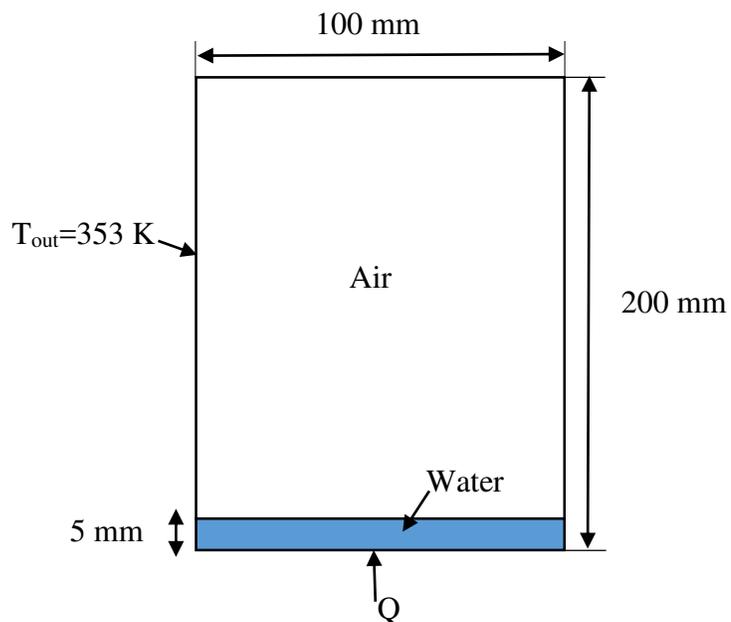


Figure IV.3: Schematic of geometric model for boiling verification

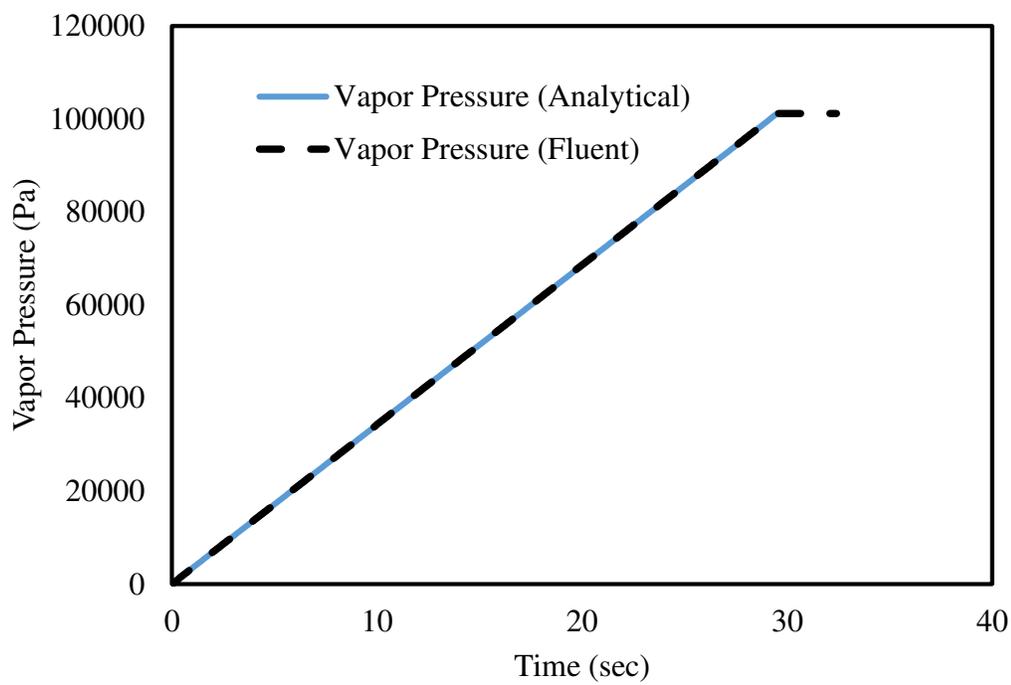


Figure IV.4: Vapor pressure vs Time for boiling model

3. Limitation of FLUENT Boiling Models

The boiling of water inside a closed container filled with helium gas would reach saturation pressure and an equilibrium condition will be reached. The mass fraction of vapor inside the canister will increase and the mass fraction of helium will decrease until equilibrium state is reached. At the equilibrium state, the vapor mass fraction of water will be constant and the summation of vapor mass fraction and helium mass fraction will be unity. A closed container (Fig IV.5) with heated rods inside was modeled in “FLUENT” [28]. The water height at the bottom of the container was 14 mm and the rest was filled with helium gas. Multiphase mixture model was used for this simulation in steady state condition.

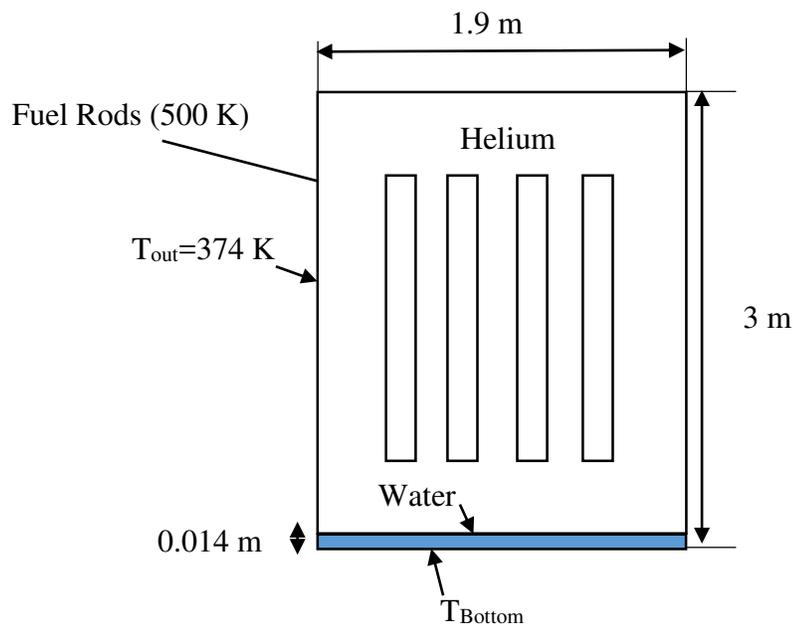


Figure IV.5: Schematic of geometric model for “FLUENT” [28] Models

Vapor mass fraction was zero initially and reached unity at steady state. The mass fraction of helium reached zero at steady state. That means there was no helium inside the container after the simulation, which is against law of mass conservation.

The same closed container simulation was done using “Species transport model” under steady state condition [28]. For this simulation also, the volume fraction of vapor reaches unity, which does not follow the law of mass conservation. So, the mass transfer rate could be modeled in “FLUENT” but the closed system evaporation could not be modeled using “FLUENT” built-in models [28].

4. FLUENT models with User Defined Function

“FLUENT” models’ simulation results (volume fraction of helium) for closed container system do not satisfy the law of mass conservation. Also the “FLUENT” mass transfer equation (“Lee model” [28]) does not consider mass transfer due to gas flow velocity or advection effect [28]. “Lee model” [28] gives mass transfer based on temperature difference only. So, to solve these problems, Carrier’s mass transfer equation [24] (described in Section 4.1 of Chapter 2) was used through “UDF” [28] programming (Appendix A.3). The mass transfer rate equation for “species transport model” and “multiphase mixture model” was given as input to “FLUENT” through “UDF” (Appendix A.3), following the “mass and momentum continuity equation” [28].

4.1. Multiphase Model

The “multiphase mixture model” [28] was used with “UDF” [28] (Appendix A.3) to use Carrier’s mass transfer equation [24] in “FLUENT” [28] simulation. The schematic of the model is shown in Figure IV.5. The boundary walls were at $T_{out} = 374$ K, bottom wall was at $T_{Bottom} = 374$ K and the fuel assemblies were at 500 K. The vapor volume fraction reaches equilibrium at steady state. The equilibrium volume fraction of vapor was 0.16 at steady state. So, the volume fraction of vapor was not unity at equilibrium and the summation of volume fraction of vapor and helium at steady state was unity, which follows

the law of mass conservation. So, the Carrier's mass transfer equation [24] through "UDF" and with "multiphase mixture model" reaches equilibrium vapor pressure condition and also follows the law of mass conservation [28]. So, this model can simulate the evaporation - boiling model with "user defined function" [28].

4.2. Species Transport Model

The same geometry as in Figure IV.5 with same boundary conditions was simulated with "UDF" (Appendix A.3) and "species Transport model" in steady state [28]. The steady state mass fraction of vapor inside the canister was 0.03. So, the "species transport model" can simulate diffusion process with "UDF" [28].

4.3. Profile of Mass Transfer Rate along Interface

Diffusion mass transfer rate depends on the concentration gradient. Helium gas flows inside the canister and over the water-vapor interface. Water vapor diffuses in helium gas as helium gas passes over the water.

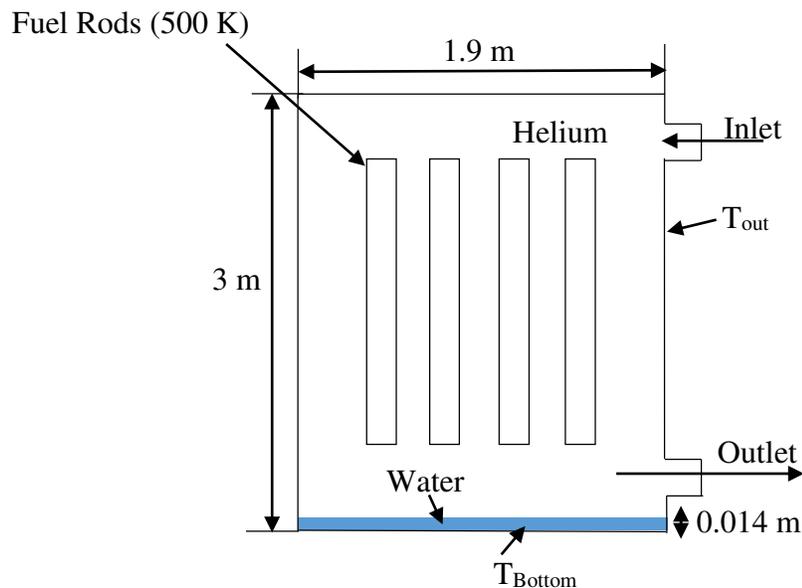


Figure IV.6: Schematic of geometric model with Helium gas flow

As the helium gas becomes saturated, the mass transfer rate from water or the diffusion rate of vapor reduces. So, the mass transfer rate from water to vapor decreases as helium flows toward the outlet. Figure IV.6 shows 2D schematic of the model with helium gas flow. “Species transport model” was used with “UDF” (Appendix A.3) to simulate the diffusion process and to get the diffusion rate profile in the canister under transient condition [28].

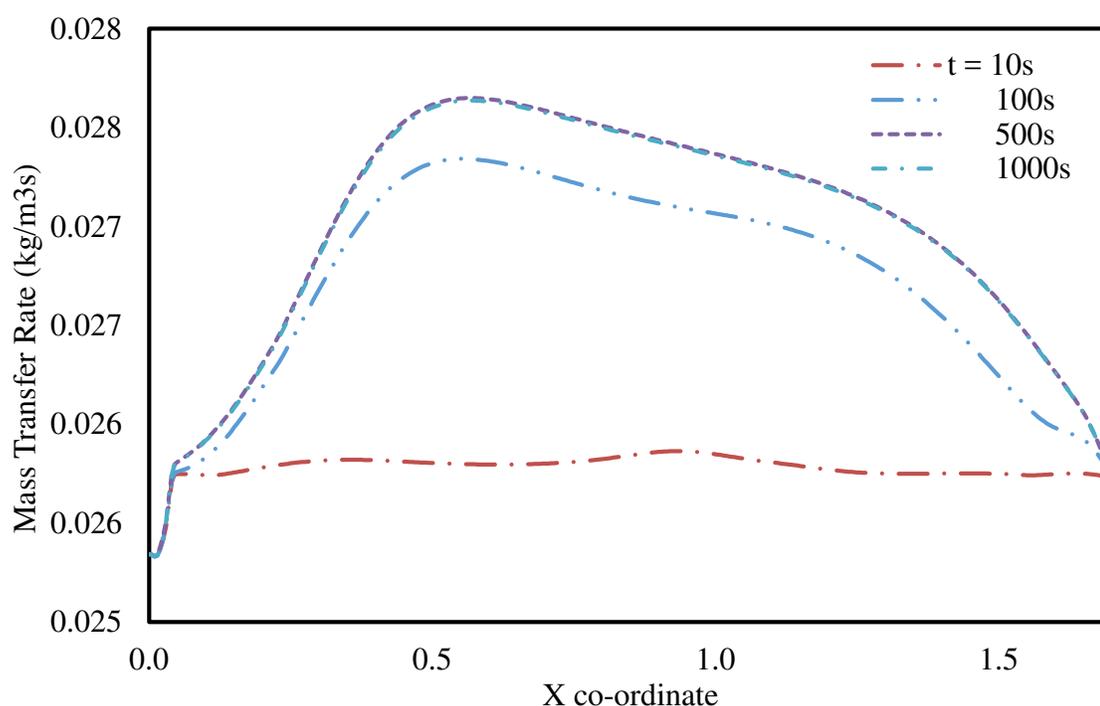


Figure IV.7: Mass transfer rate of vapor in transient state

Figure IV.7 shows the mass transfer rate of vapor inside the canister as helium flows over the water and towards the outlet. The boundary walls were at temperature $T_{out}=300$ K, the fuel rods were at 500 K, and the bottom wall at $T_{Bottom}=300$ K. The mass transfer rate increases as the gas flows over the interface and reaches highest value. Then, the mass transfer rate decreases as the helium gas becomes more saturated and concentration

gradient for water vapor decreases. The maximum mass transfer rate occurred at 1/4th distance of the total length. The mass transfer rate increased with time as the temperature of the water increased until the equilibrium temperature is reached. After 500 second, the mass transfer rate profile became almost constant as the system reaches equilibrium.

5. Simulation of “FHD” [13] in “FLUENT” [28] (2-D model)

“FLUENT” can model and simulate mass transfer rate for evaporation-boiling and diffusion using in built models, “multiphase mixture model” and “species transport model” respectively [28]. The amount of error is negligible when compared with analytical solution, as showed in section 1 and 2 of this Chapter. But there is limitation of these models in simulating the equilibrium condition in closed container as described in Section 3 of this Chapter. The limitation can be overcome using Carrier’s correlation mass transfer equation [24] instead of using “Lee model” [28] for mass transfer rate through “UDF” [28] (Appendix A.3) programming. As, the “FHD” [13] process involves evaporation-boiling and diffusion-advection during the drying process, the “multiphase mixture model” and “species transport model” with “UDF” (Appendix A.3) can simulate the “FHD” [13] in “FLUENT” [28].

5.1. Two Step Simulation

The “FHD” [13] process occurs in two steps. When water is drained from the canister, vapor is generated inside the canister due to the remaining water. So, the vapor pressure increases inside the canister in the first step. In the second step, helium gas circulation starts and water vapor is pushed by helium and taken out of the canister during drying process.

So, the simulation process was also divided in two steps. The first step was with closed container and no helium flow.

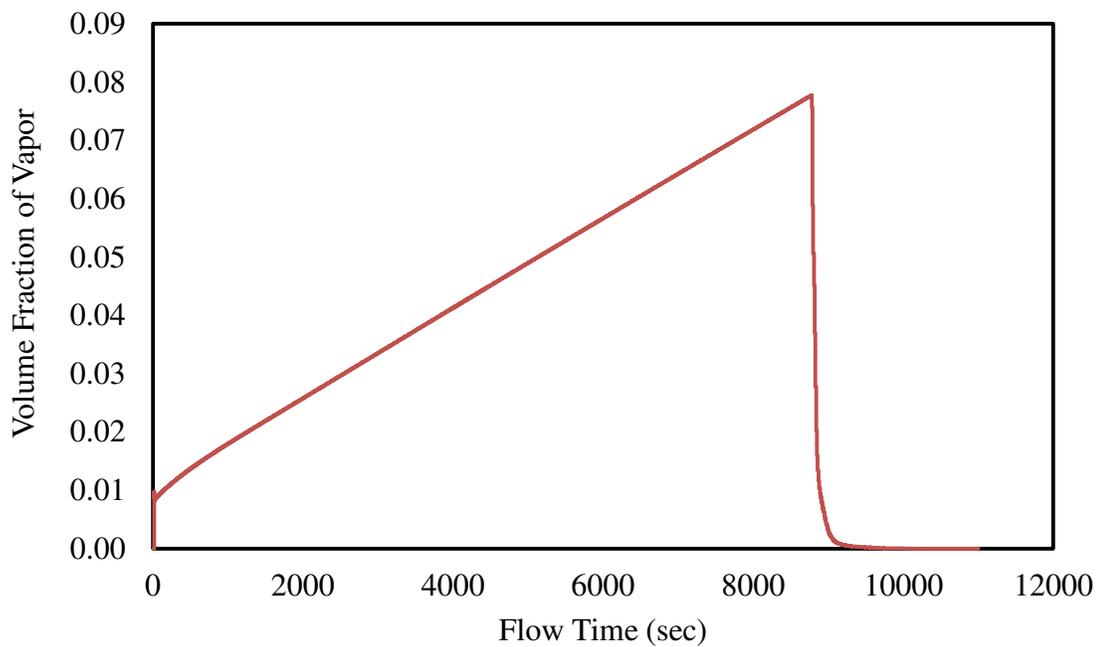


Figure IV.8: Vapor volume fraction in two step simulation

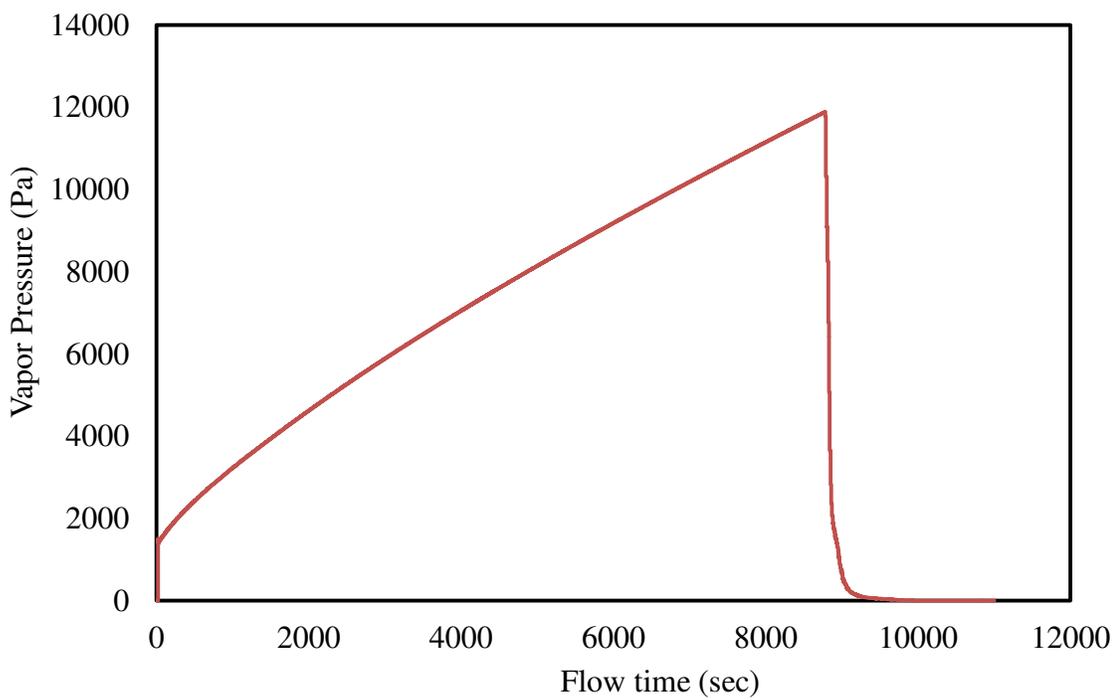


Figure IV.9: Vapor pressure in two step simulation

When the vapor pressure reached 11599 Pa (from Holtec patent for “FHD” [13], the vapor pressure is 87 Torrs or 11599 Pa before the drying process start up [13]), the helium flow inlet was opened and circulation of helium gas was started.

Figure IV.8 shows the volume fraction of vapor in mixture model with “species transport model” activated in two step simulation. Figure IV.19 shows the vapor pressure profile in two step simulation for “Multiphase mixture model” activated with “species transport model” [28]. The vapor pressure increased in the closed container until it reached 11599 Pa, then helium flow was initiated and the vapor was removed by the dry helium gas circulation.

During “forced helium dehydration” [13] process, both advection-diffusion and evaporation processes are important. “Multiphase mixture model” activated with “species transport model” considers both boiling and diffusion with the use of “UDF” (Appendix A.3) [28]. The volume fraction of water remains almost constant at the first stage with no helium gas flow. So, in the first stage very low amount of vapor is generated. In the second stage, the helium gas circulation is initiated and the water volume fraction drops rapidly with high mass transfer rate. This mass transfer rate is due to advection and diffusion causing evaporation of water.

6. Simulation in 3-D Model

“FLUNET” simulation model and “UDF” (Appendix A.3) was selected from two dimensional simulation results [28]. “Multiphase mixture model” with “species transport model” activated can simulate the “forced helium dehydration” [13] process in two dimensional model [28]. So, the model with “UDF” [28] was used in three dimensional model to simulate the “forced helium dehydration” [13] process in 3D.

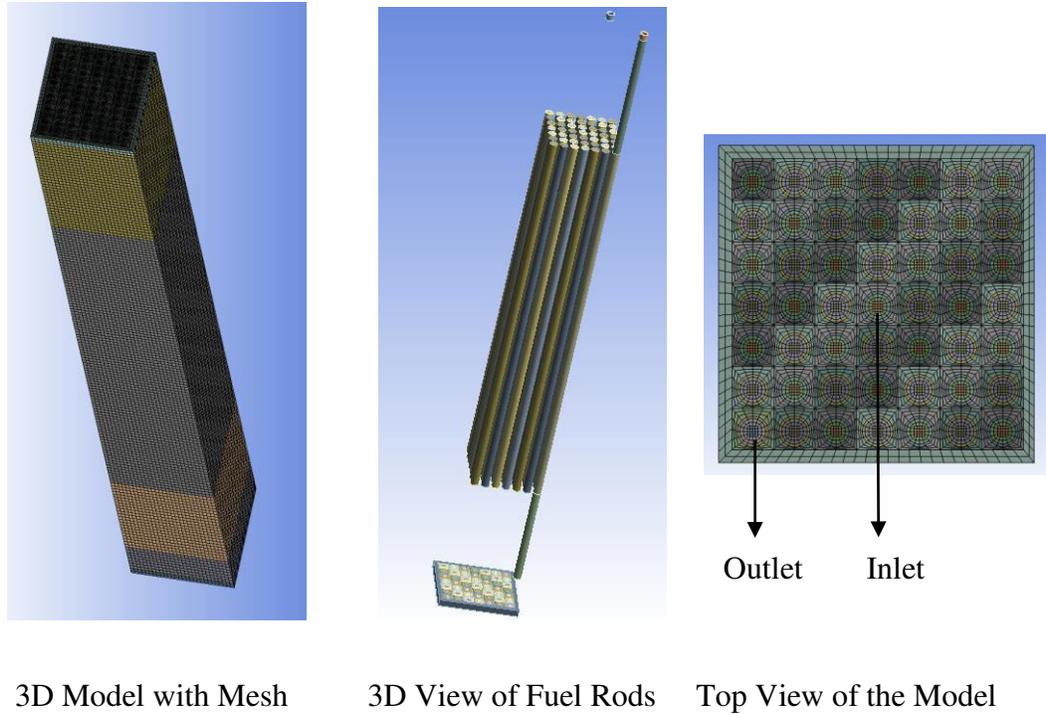


Figure IV.10: 3D Model for Two Step Simulation

The model was applied to the two step simulation. The first step was a closed system, where vapor pressure inside the canister increased. In the second step the helium gas circulation was initiated and vapor was removed from the canister through diffusion-advection and evaporation. Figure IV.10 shows the 3D model of the “cask” [13] with fuel rods and inlet-outlet. The height of the 3D model is 1 meter, length and width are 122 millimeters. A 7 x 7 array of fuel rods was used in the 3D model. The helium gas flow through the inlet and then the helium gas is distributed in the canister. The helium gas push the moisture out of the canister through the outlet tube and towards the outlet port.

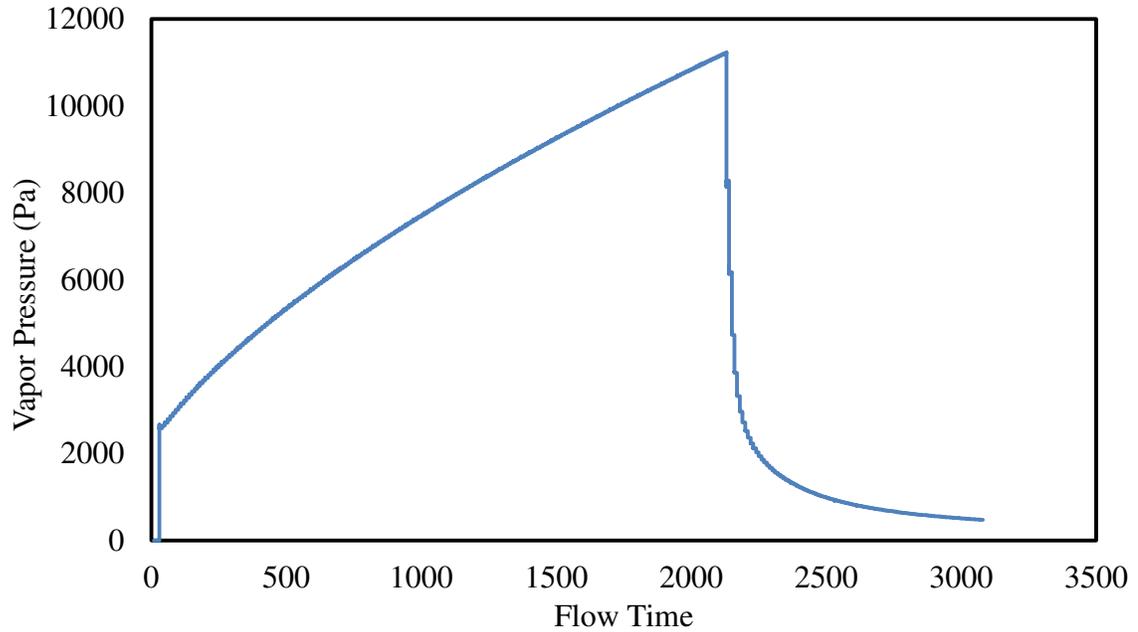


Figure IV.11: Vapor pressure in the three dimensional model under two step simulation

Boundary conditions: Fuel Rods Temperature: 500 K; Other walls: 374.85 K; Helium Inlet velocity: 1m/s. Figure IV.11 shows the vapor pressure inside the canister in two step simulation. In the first step, when the vapor pressure reaches 11599 Pa helium gas circulation is started. So, the vapor pressure drops rapidly due to moisture removal in the second step. When the vapor pressure inside the canister reached 400 Pa, helium gas flow was stopped as described in the patent of “FHD” by Holtec [13].

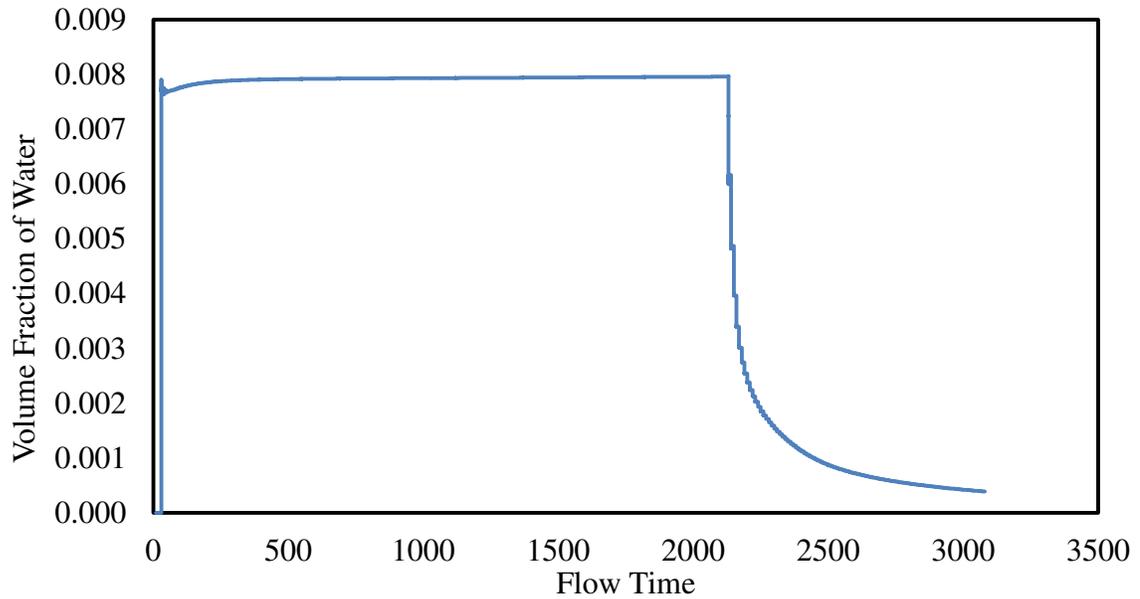


Figure IV.12: Volume fraction of water inside three dimensional model

Figure IV.12 shows the volume fraction of water inside the canister in two step simulation. During the first stage, the amount of water remains almost unchanged. But during the second stage, as helium absorbs and removes moisture from the canister, the volume fraction of water reduces rapidly. After two step simulation, we can find the required time of circulation of helium gas. The amount of water remaining inside the canister can also be calculated from the volume fraction of water.

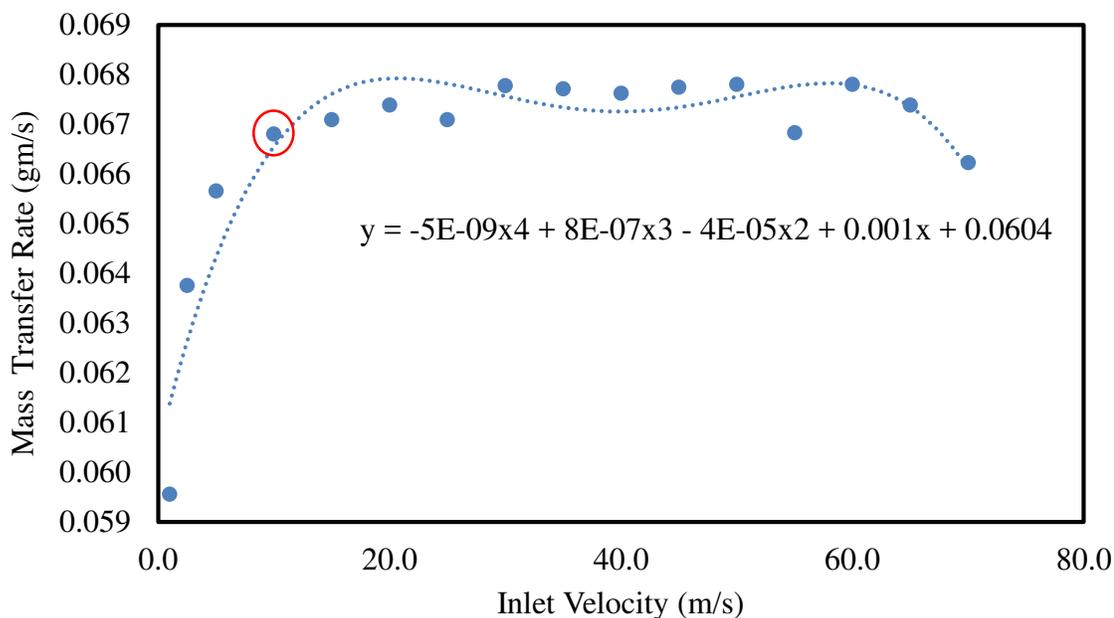


Figure IV.13: Mass transfer rate vs helium flow inlet velocity

So, the simulation model can simulate the “forced helium dehydration” [13] process and the remaining water inside the canister after the dehydration process can be estimated. The time required to dry a particular canister can also be calculated through simulation.

7. Relationship between Inlet Velocity of Helium and Mass Transfer Rate

Figure IV.13 shows the relation between the inlet velocity of helium flow and the mass transfer rate of water. The “Multiphase mixture model” with “Species Transport model” activated was used with “UDF” (Appendix A.3) in 3-D model for this simulations [28]. With the increase in inlet helium flow velocity, the mass transfer rate of water also increased. At higher velocity, the advection was increased which increased the mass transfer rate. But after certain velocity, the mass transfer rate did not increase at the same rate with velocity increment. After this velocity, the mass transfer rate was reduced due to the impact of turbulence. So, the optimum helium inlet velocity could be determined from the simulation results.

The mass transfer rate of vapor increases with the increase in helium inlet flow velocity. But after 15m/s, the mass transfer rate did not increase that much. In fact, there was a decrease in mass transfer rate with higher inlet velocity. So, after 15 m/s the mass transfer rate increment was very small and started to decrease eventually. For this three dimensional model, 15 m/s was the optimum velocity after which the increase in velocity did not impact the mass transfer rate at a significant level.

CHAPTER 5

CONCLUSION

This thesis described the development of “FLUENT” [28] simulation model for forced helium dehydration process. “FLUENT” in-built models (“multiphase mixture model” and “species transport model”) can be used to simulate mass transfer from one phase to another [28]. But for particular application, these models might not work properly. The governing equations vary from application to application. So, the required equations are to be used with these models in “FLUENT” simulation through “UDF” programming to get the accurate results [28]. The “FHD” [13] process circulation time depends on the inlet velocity of helium gas. The moisture removal rate increases with increase in inlet velocity. But after certain velocity, the mass transfer rate does not have much effect and at higher velocities, the mass transfer rate decreases. So, the optimum velocity for “FHD” [13] was determined from the simulations. With the simulation model, the remaining water and vapor pressure inside the canister can be determined after the drying operation. So, for canister or cask design, this model can be applied to find the effect of drying operation and the optimum inlet velocity.

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APPENDIX A

A.1 UDF for Stefan Diffusion Problem

```

#include "udf.h"

#include "mem.h"

#include "sg.h"

DEFINE_SOURCE(mass_source_species, c, t, dS, eqn)

{ real source = 0.0, phi0=0.0, phif=0.0, prime_grad=0.0, rho=0.0, v=0.0, area = 0.0, ds;

real mass_source = 0.0, area_vec[ND_ND], A[ND_ND], es[ND_ND], A_by_es,

dr0[ND_ND]; int n;

c_face_loop (c, t, n)

{ Thread *tf = C_FACE_THREAD (c, t, n); real SURFACE_ID = 12;

if(SURFACE_ID == THREAD_ID(tf))

{ face_t f = C_FACE (c, t, n); F_AREA(area_vec, f, tf); area = NV_MAG(area_vec);

rho=C_R(c,t); v=C_VOLUME(c,t); phi0=C_YI(c,t,1); phif=F_YI(f,tf,1);

BOUNDARY_FACE_GEOMETRY(f,tf,A,ds,es,A_by_es,dr0);

prime_grad= A_by_es*(phif-phi0)/ds;

mass_source = prime_grad*C_DIFF_EFF(c,t,1)*(C_YI(c,t,1)/(1-C_YI(c,t,1)))*rho/v;

source += mass_source;

}

}

C_UDMI(c, t, 1) = source; dS[eqn] = 0.0; return source;

}

```

```

DEFINE_SOURCE(mass_source, c, t, dS, eqn)
{
    real source = 0.0, mass_source = 0.0, area = 0.0, v=0.0, rho=0.0, phi0=0.0, phif=0.0,
    prime_grad=0.0, area_vec[ND_ND], SURFACE_ID = 12; int n;
    real A[ND_ND],ds, es[ND_ND],A_by_es,dr0[ND_ND];
    c_face_loop (c, t, n)
    {
        Thread *tf = C_FACE_THREAD (c, t, n);
        if(SURFACE_ID == THREAD_ID(tf))
        {
            face_t f = C_FACE (c, t, n); F_AREA(area_vec, f, tf); area = NV_MAG(area_vec);
            rho=C_R(c,t); v=C_VOLUME(c,t); phi0=C_YI(c,t,1); phif=F_YI(f,tf,1);
            BOUNDARY_FACE_GEOMETRY(f,tf,A,ds,es,A_by_es,dr0);
            prime_grad= A_by_es*(phif-phi0)/ds;
            mass_source = prime_grad*C_DIFF_EFF(c,t,1)/C_YI(c,t,0)*rho/v;
            source += mass_source;
        }
    }
    C_UDMI(c, t, 2) = source; dS[eqn] = 0.0; return source;
}

```

A.2 UDF for Boiling Model Verification

```

#include "udf.h"
#include "sg.h"
#include "sg_mphase.h"
#include "flow.h"
#include "mem.h"

```

```

#include "math.h"

DEFINE_LINEARIZED_MASS_TRANSFER(cav_source, cell, thread, from_index,
from_species_index, to_index, to_species_index, d_mdot_d_vof_from,
d_mdot_d_vof_to)

{ Thread *liq = THREAD_SUB_THREAD(thread, from_index);
Thread *vap = THREAD_SUB_THREAD(thread, to_index);
Thread *he = THREAD_SUB_THREAD(thread, 0);

real T = C_T(cell, liq), P_SAT = 101325, rho_l = C_R(cell, liq);
real m_dot = 0.0, dp, m_source = 0.0, h_fg = 2437426.07, rho_he = C_R(cell, he);
real, vof_l = C_VOF(cell, liq), vof_he = C_VOF(cell, he), Vol = 0.0195, p_vap_t = 0.0;
real vof_v = 1.0 - vof_he - vof_l, r_rho_lv = 1. / rho_v - 1. / rho_l, time = 0.1;
real m_dot = 1000 / h_fg, p_vap = (m_dot * time* 8315 * (80 + 273.15)) / (Vol*18.02);
if (C_UDMI(cell, thread, 2) <= P_SAT)
{ m_source = m_dot + C_UDMI(cell, thread, 1);
p_vap_t = C_UDMI(cell, thread, 2) + p_vap;
dp = P_SAT - p_vap_t; dp = MAX(dp, 1e-4); C_UDMI(cell, thread, 1) = m_source;
C_UDMI(cell, thread, 2) = p_vap_t; *d_mdot_d_vof_from = m_dot; *d_mdot_d_vof_to
= -m_dot;
}
else
{ m_dot = 0.0; m_source = m_dot + C_UDMI(cell, thread, 1); p_vap = 0.0;

```

```

p_vap_t = C_UDMI(cell, thread, 2) + p_vap; dp = P_SAT - p_vap_t; dp = MAX(dp, 1e-
4); C_UDMI(cell, thread, 1) = m_source; C_UDMI(cell, thread, 2) = p_vap_t;
*d_mdot_d_vof_from = m_dot; *d_mdot_d_vof_to = -m_dot;
}
if (NNULLP(THREAD_STORAGE(thread, SV_MT_DS_DP)))
C_STORAGE_R(cell, thread, SV_MT_DS_DP) = ABS(r_rho_lv*m_source / dp);
return m_source;
}

```

A.3 UDF for Multiphase Mixture Model and Species Transport Activated

```

#include "udf.h"
#include "sg.h"
#include "sg_mphase.h"
#include "flow.h"
#include "mem.h"
#include "math.h"
DEFINE_LINEARIZED_MASS_TRANSFER(cav_source, cell, thread, from_index,
from_species_index, to_index, to_species_index, d_mdot_d_vof_from,
d_mdot_d_vof_to)
{ Thread *liq = THREAD_SUB_THREAD(thread, from_index);
Thread *vap = THREAD_SUB_THREAD(thread, to_index);
Thread *he = THREAD_SUB_THREAD(thread, 0);
real T = C_T(cell, liq), P_SAT = exp(77.345 + 0.0057*T - 7235 / T) / pow(T, 8.2);
real m_dot=0.0, dp, m_source=0.0, p_op = RP_Get_Real("operating-pressure");

```

```

real rho_he = C_R(cell, he), rho_v = C_R(cell, vap), rho_l = C_R(cell, liq);
real vof_he = C_VOF(cell, he), vof_l = C_VOF(cell, liq), vof_v = 1.0 - vof_he - vof_l;
real r_rho_lv = 1. / rho_v - 1. / rho_l, h_fg = 2437426.07;
real p_vap = (C_P(cell, thread) + p_op)*((vof_v*rho_v) / (vof_v*rho_v +
vof_he*rho_he)); real vel = sqrt(C_U(cell, thread)*C_U(cell, thread) + C_V(cell,
thread)*C_V(cell, thread));
if (p_vap <= P_SAT)
{ dp = P_SAT - p_vap; dp = MAX(dp, 1e-4); m_dot = (0.0888 + 0.0783*vel)* dp / h_fg;
m_source = m_dot*vof_l; C_UDMI(cell, thread, 1) = m_source; *d_mdot_d_vof_from =
m_dot; *d_mdot_d_vof_to = -m_dot;
}
else
{ dp = P_SAT - p_vap; dp = MAX(dp, 1e-4); m_dot = 0.0; m_source = m_dot*vof_l;
C_UDMI(cell, thread, 1) = m_source; *d_mdot_d_vof_from = m_dot;
*d_mdot_d_vof_to = -m_dot;
}
if (NNLLP(THREAD_STORAGE(thread, SV_MT_DS_DP)))
C_STORAGE_R(cell, thread, SV_MT_DS_DP) = ABS(r_rho_lv*m_source / dp);
return m_source;
}

```