Development of a Numerical Solver for Phase-Change and Two-Phase Flow in Porous Media

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

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Porous media are used in several thermal management systems, such as loop-heat-pipes, to control the temperature of electronics and other components. It is important to understand the mechanisms of flow and phase-change in porous media to better control/increase the performance of those systems. In this work, we develop a CFD solver using the object-oriented OpenFOAM architecture that can simulate most of the relevant physics of flow and phase-change in porous media. The developed solver is based on an existing solver based on the IMPES (Implicit Pressure, Explicit Saturations) method, which is employed to solve the pressure and saturation equations due to the nonlinearity of the capillary and relative permeability equations. The solver is then modified to include the energy equation and phase-change models (empirical and interface equilibrium models) that can simulate temperature and phase-change, respectively. Hydrodynamic and thermal coupling of flow and phase-change in porous media is complex numerically, and, this complexity is achieved in the present study by coupling between all the governing equations and the phase-change models using the VOF (Volume of Fluid) approach. Different effective thermal conductivity models are implemented to calculate an effective thermal conductivity between the three phases (solid, liquid, and vapor) in every cell. The solver also uses temperature-dependent properties for density, thermal conductivity, and viscosity. The results obtained from this solver are compared with a one-dimension semi-analytical solution to validate the solver. An example of flow and phase-change in a section of the porous media of a loop heat pipe (LHP) is also presented.
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# Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_p$</td>
<td>Specific heat (J/kgK)</td>
</tr>
<tr>
<td>$D_m$</td>
<td>Molecular Diffusion (m$^2$/s)</td>
</tr>
<tr>
<td>$D_L$</td>
<td>Longitudinal Dispersion Coeff (m$^2$/s)</td>
</tr>
<tr>
<td>$d_p$</td>
<td>Hydraulic diameter (m)</td>
</tr>
<tr>
<td>$g$</td>
<td>Acceleration of gravity (m/s$^2$)</td>
</tr>
<tr>
<td>$h$</td>
<td>Specific enthalpy (J/kg)</td>
</tr>
<tr>
<td>$h_{lv}$</td>
<td>Latent heat (J/kg)</td>
</tr>
<tr>
<td>$h_{sv}$</td>
<td>Heat trans coeff of vapor (W/m$^2$K)</td>
</tr>
<tr>
<td>$h_{sl}$</td>
<td>heat trans coeff of liquid (W/m$^2$K)</td>
</tr>
<tr>
<td>$J$</td>
<td>Capillary J-function</td>
</tr>
<tr>
<td>$K$</td>
<td>Permeability (m$^2$)</td>
</tr>
<tr>
<td>$K_r$</td>
<td>Relative permeability</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure (Pa)</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandlt number</td>
</tr>
<tr>
<td>$PCV$</td>
<td>Dilatation rate</td>
</tr>
<tr>
<td>$Q$</td>
<td>Volumetric heat source (J/m$^3$s)</td>
</tr>
<tr>
<td>$Q_{sf}$</td>
<td>Convection heat flow (J/m$^3$s)</td>
</tr>
<tr>
<td>$Q_{pc}$</td>
<td>Phase change heat (J/m$^3$s)</td>
</tr>
<tr>
<td>$Q_{boil}$</td>
<td>Boiling heat flow (J/m$^3$s)</td>
</tr>
</tbody>
</table>
\( q \)  Heat flux (J/m\(^2\)s)

\( Re_p \)  Reynolds number

\( r \)  Rate parameter (1/s)

\( S \)  Saturation

\( T \)  Temperature (K)

\( t \)  Time (s)

\( u \)  Velocity (m/s)

\( \alpha_{sf} \)  Aspect ratio

\( \varepsilon \)  Porosity

\( \varepsilon' \)  Effective porosity

\( \kappa \)  Heat conductivity (W/mK)

\( \lambda \)  Displacement of particles (m)

\( \mu \)  Fluid dynamic viscosity (kg/ms)

\( \rho \)  Density (kg/m\(^3\))

\( \sigma \)  Interfacial tension (N/m)

\( \sigma^2 \)  Displacement Variance

Subscripts

\( s \)  Solid

\( r \)  Relative

\( f \)  Fluid

\( l \)  Liquid

\( v \)  Vapor
\begin{itemize}
\item \textit{c} \quad \text{Capillary pressure}
\item \textit{sat} \quad \text{Saturated}
\item \textit{Eff} \quad \text{Effective}
\item \textit{max} \quad \text{Maximum}
\item \textit{irr} \quad \text{Minimal irreducible}
\end{itemize}
1 Introduction

1.1 Overview

Transport of fluid and heat in porous media has been noticed in many engineering applications, for example, geothermal systems, underground spread of pollutants, nuclear waste materials storage, thermal insulation, electronic cooling, modeling of petroleum reservoir, ceramic engineering…etc. Moreover, porous media is used for heat transfer applications as it provides a very large surface area to volume ratio. For instance, porous fins are used in motor bikes [1]. The tortuous path in the porous fins provides more surface area than a regular straight or pin-type fins. As a result, more heat transfer takes place providing more cooling to the engine. Another key feature of porous media is capillarity, which creates pumping pressure. For instance, in the petroleum industry, the extraction of oil is done by the overcoming capillarity through the porous rocks from underground reservoirs. These two important features (i.e. cooling and capillarity) of porous media make it popular in the field of electronics industry. The miniaturization in electronics, while aiming for high performance, increases heat dissipation and the use of fan as a cooling system for transferring such high heat fluxes is inefficient. Therefore, new technologies for cooling should be introduced for efficient control of electronics temperature. A Loop Heat Pipe (LHP) containing a porous medium is an alternative cooling technology to dissipated heat from electronics. An example of electronics cooling devices for space application employing LHPs is discussed below.

For spaceships or near-earth satellites [2], thermal management or control is very important to protect power electronics, electronic devices and other systems from extreme
heat. LHPs can accommodate the best thermodynamic (surface area of porous media) and hydraulic (capillarity of porous media) performance. For example, in September 2021, NASA will launch the Surface Water Ocean Topography (SWOT) mission [3] (See Figure 1), which will collect data from 90% earth surface from the transition of water bodies. The main goal of this project is to examine the surface water of the earth. Electronic components such as Nadir Altimeter and KA-band radar interferometer will help to gather that information for weather and climate modeling, and freshwater management. For proper operation, the allowable KaRIn temperature rate of change is 20 times smaller than typical spacecraft instruments.

![Surface Ocean Water Topography (SWOT) Project](image)

**Figure 1.1** Surface Ocean Water Topography (SWOT) Project

Advanced thermal management system is required for the SWOT mission to accurately control the temperature of those equipment. NASA usually employs single-phase cooling systems for thermal control, but such a system has a very poor isothermality and requires high pumping power. On the other hand, a two-phase system, such as LHP,
can achieve higher isothermality, as the absorption of heat is achieved through phase-change (latent heat). Also, higher heat loads can be accommodated due to also the latent heat. Furthermore, no external pumping power is required for LHPs as the porous wick drives the flow. However, if higher controllability of temperature is required, a small pump may be added to the liquid line. These features make LHPs very suitable for space applications.

A two-phase LHP system [4-9] (see Fig. 2) is a passive thermal management system where heat is absorbed at evaporator (where cooling of electronic devices and other equipment takes place) by a suitable working fluid through phase-change (liquid to vapor). Inside the evaporator is a porous wick that seats on pillars that form grooves or touches the casing of the evaporator (see Fig. 2). Phase-change takes place inside the porous wick at the interface between the porous media and pillar/casing. The resulting vapor leaves through the grooves towards the vapor line. Before leaving the grooves, the vapor becomes slightly superheated. If the vapor line is not properly insulated, then a heat exchange will take place, which will cause a reduction in the vapor temperature and possible condensation. To get better performance of the LHP, the vapor line should be insulated. The vapor is then fed to the condenser, where phase-change (vapor to liquid) occurs by releasing heat to the surrounding ambient (deep-space for space applications). The produced liquid will be subcooled at the later portion of the condenser. Then, this subcooled liquid will pass through the liquid line towards the evaporator. If the liquid line is not properly insulated, the liquid will release or gain heat depending on the surrounding temperature. The liquid line also contains an accumulator (replacing the traditional compensation chamber), which controls the temperature when liquid from the liquid line
mixes with the liquid in the accumulator by maintaining two-phase equilibrium inside of it. The liquid will then seep through the porous wick inside the evaporator and a meniscus will form at the liquid-vapor interface, which develops a pressure by the action of capillarity. It is this capillary pressure that drives the fluid flow through the whole loop.

It is vital to notice that with increasing heat loads boiling might take place inside the wick, which may result in dry out of the porous wick. Also, if nucleation occurs within the porous wick it will eliminate the meniscus thus eliminate the capillary pressure.

![Figure 1.2 A schematic of a two phase LHP system](image)

**1.2 Research Objective**

From the above discussion, it clear that the porous wick within the evaporator is the most critical component of the LHP. The performance of the LHP greatly relies on the
characteristics of the porous wick used. Therefore, it is important to fully understand the
two-phase flow and phase change in porous media. The overall objective of the current
research is to develop and design an advanced two-phase LHP that can operate in
microgravity for NASA Space systems. Specifically, design a system with a ~1-m²-flat
coolant plate whose temperature can be controlled to better than 2 K isothermality with
discrete and time-varying heat loads of ~5W/cm². The main focus of this thesis is to
develop a solver in the OpenFOAM architecture that can accurately model phase-change
and two-phase flow in porous media. This solver can be used to study the performance of
different porous media for LHPs and select the porous media characteristics that can
enhance the performance of LHPs.
2 Literature Review

In this section, we will discuss how different parameters affect the LHP performance, and the modeling approaches for LHPs. Moreover, we will discuss the different approaches used to model porous wick within the evaporator, which the most important component of an LHP.

2.1 LHP Modeling

Different processes occur in different parts of an LHP; for instance, the liquid evaporates inside the evaporator, and the resulting vapor is transported to the condenser where it condenses back into liquid, which is then returned to the evaporator to repeat the cycle. These processes are hydro-dynamically and thermally coupled. As a result, the whole LHP performance depends on those processes and its performance can be altered with any adjustment in those processes. To simulate an LHP, it is essential to model the parameters influencing the LHP performance meticulously.

To maintain the fluid circulation inside the LHP, the developed capillary pressure in the porous wick should be greater than or equal to the total pressure drop in the loop.

\[ P_{\text{capillary}} \geq P_{\text{total}} \]

\[ = P_{\text{evaporator}} + P_{\text{condenser}} + P_{\text{liquid line}} + P_{\text{vapor line}} + P_{\text{accumulator}} \quad 2.1 \]

Viscous forces of the fluid can be larger than the pressure forces for low operating temperature and small applied heat load. Low or no-flow will reduce heat transport [10].
On the other hand, the vapor flow rate can increase to a sonic speed [11] (while flowing through a pipe with uniform cross-section) when mass flow is increased due to excessive phase-change (evaporation). Also, if the cross-sectional area of the vapor duct decreases while in operation, choked flow will occur. All these phenomena alter the performance of LHPs. Therefore, it is important to understand the parameters that affect them.

Pore diameter, porosity, permeability, and the effective thermal conductivity of the porous wick has a great effect on the LHP performance.

The effective thermal conductivity [12-13] is calculated as a function of the fluid and solid conductivities. LHP operating temperature and heat leak are directly influenced by the effective thermal conductivity. Baumann and Rawal [14] observed that a low thermal conductivity of the working fluid will reduce the heat transportability of the evaporator by decreasing the heat transfer coefficient, which results in reducing the LHP operating temperature.

The capillary and boiling limit may change with different porosity and permeability of the wick. Reduction in pore size enhances the capillary pressure as well as the pressure loss due to friction. So, depending on the applied heat flux, an optimal value for pore diameter exists. A porous wick with higher permeability will provide easier vapor flow as discussed by C. Figus et al. [15]. Boo and Chung [16] observed that with the decrease in pore size, system thermal resistance was reduced by 33% and the maximum thermal load was enhanced by 45%. When LHP operates at the capillary limit it is advised to use porous wick with small pore size.

Yao et al. [17] found that the number of vapor grooves raise the boiling limit of an LHP. A fin(casing)/groove width ratio of 0.5 provides a maximum boiling limit. The fin
width also enhances the capillary limit and with the decrease in wick thickness both the capillary limit and boiling limit increase. The working fluid used in this study was ammonia and the porous wick was made of a sintered nickel.

Working fluids used in LHP affect its performance greatly. Ammonia is the most common working fluid used in LHPs. However, other fluids, such as water, acetone, and propylene are also used. Kaya and Ku [18] compared the effect of using ammonia, water, and acetone on the performance of LHP. Absolute vapor pressure limits water and acetone. On the other hand, ammonia has most of the quality to be a perfect working fluid for LHP but it has a relatively high freezing temperature, which causes freezing in the condenser at low-temperature applications. For low sink temperature, propylene exhibits better LHP performance because of its low freezing point.

Sink temperature and ambient temperature has also an effect on LHP performance. Working fluid’s thermophysical properties rely on the sink and ambient temperature. As a result, variation in the sink and ambient temperature will affect the thermo-hydraulic behavior of an LHP.

The heat transfer performance of an LHP also depends on the working fluid fill ratio (volume of liquid in the reservoir to total reservoir volume). Lee et al. [19] measured the best heat transfer performance when the filling ratio is 51.3 vol% for any porous materials and any imposed heat flux.

The presence of non-condensable gases (NCG) has also an effect on LHP performance. An experiment was conducted by Nikitkin et al. [20] to observe the influence of NCGs on LHP performance. Different amounts of hydrogen were added to the LHP where ammonia was the working fluid. Operating temperature and start-up time of the LHP
were increased with the addition NCGs, but not as much as anticipated because the working fluid and wick materials ingested the gas.

Gravity is another vital factor that influences the LHP performance at low heat loads as observed by Y. Chen et al. [21]. Elevation in LHP refers to the relative position of the evaporator to the condenser. When the evaporator is placed above the condenser, it is known as an adverse elevation. When the heat loads are low, the operating temperature of LHP increases while maintained at adverse elevation. With higher heat loads, the effect due to elevation started vanishing and at some value, it completely vanishes. Boo and Chung observed [16] that the operating temperature of LHP changes from 50°C to 72°C for elevation changing from 5cm positive elevation to 10cm adverse elevation. Deli et al. [22] observed that adverse elevation affects evaporation negatively thus hinders LHP performance.

Pressure drops in LHP contribute also to its performance. At a constant heat load, the pressure is controlled by closing/opening the metering valve at the vapor line. Ku et al. [23] observed that with the increasing external pressure drop (due to the temperature difference between evaporator and compensation chamber), operating temperature is increased.

### 2.2 Porous Media Modeling

From section (1.1), it can be easily portrayed that the evaporator is the most important component of an LHP because it contains the porous wick. Both the phase change and capillary pressure development takes place in the porous wick. Three different properties can define a porous media [24]: (a) space filled with multiphase matter, consisting of at least the solid and fluid phases (fluid-phase occupies the pore space around
the solid matrix), (b) distribution of the solid phase throughout the porous medium, which affects the solid surface area, and (c) interconnection between the pores (interconnected pore space is called effective pore space and pores that are not connected are considered as a segment of the solid phase). Generally, in two phase system, porous media is occupied with two different fluids, one is wetting and another is non-wetting [25]. Wetting fluid flows in the porous medium by the action of capillarity and while wetting fluid is advancing through the porous media, the non-wetting one is receding. The capillary pressure that is developed inside the porous media is defined by the pressure difference between non-wetting and wetting fluid. This capillary pressure is typically calculated as a function of saturation of the wetting fluid. Saturation of the wetting fluid is the ratio of the portion of pore space occupied by the wetting fluid to total pore space.

Pore space inside the porous medium can be characterized by two parameters: porosity and permeability. Porosity is the ratio of the volume of pore space to the total volume of porous media. Permeability defines the resistance of the porous media to the flow of a fluid. High permeability allows fluid to flow with less resistance through the porous media. Two fluid phases inside the porous media will experience relative permeability. Relative permeability of a phase is defined as the ratio of effective permeability of that phase to the absolute or intrinsic permeability. When porous medium is fully saturated with either wetting fluid or non-wetting fluid, the obtained permeability from this system is referred to absolute permeability. Relative permeability is also calculated as a function of wetting fluid saturation.

The above-mentioned parameters define the porous medium. These parameters have an important role to model the porous media and construct the governing equation for
fluid flow and heat transfer. It is difficult to model porous media considering hydrodynamic, thermal behavior, and structural complexity of the solid matrix. There are four different [26] scales (see Fig. 2.1) to model porous media depending on the application i.e. pore scale, Darcy scale, core scale, and field scale.

![Figure 2.1 Different scales of porous media modeling [27]](image)

At the pore scale, a continuum is described by each of the phases within a domain of interest. The pore scale is defined by the microscale level where a microscale level [26] refers to what occurs at a point of a specific phase (solid, liquid or gas) in porous media. The typical scale is in micro meter. For example, vapor is flowing through the porous domain. At the pore scale, all the behavior for the flow of vapor, for example, velocity, pressure, etc. will be calculated for every point where the vapor flows through. Ranjan et al.
al [28] studied the porous wick region of a flat heat pipe for evaporation and condensation by considering micro (microstructure level evaporation model) and macro (device-level model) models. These two models are integrated to understand the performance of the heat pipe with screen mesh porous medium at the pore scale. It is observed that the vapor chamber performance is affected by the thermal resistance of liquid-vapor interface inside high-conductive thin wick. Raeini et al. [29] developed a model, for two-phase flow, employing volume of fluid (VOF) method in porous media at a pore scale. A semi-sharp surface force model is adopted to determine the capillary forces. A numerical solver is extended to develop this two-phase model at the pore scale. To validate the model, several test cases including stationary droplet, moving droplet, and two-phase flow through capillary tubes are modeled. The stability and accuracy of the VOF method were benchmarked by those test cases.

At the Darcy scale, a continuum is described by the volume average porous domain of interest. Also, every phase in the domain is considered as a continuum. For the entire domain, variables of state are defined regardless of the phase. The typical scale is in centimeter and meter. Geological formations, i.e. oil reservoirs and aquifers are modeled in this scale. In this macroscopic level, interest leans towards average fluid flow, solute transport, heat transport, etc than specific at a point as discussed in pore scale. For some specific case, for example, dissolution during acid injection, a little upscaling is required and it is referred to as ‘core scale’. A macroscale numerical model for porous media is developed by Niessner et al. [30] by implementing an extended form of Darcy’s law. This extended model captures the fluid-fluid interfacial area as a parameter for capillary pressure and includes physical processes, for example, hysteresis (difference in the angle
of wetting during imbibition and drainage of porous media, where angle of wetting computed from front of the wetting fluid for imbibition and from back of the wetting fluid for drainage. It is basically the contact angle between fluid and solid porous medium). Capillary pressure and saturation are independent of each other in this model. Furthermore, the inclusion of the interfacial area makes this model unique for new applications in porous media. To avoid local volume average closure problems in heterogeneous porous media where complex architecture of porous media causes different flow directions and velocities, Quintard et al. [31] introduced the method of large scale averaging. In this method, Darcy equations are averaged over a heterogeneous region. Local Mechanical Equilibrium (capillary pressure-saturation relations determines the local fluid distribution) eliminates the closure problem of the homogeneous medium. In this research, the authors extend the work from single-phase to two-phase flow to investigate the phenomena for two-phase flow in heterogeneous porous media.

At the ‘field scale’, also known as formation scale, the transport behavior in heterogeneous (Layers of different permeability) geological formations is considered. Distance is typically from meters to kilometers. Space is a key consideration in this kind of porous domain. Hillfer et al. [32] presented a macroscopic equation of motion at field scales that are used to perform the numerical analysis of the reservoir. Dimensional analysis is shown where capillary number is used instead of Darcy’s law to normalize the pressure field. Macroscopic Capillary Number refers to the ratio of macroscopic viscous forces to macroscopic surface tension. Capillary force will be dominant for low capillary number and viscous forces will be dominant for high capillary number. Two different experiments are performed for unconsolidated sand, sandstones, and limestone in field-
scale (field flood) and laboratory-scale (laboratory flood), and the obtained capillary number from these experiments showed the difference in oil saturation. For different media, this field-scale model agrees with the experiment to measure the gravitational relaxation time and segregation front widths.

Motte et al. [33] investigated a capillary evaporator employing a mixed pore network model representative of unit cells to compute heat and mass transfer with liquid-vapor phase change. In vapor and liquid pores, temperature and pressure fields are integrated using the mean-field approach and this method relies on the capillary pressure threshold, which is related to each local blockage between two pores. The heat source was also considered in the simulation. Classical pore network is used to model the capillary pressure and simulations are performed under the mesoscale approach. Numerical simulation results show agreement with the visualization experiment results.

Selih et al. [34] developed a general transient numerical model for multiphase flow with phase-change in porous media. An alternating direction block iterative method and the tridiagonal matrix algorithm are used in this model. To validate the model, gravimetric experimental data for concrete is used. The capillary pressure is not considered in this model for the flow of moisture content. Extreme conditions, for example, a porous media is exposed to high-intensity fire, can be analyzed with this numerical model.

Raffray et al. [35] observed that most of the thermal-hydraulic porous models were based on a semi-empirical approach, which was limited to the only estimation of the overall heat transfer coefficient. The author proposed MERLOT (Model of Energy-transfer Rate for fLow in Open-porosity Tailored-media) model, which provides the data for velocity profile and temperature distribution in the porous region, and solid-fluid local heat transfer.
This model is based on the polar coordinate system and it does not consider capillary pressure.

Xin et al. [36] developed a modified separate flow model including capillarity, liquid phase change, non-isothermal two-phase region, and local thermal non-equilibrium (LTNE) to observe the characteristics of mass and heat transfer in porous media. It was long assumed that solid and fluid temperatures are equal locally. But Shi and Wang [36] and Yuki et al. [37] studied found that there is a temperature difference between the solid and liquid locally at higher heat loads in the two-phase region. Neither of them used the separate flow model (SFM) where two phases are recognized as separate fluid, instead, they use a two-phase mixed model (TPMM) where the two-phase temperature is considered isothermal and at any point, local fluid and the solid temperature is same. Xin et al. [36] used a modified separate flow model employing a front capturing method where two phases are considered separately, which results in a larger set of governing equations. They studied this porous model for parallel and vertical high heat flux to the fluid flow direction. In a two-phase region, non-isothermal behavior is evident for former and LTNE behavior is noticed for the latter.
3 Numerical Approach

Different numerical approaches for porous media modeling have been discussed in the previous chapter (2). These models are reviewed for different scales, for instance, pore-scale, Darcy scale, field-scale, etc. In the next sections, two different models are presented; the flow model and the heat transfer model for the modeling of flow and phase-change in porous media.

3.1 Existing Numerical Models

In this section, different numerical approaches to model flow and/or heat transfer and phase change in porous media are described.

3.1.1 Pore Space Image Modeling

A Stokes solver is used to model the pore space image (a 3-D representation of pores in rocks) [37] for flow and transport of liquid limited to low Reynolds number flows. The idea of the pore space image is to explicitly model the voids or the pore spaces. For the flow field, a lattice Boltzmann technique is used. A numerical solver, simpleFoam, is used to simulate the fluid flow and heat transport. The governing equations for this model are

\[ \nabla \cdot \mathbf{u} = 0 \quad 3.1 \]

\[ \mu \nabla^2 \mathbf{u} = \nabla p \quad 3.2 \]

\[ \mathbf{u} = 0; \text{ on grains} \quad 3.3 \]

where \( \mathbf{v} \) is the velocity vector, \( \mu \) is the fluid viscosity and \( p \) is the pressure. A zero-velocity condition is applied at the pore wall. The author compared different porous materials by simulating a sand pack, sandstone, and carbonate.
3.1.2 Modified Separate Flow Model (MSFM)

To observe heat and mass transfer phenomena numerically in porous media, Xin et. al. [36] developed a modified separate flow model. The model included capillarity effect, phase change of liquid, local thermal non-equilibrium (LTNE), and non-isothermal two-phase region. The corresponding equation for fluid phase mass conservation is

$$\varepsilon \frac{\partial (\rho_l S_l + \rho_v (1 - S_l))}{\partial t} + \nabla \cdot (\rho_l u_l + \rho_v u_v) = 0$$

where $S$ is the saturation, $\varepsilon$ is the porous media porosity, $\rho$ is the density, and $u$ is the velocity respectively. The subscripts $l$ and $v$ are for liquid and vapor, respectively. The velocity of a phase, $\beta$ (liquid, $l$, or vapor, $v$), is calculated from the Darcy equation as

$$u_\beta = -\frac{K K_r \beta}{\mu_\beta} \left( \nabla p_\beta + \rho_\beta g \right)$$

where $K$ is the permeability, $K_r$ is the relative permeability, and $g$ is the gravity.

Local convection or solid-fluid boiling heat exchange are modeled using the LTNE equations

$$\varepsilon \frac{\partial}{\partial t} \left( \rho_l s_h + \rho_v (1 - s) h_v \right) + \nabla \cdot \left( \rho_l u_l s_l + \rho_v u_v h_v \right) = \nabla \cdot (\kappa_{f,eff} \nabla T_s) + Q_{sf}$$

$$\varepsilon (1 - \varepsilon) c_p \frac{\partial T_s}{\partial t} = \nabla \cdot (\kappa_{s,eff} \nabla T_s) - Q_{sf} + Q$$

where $T$, $c_p$, and $h$ are the temperature, specific heat at constant pressure, and specific enthalpy. $Q$ and $Q_{sf}$ are the volumetric heat source and convection or boiling flow per
volume, respectively. $\kappa_{f,\text{eff}}$ and $\kappa_{s,\text{eff}}$ are the effective thermal conductivities of the solid and fluid phases, respectively.

In this model, the capillary pressure, $p_c$, is a function of porosity, permeability, surface tension, $\sigma$, and saturation as [38]

$$p_c = p_v - p_l = \sigma J(S_l) \frac{\varepsilon}{K}$$  \hspace{1cm} 3.8

where

$$J(S_l) = 1.417(1 - S_l) - 2.12(1 - S_l)^2 + 1.263(1 - S_l)^3$$  \hspace{1cm} 3.9

The relative permeability model is derived based on the liquid saturation-relative permeability relation, which reads [39]

$$\begin{align*}
K_{rl} &= S_l^3 \\
K_{rv} &= (1 - S_l)^3
\end{align*}$$  \hspace{1cm} 3.10

The absolute permeability of the porous media depends on both pore size and the porosity as [39]

$$K = \frac{\varepsilon^3 d_p^2}{150(1 - \varepsilon)^2}$$  \hspace{1cm} 3.10

where $d_p$ is a characteristic pore diameter.

Finally, for MSFM, the phase-change model is developed based on the saturation temperature and latent heat of the liquid as

$$Q_{sf} = \begin{cases} 
  h_{sl}\alpha_{sf}(T_s - T_l); & \text{for Liquid region} \\
  h_{sv}\alpha_{sf}(T_s - T_v); & \text{for Vapor region} \\
  Q_{\text{boil}} + (1 - s)h_{sv}\alpha_{sf}(T_s - T_l); & \text{for two phase region}
\end{cases}$$  \hspace{1cm} 3.11

where $\alpha_{sf}$ is the aspect ratio and boiling heat flow $Q_{\text{boil}}$ is
\[ Q_{\text{boil}} \]
\[ = s \alpha_{sf} \mu h_{lv} \left( \frac{g (\rho_l - \rho_v)}{\sigma} \right)^{1/2} \left( \frac{c_{pf} (T_s - T_{sat})}{0.006 h_f g} \right)^{3} \left( \frac{1}{\Pr_f} \right)^{\frac{1.7}{0.33}} \]  

3.12

In this equation, \( h_{lv} \) is the latent heat of evaporation, and \( T_{sat} \) is the saturation temperature. For the calculation of the Prandtl number, \( Pr \), the following equation can be used

\[ h_{s\beta} = \left( \frac{K_{\beta}}{d_p} \right) \left( 2 + 1.1 \Pr_{\beta}^{\frac{1}{5}} Re_{p}^{0.6} \right) \]; with \( Re_{p} = \frac{\rho_{\beta} u_{\beta} d_{p}}{\mu_{\beta}} \)  

3.13

3.2 Numerical Models Inspiring our Research

For our numerical study, an OpenFOAM [40] flow solver, impesFOAM is adopted and modified to include the energy equation and phase-change models. OpenFOAM is open source field operation and manipulation. This is an open source software for computational fluid dynamics. This OpenFOAM platform is based the object oriented c++ code and the source code is available to all the users. The users can customize and manipulate the c++ code to build their own numerical solver to solve specific problems. For CFD analysis all numerical solver employs finite volume method (FVM) unless otherwise defined. Numerical analysis of multiphase flow, heat transfer, incompressible or compressible flow of fluid, DNS, combustion, stress can be performed in OpenFOAM.

The original impesFOAM solver is developed by Horgue et. al. [41]. In the article, a toolbox is introduced to solve multiphase flow problems in porous media where mass conservation for each phase combined with the phase velocity derived from Darcy’s Law [42] are solved instead of the modified Navier-Stokes equations. To develop the toolbox,
a sequential approach, IMPES (Implicit Pressure Explicit Saturation) method, is embraced because of the sequential character of OpenFOAM where, except the transient term, all the terms are a function of saturation. When saturation and pressure in a system are independent, the sets of governing equations can be presented implicitly. This can reduce computation time greatly. On the other hand, when the equations depend on an explicit term and nonlinear relations between variables presented in the system, it will make the system unstable and more computational time is required. The formulation of the governing equations for impesFOAM solver is discussed in the next sub-sections.

3.2.1 Fluid Flow Model

This open-source solver, impesFOAM, is slightly customized to match our case by neglecting the wellbore (an opening to the underground resources) terms. At macro-scale, the volume-averaged equations define the flow through the porous medium. The finite volume method is applied for numerical analysis in the ‘porousMultiphaseFoam’ toolbox. In this two-phase system, instead of solving the Navier-Stokes equations, system equation of mass conservation for each phase combined with the Darcy velocity derived from Darcy’s law, and a pressure-saturation (Eqns. 3.20-3.21) is constructed and solved using the IMPES approach. This approach is a segregated method introduced by Sheldon et. al. [43] where the pressure equation is solved implicitly and the saturation equation is solved explicitly. All terms, except the transient ones, in this IMPES method are expressed as a function of saturation. This method is illustrated in detail in Hourge et. al. [41].

To compute the saturation of liquid and vapor, the saturation equation is solved as

$$\varepsilon \frac{\partial S_l}{\partial t} + \nabla \cdot \mathbf{u}_l = q_l$$  \hspace{1cm} (3.14)
To compute the total velocity and pressure, the pressure equation is solved as

\[
\nabla \left( - \frac{KK_{rv}(S_l)}{\mu_v} (\nabla p_v - \rho_v g) \right) + \nabla \left( - \frac{KK_{rl}(S_l)}{\mu_l} (\nabla p_l - \rho_l g - \nabla p_c(S_l)) \right) = q_v + q_l
\]

Capillary pressure is calculated from the saturation dependent capillarity model (Eqns. 3.13 and 3.14) which eliminates an unknown from the system.

In the above equations (3.20 and 3.21), \( q_v \) and \( q_l \) are the wellbore terms that indicate the extraction and injection flow rates. These terms mostly applied to earth science modeling and are not used in our model.

The dependency of relative permeability and capillary pressure with saturation is nonlinear, as a result, ‘IMPES’ algorithm is adopted. At each time step, using the PISO method, the corrected velocity field is obtained after the pressure equation is solved.

### 3.2.1.1 Porous Models

For the calculation of the capillarity and relative permeability, seven different parametric models are analyzed. Among them, the Van Genuchten model [44-46] shows the most aligned result with experimental data. Van Genuchten capillarity and relative permeability model are available in the porousMultiphaseFoam toolbox library. Both the models are developed based on the effective saturation.

Using the van Genuchten model, the relative permeability for vapor and liquid phases are defined as

- Vapor
\[ K_{rv}(S_{l,eff}) = K_{rv,\text{max}}(1 - S_{l,eff})^{\frac{1}{2}}(1 - S_{l,eff}^m)^{2m} \]

3.16

- Liquid

\[ K_{rl}(S_{l,eff}) = K_{rl,\text{max}}(S_{l,eff})^{\frac{1}{2}}(1 - (1 - S_{l,eff}^m)^m)^2 \]

3.17

with

\[ S_{l,eff} = \frac{S_l - S_{l,irr}}{1 - S_{v,irr} - S_{l,irr}} \]

3.18

Here, \( K_{rv,\text{max}} \) and \( K_{rl,\text{max}} \) are the maximum relative permeabilities for vapor and liquid, respectively, and are normally set to 1 if not defined otherwise. \( S_{l,eff} \) is effective saturation, which is calculated from the user-defined minimal irreducible saturations \( S_{v,irr} \) and \( S_{l,irr} \).

Using the same model, the capillarity is defined as

\[ p_c(S_{l,p_c}) = p_{c,0}(S_{l,p_c}^{-\frac{1}{m}} - 1)^{\frac{1}{n}}, \quad \frac{1}{n} = 1 - m \]

3.19

where, \( p_{c,0} \) is the entry capillary pressure, \( S_{l,p_c} \) is the effective saturation of the capillary pressure and \( m \) is the van Genuchten coefficient. The effective saturation of the capillary pressure can be written as

\[ S_{l,p_c} = \frac{S_l - S_{p_c,irr}}{S_{p_c,\text{max}} - S_{p_c,irr}} \]

3.20

In this equation, \( S_{p_c,\text{max}} \) is the maximum saturation of wetting fluid, and \( S_{p_c,irr} \) is the residual saturation, which is a user-defined parameter.
3.2.2 Phase Change Model

Two-fluid Eulerian averaging of dispersed features, Lagrangian tracking of individual particles, interface capturing and tracking techniques, etc. are different numerical approaches used to compute phase-change heat transfer. In the current solver, VOF interface capturing approach is used. This approach tracks the generation of liquid or the transfer of mass from one phase to another caused by phase-change heat transfer. A library of thermal phase-change model is implemented into the IMPES solver with two different phase-change models; The first one is the empirical rate parameter model that estimates the volumetric phase-change heating rate. This is the most common and simple approach that was developed by Yang et. al [47-48]. In this model, the phase change is applied to every cell along with the liquid-vapor interface. The evaporation and condensation heat transfer, $\dot{Q}_{pc}$, with evaporation and condensation rate parameters $r_l$ and $r_v$ respectively, can be expressed as

- Evaporation when the temperature of the domain is greater than saturation temperature,

$$\dot{Q}_{pc} = r_l S_l \rho_l h_{lv} \frac{T - T_{sat}}{T_{sat}}, \quad T \geq T_{sat} \quad (3.21)$$

- Condensation when the temperature of the domain is less than the saturation temperature

$$\dot{Q}_{pc} = r_v (1 - S_l) \rho_v h_{lv} \frac{T - T_{sat}}{T_{sat}}, \quad T < T_{sat} \quad (3.22)$$

The rate parameters $r_l$ and $r_v$ must be tuned for different meshes and studies as they depict thermal time constants of mesh cells.
Interface equilibrium is another model for phase change heat developed by Rattner et al. [49]. In this model, saturation temperature is regained by defining the phase change heat source from the liquid-vapor interface at every time step. The mesh cells of the domain are represented as a graph of nodes and edges. A scan is undertaken over the graph edges to determine the location of the interface of liquid and vapor or the two phase zone and the phase change model is then applied to that location of a two-cell thick layer interface. The phase change heat, \( \dot{Q}_{pc} \), in this model is calculated by taking fluid density, \( \rho_f \), and fluid specific heat, \( c_{pf} \), into account,

\[
\dot{Q}_{pc} = \rho_f c_{pf} \frac{T - T_{sat}}{\Delta t}
\]  

3.23

Here, \( \Delta t \) is the time step size.

3.3 Our Model Development

We have started our development by customizing the impesFOAM solver. ImpesFOAM is based on pressure and saturation equations and only models multiphase flow through the porous media, which provides the pressure field, corrected velocity field, and the saturation of different phases. In our research, heat is supplied to the porous media, as a result, we need to find a way to obtain the information of temperature distribution over the porous media as transport of heat will take place inside the porous media. For that, the inclusion of the energy equation becomes a precondition. Furthermore, as we are dealing with the latent heat, phase change will occur inside the porous media. As a result, we need a phase change model inclusion into our governing equations. Finally, a new model formulation for two-phase flow and phase-change in porous media is required and the modified formulation is discussed below.
3.3.1 Flow Equations

The governing equations of impesFOAM are constructed by including the injection and extraction flow rates because it is very common in earth applications, for example, oil/gas extraction. But for our case, LHP modeling, the need for injection and extraction is not usual. The injection and extraction flow rates are denoted by the wellbore terms in the pressure and saturation equations (Eqn. 3.20 and 3.21). We can neglect the wellbore terms by setting their value to zero. As a result, the saturation and the pressure equations become

\[
\varepsilon \frac{\partial S_l}{\partial t} + \nabla \cdot \mathbf{u}_l = 0 \tag{3.24}
\]

\[
\nabla \left( - \frac{K K_{rv}(S_l)}{\mu_v} (\nabla p_v - \rho_v g) \right) + \nabla \left( - \frac{K K_{rl}(S_l)}{\mu_l} (\nabla p_l - \rho_l g - \nabla p_c(S_l)) \right) = 0 \tag{3.25}
\]

3.3.1.1 Capillarity and Relative Permeability Model

Along with the saturation dependent van Genuchten relative permeability and capillary models presented in the previous section, a new capillarity and relative permeability model is implemented as a library in the current solver. The Leverett [38] capillarity model is a function of porosity, permeability, surface tension and saturation and is described using Eqns. 3.13 and 3.14. The Carman-Kozeny [39] saturation-dependent relative permeability model is described using Eqn. 3.15.

3.3.2 Heat Transfer in Porous Medium

The first extension to the impesFOAM solver in the path of developing the new phase-change and two-phase solver is the inclusion of the thermal energy transport
equation to solve for temperature in the simulation domain. To solve heat transfer [50] in porous media, the following energy equation is implemented in the impesFOAM solver

$$\left( \varepsilon (\rho c_p)_f + (1 - \varepsilon)(\rho c_p)_s \right) \frac{\partial T}{\partial t} + (\rho c_p)_f \nabla \cdot (uT) = \nabla \cdot (\kappa_{eff} \nabla T)$$

3.26

where $c_{pf}$ and $c_{ps}$ are heat capacity of the fluid and solid, respectively, and $\kappa_{eff}$ is the effective thermal conductivity. $u = u_l + u_v$ where $u_l$ and $u_v$ are the velocities of liquid and vapor phases, respectively, which can be obtained from the corrected velocity field.

### 3.3.2.1 Temperature-Dependent Fluid Properties

The fluid material properties (density and heat capacity) are defined as a weighted average of the liquid and vapor saturation as

- **Fluid Density**

$$\rho_f = S_l \rho_l + (1 - S_l) \rho_v$$

3.27

- **Fluid Heat Capacity**

$$c_{pf} = \frac{S_l \rho_l c_{pl} + (1 - S_l) \rho_v c_{pv}}{\rho_f}$$

3.28

In this equation, $c_{pl}$ and $c_{pv}$ are the specific heat of liquid and vapor, respectively.

- **Fluid thermal conductivity**

$$\kappa_f = S_l \kappa_l + (1 - S_l) \kappa_v$$

3.29

where $\kappa_l$ and $\kappa_v$ are the thermal conductivity of liquid and vapor, respectively.

Temperature-dependent densities, viscosities, and conductivities of the vapor and liquid phases are implemented in the solver through first or second-order correlations obtained from available experimental datas [51] as follow
- **Density**

\[
\rho_l = -3.61131018 \times 10^{-3}T^2 + 1.906819T + 749.06563 \\
\rho_v = 1.415309 \times 10^{-6}T^2 - 2.3466872 \times 10^{-3}T + 1.261127
\]

- **Dynamic Viscosity**

\[
\mu_l = 1.42590047 \times 10^{-7}T^2 + 1.0393536 \times 10^{-4}T + 0.01192442 \\
\mu_v = 4.05848016 \times 10^{-5}T - 0.00301655
\]

- **Thermal Conductivity**

\[
\kappa_l = -9.6739824 \times 10^{-6}T^2 + 7.43735 \times 10^{-3}T - 0.75224861 \\
\kappa_v = 1.253 \times 10^{-4}T - 0.0217497
\]

These temperature-dependent correlations are implemented as a library and used in the solver where called upon.

### 3.3.2.2 Effective Thermal Conductivity Model

There are different models available in the literature for effective thermal conductivity for the porous media, which depends both on the thermal conductivity of the solid and fluid phases [52]. A library for effective thermal conductivity models is developed and implemented in the solver to have freedom of using related model for a given problem. Below is a list of the effective thermal conductivity models implemented in the solver. In all of these models, \(\kappa_s\), is the solid thermal conductivity.

- **Parallel Model**

\[
\kappa_{eff} = \varepsilon \kappa_f + (1 - \varepsilon)\kappa_s
\]

- **Series Model**
\[
\frac{1}{\kappa_{\text{eff}}} = \frac{\varepsilon}{\kappa_f} + \frac{1 - \varepsilon}{\kappa_s}
\]  \hspace{1cm} 3.37

- Alexander Model

\[
\kappa_{\text{eff}} = \kappa_f \left( \frac{\kappa_s}{\kappa_f} \right)^{(1 - \varepsilon)\alpha}
\]  \hspace{1cm} 3.38

where \(\alpha\) is an empirical parameter that depends on the types of porous media. For a sintered powder \(\alpha = 0.53\).

- Chi model

\[
\kappa_{\text{eff}} = \frac{\pi}{8} \left( \frac{r_c}{r_s} \right)^2 \kappa_s + \left[ 1 - \frac{\pi}{8} \left( \frac{r_c}{r_s} \right)^2 \right] \left[ \frac{\kappa_s \kappa_f}{\varepsilon' \kappa_f + (1 - \varepsilon') \kappa_s} \right]
\]  \hspace{1cm} 3.39

With

\[
\varepsilon' = \frac{\varepsilon}{1 - \frac{\pi}{8} \left( \frac{r_c}{r_s} \right)^2}
\]  \hspace{1cm} 3.40

This model is developed to evaluate the effective thermal conductivity for packed-spheres porous media.

### 3.3.3 Governing Equations for Our Model

Mahdi et al. [47] worked on implementing phase-change in the multiphase solver interFoam of OpenFOAM. They employed the phase-change closure model described by Yang et al. [53]. Therefore, interThermalPhaseChangeFoam is developed by implementing the phase-change source term in the governing equation. We adopt the same technique employed to incorporate phase-change in our solver.

All the governing equations are coupled with phase change term, \(\dot{Q}_{pc}\) calculated from the phase-change model, which contributes to the pressure, saturation, and energy
equations in terms of dilatation rate, $PCV$, and saturation generation, $S_{l,pc}$, respectively, with

$$PCV = \frac{\dot{Q}_{pc}}{h_{lv}} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right)$$  \hspace{1cm} 3.41

and

$$S_{l,pc} = -\frac{\dot{Q}_{pc}}{\rho_l h_{lv}}$$  \hspace{1cm} 3.42

The liquid saturation equation coupled with the phase-change heat can be expressed as

$$\varepsilon \frac{\partial S_l}{\partial t} + \nabla \cdot \mathbf{u}_l = -\frac{\dot{Q}_{pc}}{\rho_l h_{lv}}$$  \hspace{1cm} 3.43

The pressure equation from the IMPES model coupled with the phase-change heat can be written as

$$\nabla \left( -\frac{Kk_r v(S_l)}{\mu_v} \left( \nabla p_v - \rho_v g \right) \right)$$

$$+ \nabla \left( -\frac{Kk_r l(S_l)}{\mu_l} \left( \nabla p_l - \rho_l g - \nabla p_c(S_l) \right) \right)$$

$$= \frac{\dot{Q}_{pc}}{h_{lv}} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right)$$

Finally, the energy equation for the porous media is solved for the saturation range of $[0-1]$ coupled with the phase change heat where conduction and convection heat fluxes are dominant [47], radiation is neglected here.
\[
\left( \varepsilon (\rho C_p)_f + (1 - \varepsilon)(\rho C_p)_s \right) \frac{\partial T}{\partial t} + (\rho C_p)_f \nabla \cdot (uT) = \nabla \cdot \left( \kappa_{eff} \nabla T \right) - \dot{Q}_{pc} 
\]

Phase change source terms are formulated in a new library called ‘thermalPhaseChangeModel’ which is included in our code to serve as the source term for governing equations.

After implementing all the changes, the new solver is named ‘phaseChangeImpesFOAM’ and its flow diagram is shown in Fig. 3.1.
Figure 3.1 Flow diagram for the ‘phaseChangeImpesFOAM’ solver
4 Result and Discussion

In this section, we present two examples of results for two-phase flow and phase-change in 1-D and 2-D configurations using the developed phaseChangeImpesFOAM solver. First, the 1-D simulation results are presented and compared to a semi-analytical model. Second, a 2-D simulation domain that represents a section of the evaporator porous media of an LHP is used and results are presented.

For all numerical simulations presented in this chapter, we have used water as the working fluid. The thermo-physical properties of water liquid and vapor are shown in Table 1 at 1 atm pressure and 273.15K (0°C) temperature.

Table 4.1 Properties of water at STP (Standard temperature and pressure condition) [54]

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Vapor</th>
<th>Unit (SI)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity (Dynamic)</td>
<td>2.79×10⁻⁴</td>
<td>1.202×10⁻⁵</td>
<td>Ns/m²</td>
</tr>
<tr>
<td>Density</td>
<td>1,000</td>
<td>0.6</td>
<td>Kg/m³</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.68</td>
<td>0.0248</td>
<td>W/m-K</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>4,217</td>
<td>2,029</td>
<td>J/kg K</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>0.0589</td>
<td>-</td>
<td>N/m</td>
</tr>
<tr>
<td>Latent Heat (Evaporation)</td>
<td>2,675,710</td>
<td>-</td>
<td>J/kg</td>
</tr>
<tr>
<td>Saturation Temperature</td>
<td>373.15</td>
<td>-</td>
<td>K</td>
</tr>
</tbody>
</table>

4.1 1-D Simulation Results

A simple 1-D simulation case is chosen to demonstrate the capability of the newly developed phaseChangeImpesFOAM solver. The simulation domain consists of a 10 cm
long porous media with a porosity of 0.38, a permeability of 2×10^{-12} \text{ m}^2, and thermal conductivity of 2.48 \text{ W/m-K}. The Leveret model for capillarity (Eqns. 3.13 – 3.15) and Carman-Kozeny model for relative permeability (Eqn. 3.15) and empirical rate parameter model for phase-change (Eqns. 3.27 and 3.28) are employed in this simulation.

Figure 4.1 shows the applied boundary condition on the simulation domain. Liquid enters the porous domain at a temperature of 300K with a saturation of \( S_l = 1 \). A liquid velocity of \( 3 \times 10^{-4} \text{ m/s} \) is imposed at the inlet. Gravity is taken into account in this simulation and is in the direction of flow (see Fig. 4.1). The flow of liquid in the domain is due to the action of the inlet velocity, capillarity, and gravity. At the outlet, a temperature of 1580 K and a zero gage pressure are prescribed. The other conditions are zero-gradient for pressure at the inlet, and zero-gradient for vapor velocity at the outlet, which allows vapor to leave the domain.

\[
\begin{align*}
T_{in} &= 300 \text{ K} \\
u_l &= 3 \times 10^{-4} \text{ m/s} \\
S_l &= 1 \\
T_{out} &= 1580 \text{ K} \\
P_{out} &= 0 \text{ Pa}
\end{align*}
\]

Figure 4.1: 1-D simulation domain with boundary conditions

A transient simulation is conducted with the domain initially saturated with liquid. Condensation takes place when the temperature of the vapor is below the saturation temperature, \( T_{sat} = 373.15 \text{ K} \), and evaporation occurs when the temperature of the liquid is above the saturation temperature. Due to the action of capillarity and the imposed liquid velocity at the inlet, liquid advances towards the outlet and starts evaporating. The liquid completely converts to vapor close to the outlet as it is set at a high temperature of 1580K.
This leads to three distinct zones in the porous domain, i.e. the liquid zone, the two-phase zone, and the vapor zone.

Figure 4.2 shows the liquid saturation contour in the simulation domain and Fig. 4.3 shows the profile of the liquid saturation along the length of the simulation domain. From these two figures, it can be seen that below roughly 6.7 cm, the domain is fully saturated with liquid (liquid zone) and above 8 cm it is fully saturated with vapor (vapor zone). Between 6.7 cm and 8 cm, the liquid saturation changes from 1 to 0 in an S-like shape (two-phase zone). The saturation profile (S-shape) in the two-phase zone is mainly due to the relation between the capillary pressure and saturation (Eqns. 3.13 and 3.14), which also exhibits an S-shape.

![Saturation contour for the 1-D case.](image)

Figure 4.2 Saturation contour for the 1-D case.

Figure. 4.4 shows the liquid velocity profile along the length of the porous domain. At the inlet, the liquid velocity is $3 \times 10^{-4}$ m/s, then it suddenly decreases in the first a few millimeters to a constant value of $7.25 \times 10^{-5}$ m/s, and remains at this value in the liquid region. This decrease in liquid velocity is not yet well understood, as the liquid velocity is supposed to remain constant throughout the liquid zone at the inlet value. It seems that the solver forces the liquid to flow at the constant velocity of $7.25 \times 10^{-5}$ m/s and ignores the inlet velocity condition. Other cases were simulated with an increased inlet velocity, and it was found that the solver always brings the velocity to the same constant value in the liquid
zone for a given permeability. If the permeability is changed, then the constant velocity in the liquid zone will change also. This issue will be investigated as part of future work. In the two-phase zone, the liquid velocity increases slightly due to the effect of capillary pressure, then suddenly drops to zero at the end of the two-phase region, where there is nearly no liquid due to complete evaporation. In the vapor zone, there is no liquid, therefore, a liquid velocity of zero is obtained.

![Figure 4.3 Liquid saturation of the domain](image)

Figure 4.3 Liquid saturation of the domain
Figure 4.4 Liquid velocity profile along the length of the domain

Figure 4.5 Vapor velocity profile along the length of the domain
Figure 4.5 shows the vapor velocity profile along the length of the porous domain. In the first zone (liquid), there is no vapor, therefore, the vapor velocity is zero. In the two-phase zone, the vapor velocity is negative, meaning that vapor flows in the opposite direction to the liquid flow. As discussed in Sec. 2.2, when the wetting fluid (liquid) advances due to capillary action, the non-wetting fluid (vapor) recedes, which is observed here as well. It can be also noticed from this profile that the vapor velocity magnitude increases as the saturation of liquid decreases (increase in vapor saturation, see Fig. 4.3) close to the vapor zone, and its value is a few orders of magnitude larger than the liquid velocity. The net sum of flow in the two-phase region is zero. In the vapor region, the vapor velocity increases considerably to reach $6.8 \times 10^{-2}$ m/s at the exit.

Figure 4.6 shows the temperature profile in the domain. In the liquid zone, the temperature is increasing slowly as the effective thermal conductivity in this region is relatively high. The temperature reaches 326K at the end of the liquid zone. In the two-phase zone, the temperature starts increasing more rapidly, due to a decrease in the effective thermal conductivity as the vapor starts forming in this region. At the end of this zone, the temperature reaches 377.5K. Finally, when the liquid completely changed its phase to vapor in the vapor zone, the increase in temperature becomes rapid and the temperature increases to 1580K at the end of the domain, which is the outlet boundary condition. The rapid increase in temperature in this zone is due to the relatively lower effective thermal conductivity. It should be noted here that in the two-phase zone, the temperature should be nearly isothermal as the phase-change occurs in that zone. Whereas, in our simulation, the temperature increases in the two-phase zone by 51.5K. Also, it seems that evaporation
takes place at a temperature much lower than the saturation temperature. These behaviors will be investigated as part of future work.

Figure 4.6 Temperature profile of the Domain

Figure 4.7 presents the pressure profile along the axis of the domain. The pressure is nearly constant in the liquid zone. However, in Figure 4.4, it is found that liquid is moving towards the outlet in that zone. As a result, there should be a pressure gradient in this zone to drive the liquid. The pressure difference in that zone is 0.45 Pa, which is not enough to drive the liquid in that zone. This irregularity in the pressure profile is not well understood, and it is believed to be related to the drop of liquid velocity at the inlet of the domain (see Fig. 4.4). This will also be investigated as part of future work. In the two-phase region, the pressure rises (see Figure 4.7) significantly due to the capillary pressure. As liquid saturation decreases from the beginning of the two-phase zone, the transfer of
momentum from liquid to vapor begins. The generation of vapor due to phase-change in the two-phase zone causes an increase in the vapor pressure. This vapor pressure adds to the pressure rise in the two-phase zone and the pressure finally rises to 2281Pa. However, with an increase in vapor generation in the two-phase zone, transport of momentum from liquid to vapor increases, which causes liquid pressure to decrease toward the end of the two-phase zone. At the interface of two-phase and vapor zones, liquid converts into vapor fully. The full liquid momentum transferred to vapor, as a result, with the increase in vapor momentum, vapor velocity increases from negative to positive. In the vapor zone, the pressure decreases to 0 Pa, which is our outlet pressure boundary condition, and it causes vapor velocity to increase very quickly as seen in Fig. 4.5.

Figure 4.7 Pressure profile of the domain
4.1.1 Comparison with a Semi-Analytical Model

In this section, we compare our numerical results with a semi-analytical model developed by He et al. [54]. In their work, they presented a set of governing equations (mass, momentum, and energy) for phase-change in porous media. In momentum and energy equation, they adopted the vapor compressibility. In the momentum equation, a momentum transfer term is added as momentum transfer occurs at two-phase region between liquid and vapor. Finally, a change in temperature and pressure in the two-phase region is addressed in the energy equation. In their model, they employed governing equations for every zone separately for phase change, wherein our model we adopted a phase change model to observe phase change in porous media. The Leveret model for capillarity and Carman-Kozeny model for relative permeability (Eqns. 3.13 – 3.15) model is used in their numerical analysis.

They presented a numerical analysis in a 10 cm 1-D domain of porous media. The parameters that we discussed above for our case are the same parameters used in their numerical analysis. Therefore, a direct comparison can be made. Table 2 shows the comparison between the two models where we are comparing the length of different zones in the domain.

Table 4.2: Comparison of the single and two-phase region lengths between our CFD model and the semi-analytical model by He et al. [54]

<table>
<thead>
<tr>
<th></th>
<th>Current Model</th>
<th>He et al. [54]</th>
</tr>
</thead>
<tbody>
<tr>
<td>length of the vapor region [cm]</td>
<td>2</td>
<td>2.1</td>
</tr>
<tr>
<td>Thickness of the two-phase region [cm]</td>
<td>1.5</td>
<td>0.7</td>
</tr>
</tbody>
</table>
There are some dissimilarities between the two models. However, the shape of the plots is similar, for example, the ‘S’ shaped two-phase zone in saturation profile (see Fig. 4.3). Our model qualitatively produces similar two-phase zone behavior, where saturation decreases from 1 to 0, liquid velocity increases because of the capillary forces, and vapor velocity is negative to maintain the mass conservation, and finally pressure increases due to the capillarity. However, due to the above-mentioned issues with our model (drop in velocity at the inlet, non-isothermal two-phase region, and constant pressure in the liquid zone), we are not yet able to get accurate quantitative results.

4.2 2-D Simulations

In this section, a two-phase flow and phase-change simulation in a small segment of the porous domain of an LHP evaporator is conducted. In an LHP evaporator, liquid advances through the porous media and evaporates at the interface between the porous media and the casing/pillar (where heat is provided). The produced vapor leaves through the vapor grooves between the pillars. Figure 4.8a shows a simple schematic of a typical flat evaporator and Fig. 4.8b shows the simulation domain considered in this study.

The simulation domain shown in Fig. 4.8b consists of a 1×1 cm² porous media with a porosity of 0.5 and a permeability of $10^{-11}$ m². The thermal conductivity of the porous media is 0.01 W/m-K. Temperature-dependent fluid properties (Eqns. 3.36 – 3.41) are used for this numerical analysis. For the capillarity and the relative permeability, the Van Genuchten model (Eqns. 3.22 – 3.26) is employed. The empirical rate parameter model (Eqns. 3.27 – 3.28) is adopted for the phase-change process.
Figure 4.8b shows the boundary conditions for the simulation. The inlet (the top boundary of the domain) is set at a temperature of 368K with an imposed liquid saturation of $S_l = 1$. The left and right walls of the domain are set to symmetry boundary conditions. The heated wall (half of the bottom boundary) is set to a temperature of 378K. The other half of the domain bottom is an outlet with zero-gradient for velocity vapor and zero-
velocity for liquid. This condition allows for vapor to leave through the outlet but blocks liquid. Also, a gauge pressure of zero is imposed at the outlet.

A transient simulation with a variable time step based on the CFL (Coats) condition is conducted. Initially, the porous domain is assumed to be fully saturated with liquid water. Figure 4.9 shows the temperature contour in the simulation domain. The heated plate is at 5K above the saturation temperature and the inlet temperature is at 5K below it. This causes a temperature gradient within the domain, with the regions surrounding the heater plate being above saturation. We expect evaporation to occur in those regions.

Figure 4.10 shows the saturation contour in the domain. When the simulation starts, vapor begins forming close to the heated plate and more vapor is produced as regions farther from the heated plates increase in temperature. A minimum saturation of 0.74 for liquid (maximum of 0.26 for vapor) is reached close to the heated plate. The liquid close the heated plate does not completely change into vapor, because of the low heat flux provided to the domain as the heated plate temperature is very close to the saturation temperature. If the temperature of the heated plate is increased, the liquid saturation will decrease. It can also be noticed from Fig. 4.10 that liquid saturation at the outlet is close to 1. This is due to the restriction imposed on the liquid not to leave the domain. This condition was applied to simulate the actual behavior of a porous media, where the capillary pressure acts as a barrier for the liquid to leave the porous media. Therefore, in our simulation, only vapor leaves the domain through the outlet (see Figure 4.10). It should also be noted here that vapor condensation does occur in the porous domain where the temperature is below the saturation temperature.
Figure 4.9 Temperature Contour

Figure 4.10 Saturation Contour
Figure 4.11 shows the normal (y-direction) liquid velocity profile along the inlet. The liquid velocity is not uniform along the inlet. It is larger in the region above the heated wall. Because of evaporation, vapor continues to form at the heated wall, which means liquid saturation is decreasing in that region. As a result, liquid saturation is lower at the right side of the domain than on the left side. The capillarity model describes that capillary pressure increases with a decrease in saturation. As a result, due to the capillarity liquid is pulled more at the right side of the inlet than the left side.

The normal (y-direction) vapor velocity along the outlet is shown in Fig 4.12. As vapor forms above the heated plate, it converges toward the outlet. Therefore, as expected, the highest vapor velocity is obtained close to the heated plate, then it decreases with increasing distance from the heated plate.

![Figure 4.11 Axial liquid velocity profile at inlet](image-url)
Figure 4.12 Axial vapor velocity profile at outlet
5 Conclusion

In this thesis, a numerical solver for two-phase flow and phase-change in porous media in the OpenFOAM architecture. The new solver, named phaseChangeImpesFoam, is developed based on an existing flow solver, impesFoam, by implementing and customizing it with phase-change, capillarity, relative permeability, and effective thermal conductivity models and temperature-dependent fluid properties. All the governing equations and the models implemented in this solver are detailed in this thesis.

Two simple example cases are presented to demonstrate the capabilities of the new solver. The first case is a 1-D simulation performed with constant fluid properties and the obtained results were compared with a semi-analytical model developed by He et al. [54]. The result showed that our solver was able to qualitatively predict the correct behavior for the flow and phase change. However, it wasn’t able to predict the correct pressure profile in the liquid zone, and temperature profile in the two-phase region. Also, we found that it cannot impose a constant mass flow at the inlet. We ran simulations imposing higher velocities and we have found that the velocity drops to the same constant value. When we performed simulations changing permeabilities, we found that the velocity increases with permeability. This result gives us a sense that the velocity was calculated from the Darcy velocity and imposing velocity at the inlet over defines the system. Adding a source term for velocity in the pressure equation might solve the issue. As velocity and pressure are coupled, fixing this velocity imposing issue at the inlet will fix the liquid zone pressure of the domain and this is our prediction. For this temperature issue we run simulations when the domain is fully saturated with vapor and we have found a nearly isothermal two phase
zone, but the two phase length becomes very larger in this case. We will be undertaking different approaches to solve this issue.

The second simulated case was a 2-D domain representing a segment of the porous wick of an LHP evaporator. The results obtained from the simulation were analyzed and it is found that liquid does not fully convert into vapor when the heated plate temperature is slightly above the saturation temperature. Higher vapor velocity and temperature are observed near the heated plate. Our porous media research group is also building a quasi 2-D experiment and we will validate the 2-D results when the experiment is completed.

As shown above, the solver is still not yet complete and it is still in the development process, as not all the issues are solved. For the future, we will continue improving the solver and we will couple it with a flow and phase-change solver in open-spaces (not porous media). This will create a robust solver that can be used for multiple applications.
6 References


