ANL/NSE-19/42

Initial Evaluation of Nek-2P for Modeling of Liquid Metal Heat Pipes

Nuclear Science and Engineering Division

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prepared by

Dillon Shaver and Adrian Tentner

Nuclear Science and Engineering Division, Argonne National Laboratory

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Abstract

A heat pipe is two-phase heat transfer device which relies on surface tension and capillary pressure to provide a very efficient heat transfer mechanism. Currently, there is interest in designing micro nuclear power reactors using high temperature heat pipes to provide totally passive cooling. To support this, heat pipe simulation capabilities must be developed. The spectral element multiphase CFD code, Nek-2P is being considered for use in providing high-fidelity results which will drive the development of reduced order models. This work is focused on an initial evaluation of the capabilities of Nek-2P to meet this goal.

The two-fluid model is used in Nek-2P along with a set of closure models formulated for simulating heat pipes. Specifically, an interfacial force modeling the surface tension effect in the pores of the wick is included. Initial simulations using this model have been performed for conditions approaching nominal values for a sodium heat pipe. Nek-2P is able to qualitatively reproduce the expected results for the volume fraction, velocity, and pressure distributions with reasonable results for the phasic temperatures. This indicates the viability of using Nek-2P to perform more in-depth investigations. However, significant quantitative differences are noted between results and conditions typical of a sodium heat pipe. These differences in results are expected to diminish as the differences between the simulated conditions and the target conditions decreases. Additionally, challenges in simulating heat pipes with Nek-2P have been identified. Future work will focus on addressing these challenges and performing investigations of the operational limits of sodium heat pipes.

1 Introduction

Sodium heat pipes are being considered in the design of simpler, safer, and more reliable small nuclear reactors. Heat-pipe-cooled reactors are nearly "solid-state" and avoid many of the complexities and issues arising from the traditional reactor concepts that rely on a coolant pumped through the reactor core. They are able to accomplish this through complex multiphase dynamics which allow heat pipes to achieve very high heat transfer coefficients.

A heat pipe is a capillary two-phase heat transfer device that transports heat from a heat source to a heat sink. It consists of a sealed tube with a wick outer region as seen in Fig. 1 – typically a ribbed or grooved geometry (shown in Fig. 2) or a wire mesh are used – and a central channel. In wire mesh designs, a gap can be included between the mesh and the outer wall which has the effect of further increasing heat transfer rates by providing an unobstructed flow path for the liquid. Heat pipes rely on boiling and condensation of the working fluid to achieve high efficiency heat transfer. As liquid is vaporized in the evaporator region the vapor pressure builds up, forcing vapor to flow axially along the central channel to the condenser. Vapor condenses in the condenser region. Liquid is drawn back to the evaporator by the capillary force along the grooves of the wick region. The pressure difference between the vapor and liquid phases is sustained by the surface tension force of the fluid. The capillary two-phase system is passive (no external pumping power), self-regulating (no flow control devices), and requires no moving parts. When the condenser is located above the evaporator in a gravitational field, gravity helps return the liquid to the evaporator. In the opposite configuration, the presence of the wick allows the surface tension and capillary forces to overcome the gravitational effect.

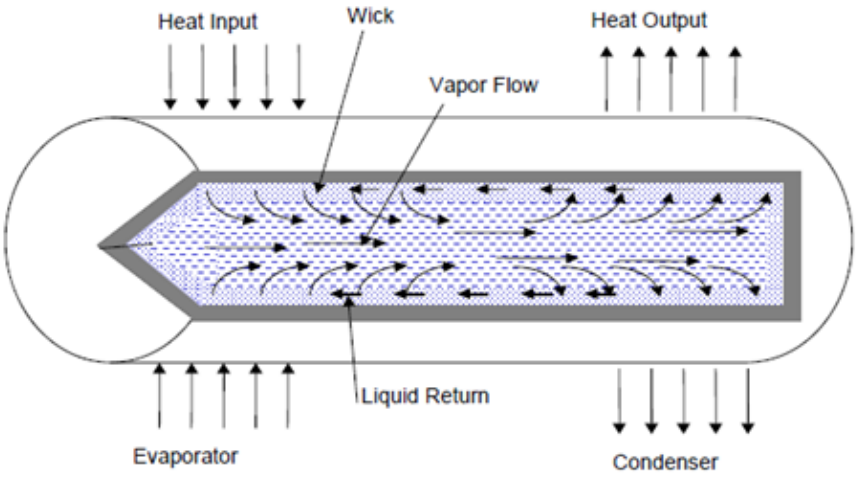


Figure 1: Heat pipe schematic

Various material combinations have been used for heat pipe design. More typical applications call for copper heat pipes filled with water or refrigerant. There have been significant experimental and theoretical investigations into these variations, with recent simulation efforts focused on thermosyphons [1, 2] (wick-less heat pipes). However, some investigations have been driven by space applications [3] where the ability to function without gravity is an attractive feature, and external

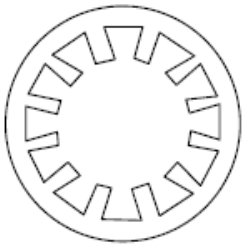


Figure 2: Heat pipe cross section with grooved wick region

combustion systems [4], which require efficient heat transfer over relatively large distances without suffering from large temperature drops. For these applications, metal heat pipes were investigated. More recently, interest has been motivated by nuclear applications [5], where heat pipes may be an attractive option for totally passive cooling of micro reactors. The focus has been largely motivated by understanding the operational limits: dryout in the evaporator, choked flow of the vapor, liquid entrainment from the wick, and the viscous limit.

The objective of this work it to perform exploratory simulations using the Nek-2P CFD two-phase code developed at Argonne to gain a better understanding of the two-phase flow and phase-change processes associated with a heat pipe using sodium as the working fluid. Modeling the heat transfer and phase changes in the wick region takes advantage of the Advanced Boiling Framework (ABF) models implemented in Nek-2P.

The exploratory simulations are used to evaluate the current Nek-2P capabilities for modeling the heat pipe phenomena and will identify areas of future development for the Nek-2P code, including: a) extension of the ABF models developed for modeling water phase change phenomena to the modeling of sodium boiling and condensation phenomena and b) modeling of surface tension effects that play an important role in the heat pipe capillary two-phase flow. The long term goal of the project is to develop a Nek-2P-based tool for the analysis and design of heat pipes with increased efficiency and safety for nuclear reactor applications. This tool will then be used for deeper investigations of complex phenomena associated with the operational limits of sodium heat pipes. These investigations can then be leveraged to support the development of fast-running tools, such as the Sockeye code, which is being developed to aid with industry designs of heat pipe cooled micro reactors.

2 Model Description

As a starting point, the typical two fluid model as implemented in Nek-2P was used. This model solves the conservation equations for mass fraction, momentum, and energy as well as a mixture equation for pressure. This implies that a single continuous pressure field is used for both phases. The governing equations for the implemented model are briefly outlined below along with the included interfacial interactions.

The presented model has been implemented in the spectral element code, Nek-2P. Nek-2P

is computational multiphase fluid dynamics code that has been under development at Argonne National Laboratory as a two phase version of Nek5000 [6, 7]. It is based on a novel splitting scheme [8] originally developed for reactive flows which couples the changing density to the energy equations, yielding a low-Mach formulation.

2.1 Governing Equations

The conservation equations for mass fraction, momentum, and energy are given as

$$\rho_m \left(\frac{\partial Y_k}{\partial t} + \vec{u}_m \cdot \vec{\nabla} Y_k \right) = -\vec{\nabla} \cdot \left(\rho_m Y_k \vec{U}_k \right) + \Gamma_k - \Gamma_j, \tag{1}$$

$$\rho_k \frac{D\vec{u}_k}{Dt} = -\vec{\nabla} P_k + \vec{\nabla} \cdot \underline{\boldsymbol{\tau}}_k + \rho_k \vec{g} + \frac{1}{\alpha_k} \left[\vec{F}_k + \Gamma_{net,k} \left(\vec{u}_j - \vec{u}_k \right) \right], \tag{2}$$

and

$$\rho_k \left(\frac{\partial h_k}{\partial t} + \vec{u}_m \cdot \vec{\nabla} h_k \right) = -\rho_k \vec{U}_k \cdot \vec{\nabla} h_k + \vec{\nabla} \cdot \vec{q}''_k + \frac{1}{\alpha_k} \left[q'''_k + \left(\Gamma_k - \Gamma_j \right) \left(h_{sat,k} - h_k \right) \right]. \tag{3}$$

These are typically combined with appropriate interfacial jump conditions to solve for the phasic velocities, mass fractions, enthalpies, and pressures. In Nek-2P, the pressure is assumed constant across the interface, leading to the phasic pressures being identical to the mixture pressure and the mixture equation is solved. This is given by

$$\vec{\nabla} \cdot \frac{1}{\rho_m} \vec{\nabla} P = \vec{\nabla} \cdot \left(-\frac{\partial \vec{u}_m}{\partial t} + \vec{u}_m \cdot \vec{\nabla} \vec{u}_m + \vec{g} \right) + \vec{\nabla} \cdot \nu_m \left(2\vec{\nabla} \xi - \vec{\nabla} \times \omega \right), \tag{4}$$

where the subscript 'm' indicates a mixture quantity, $\xi = \vec{\nabla} \cdot \vec{u}_m$ represents the divergence constraint, and $\omega = \vec{\nabla} \times \vec{u}_m$ is the mixture vorticity. Further details of the two-fluid model formulation in Nek-2P are available in literature [9, 10].

2.2 Wick Model

The wick is included in the model by defining a region in the domain via a scalar, ψ. This scalar takes a value of one in the wick region and zero elsewhere. This allows the closure models to be formulated with an explicit dependence on the presence of the wick

$$\psi = H_s(r - r_0)[1 - H_s(r - r_1)]. \tag{5}$$

Here, H_s is a smoothed Heaviside function, r_0 is the internal radius of the wick, and r_1 is the external radius of the wick. This formulation allows the wick to be prescribed fully independently from the computational mesh.

In addition to modeling the presence of the wick explicitly, a porous media model is included to mimic the effect of a wire mesh wick on obstructing the flow. This is accomplished through a body force formulated based on a Darcy-type porous media model. The force applied to each fluid

phase 'k' is given by

$$\vec{F}_{pm,k} = -\frac{\mu_k}{\varepsilon}\vec{u}_k\psi. \tag{6}$$

A permeability of $\varepsilon = 3(10^{-4})$ m^2 was used for the wick. This provides a reasonable amount of flow resistance to the liquid. It should be noted, however, that the flow resistance to the vapor will be significantly lower.

2.3 Closure Models

A standard set of interfacial force models was not included in this work as most models have been developed explicitly for channel or reactor sub-channel flows. It is expected that many of the typically modeled forces may be insignificant for heat pipe simulations or altogether inappropriate. The included interfacial force models are the drag force, dispersion force, and an effective surface tension force. The drag force on the dispersed fluid component 'd' surrounded by the continuous component 'c' is given by

$$\vec{F}_{D,d} = -C_D\frac{3}{4}\alpha_d\frac{\rho_c}{D_d}|\vec{u}_d - \vec{u}_c|(\vec{u}_d - \vec{u}_c). \tag{7}$$

Whether each phase is dispersed or continuous is determined based on the local volume fraction and flow topology according to the model presented in [9]. This allows the flow configuration to change smoothly from continuous liquid through continuous vapor.

In addition to the drag force, a dispersion force was included in the interfacial force model. This force was included as it tends to smooth out gradients in the volume fraction, having a stabilizing effect on the overall model. The dispersion force is included as

$$\vec{F}_{TD,d} = -C_{TD}\alpha_d\rho_c k_c\vec{\nabla}\cdot\alpha_d. \tag{8}$$

This is based on a formulation proposed by Podowski [11], where the turbulent kinetic energy is estimated from a correlation for turbulent intensity. This force was found to be necessary in simulating the liquid metal heat pipe, as the physics of the problem lead to a strong phasic separation with a very sharp gradient in volume fraction.

In the two-fluid model the interface is modeled, rather than explicitly resolved. Using this framework, an interfacial surface tension force is modeled similarly to an interfacial dispersion force.

$$\vec{F}_\sigma = -C_\sigma\frac{\sigma}{\delta_w}A_i'''\frac{\vec{\nabla}\alpha_v}{|\vec{\nabla}\alpha_v|}\psi \tag{9}$$

where C_σ is a calibrating coefficient, σ is the surface tension, and δ_w is the width of the pores in the wick. The interfacial area density in this model, A_i''', represents an effective area density which includes the meniscus formed between pores in the wick and will be a function of the local volume fraction and mass transfer rate. As a first approximation, this force is fixed to the location where the interface is expected to occur, i.e. the inner edge of the wick, and the magnitude is varied based on the local heat flux. This eliminates some of the complex dependences of the velocity on the

energy and mass fraction equations, keeping the force stable. Various values for C_σ have been tested to determine its effect on the results.

To model the effects of boiling and condensation, typical models for interfacial heat and mass transfer were included. Note that a wall boiling model was explicitly not included as the mass transfer should occur purely on the interface. In future work, a wall model may be included for use as a predictor of operational limits. Interfacial heat transfer is modeled between each phase and an interface at a given saturation temperature

$$q_k''' = -A_i''' \frac{H_k}{c_{p,k}} \left(h_{sat,k} - h_k\right). \tag{10}$$

A complex model for heat transfer accounting for the presence of dispersed vapor, continuous vapor, dispersed liquid and continuous liquid has been included. The net boiling rate is then given by

$$\Gamma_v = -\frac{q_l''' + q_v'''}{h_{fg}} \tag{11}$$

For further details on the interfacial heat and mass transfer model, see [9].

3 Results

Using the above presented model, a series of axisymmetric simulations of heat pipes has been performed in Nek-2P. Initial simulations began with scoping the applicability of the model and the capability of Nek-2P with simplified cases. As these cases were completed, the modeled physics, problem definition, and fluid properties were adjusted to more closely match a case of a sodium heat pipe. The presented results correspond to a heat pipe with the conditions given in Table 1.

Table 1: Parameters for the presented heat pipe simulation

parameter	Nek-2P	nominal
density ratio	100	5295
total power	60 W	4.08 kW
total length	0.39 m	3.9 m
diameter	7.875 mm	7.875 mm
evaporator length	39 mm	1.5 m
condenser length	39 mm	2.1 m

The predicted distribution of vapor volume fraction is shown in Fig. 3. Most of the heat pipe is observed to be occupied by sodium vapor. The core region is predicted to be approximately 80% vapor while the condenser and the gap are almost entirely liquid. Interestingly, the wick is predicted to be nearly half liquid and half vapor. The liquid pools in the condenser and flows through the gap between the wick and the outer wall towards the evaporator. As the liquid reaches the evaporator, it boils off relatively quickly. Overall, the result predicted by Nek-2P qualitatively matches the expected behavior of a sodium heat pipe. It could be improved with increased penetration of the

liquid into the evaporator, which should be achieved as the simulation parameters approach the desired operating conditions.

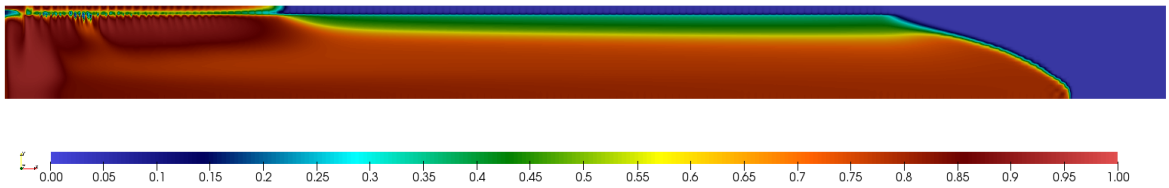


Figure 3: Distribution of vapor volume fraction

It is worth noting that in both the evaporator and the condenser, a strong gradient in the volume fraction is predicted, forming a sharp pseudo-interface between liquid and vapor. Some numerical instability is observed in the result, as the two-fluid model is generally not intended for flows with such strong phasic separation. However this does not seem to effect the overall stability of the case. This instability initially appears to be related to the resolution of the underlying mesh, however the effect of increasing the polynomial order was to merely make the interface sharper. It is likely that the underlying mass and heat transfer models need to be adjusted to correct the instability.

The distribution of the rate of mass transfer is presented in Fig. 4, where positive values indicate boiling and negative values indicate condensation. It can be seen from the figure that both boiling and condensation are practically entirely restricted to the interface. It is somewhat surprising that this distribution can be maintained, and there is evidence from the boiling rate that these conditions are on the verge of instability. Through the adiabatic region between the evaporator and condenser, both liquid and vapor are at thermal equilibrium and no mass transfer occurs.

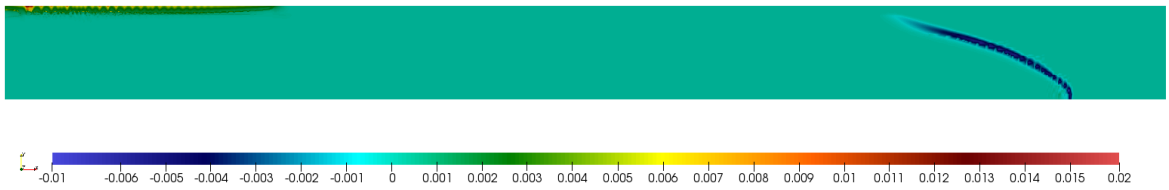
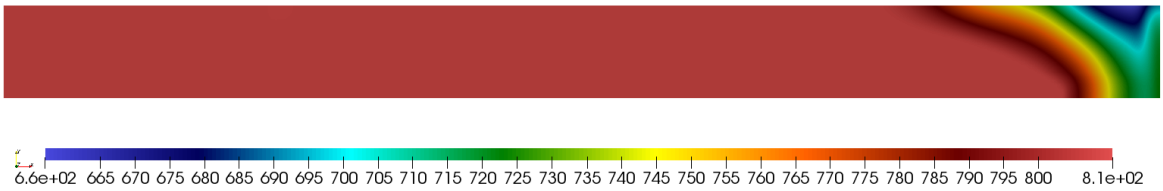


Figure 4: Distribution of vapor generation rate [kg/m^3-s]

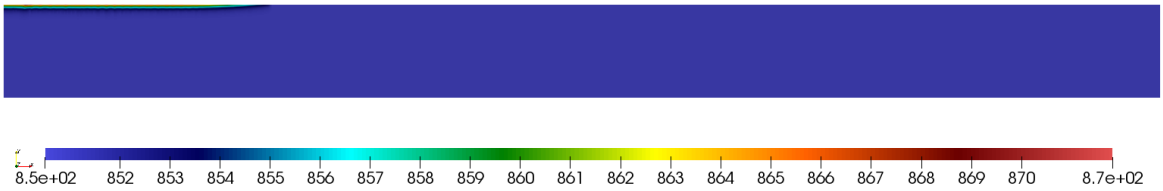
It should be noted that due to the nature of Nek-2P as a low-Mach solver and a heat pipe representing a closed system, the overall net mass transfer rate must always remain zero, i.e. no net change in the volume fractions can be predicted. This is currently a significant limitation and care must be taken to ensure the model predictions do not result in instabilities with the code.

The liquid and vapor temperature distributions are shown in Fig. 5. It can be seen that the liquid is practically saturated throughout most of the heat pipe, except for in the condenser where a strong subcooling is evident. The opposite is shown for the vapor, which is saturated practically everywhere except for some superheating near the wall in the evaporator. Comparing the

temperature distribution to the mass transfer and volume fraction distributions shown in Figs. 3 & 4, the temperature isocontour corresponding to the saturation point very closely follows the sharp interface where condensation occurs.



(a) liquid



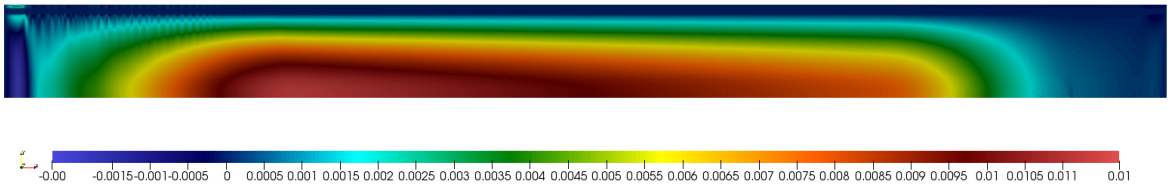
(b) vapor

Figure 5: Distributions of phasic temperatures [°C]

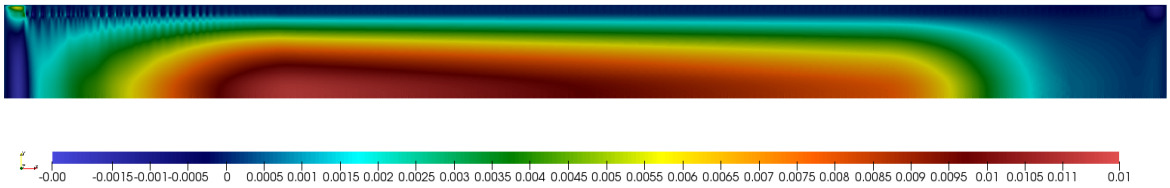
The axial component of the liquid and vapor velocity distributions are shown in Fig. 6 where a positive value indicates flow towards the condenser and a negative value indicates flow towards the evaporator. Both phases flow with practically the same velocity through most of the heat pipe. This is mostly a consequence of the strong phasic separation and the implementation of the interfacial force model, which tends to fully entrain a dispersed phase with very low volume fraction with the continuous phase. The vapor is observed to flow strongly towards the condenser through the core region, reproducing the expected behavior typical of an operating heat pipe. It is expected that as the density ratio is increased in the simulations, the predicted velocities will increase correspondingly.

A line plot of the pressure distributions in the vapor core and liquid gap are shown in Fig. 7. This shows the effect of the modeled surface tension force. The predicted distributions match reasonably well with distributions predicted by lower fidelity models [4]. By varying the magnitude of the force based on the local mass transfer rates, a larger pressure difference between the gap and the vapor core is achieved in the evaporator compared to the condenser. This also has the result of causing a pressure drop from the evaporator to the condenser in the vapor core, which forces the vapor to flow towards the condenser as expected. Similarly, a reverse pressure gradient is established in the gap between the wick and the outer wall, forcing the liquid towards the evaporator. Overall, it is this effect that drives the fluid motion in the heat pipe, indicating that an accurate model for the surface tension force is important to being able to predict the behavior. The results from Nek-2P are encouraging as it is able to qualitatively reproduce the expected profiles for pressure distribution.

The profiles of axial velocity are shown in Fig. 8. In the presented locations, both the liquid



(a) liquid



(b) vapor

Figure 6: Distributions of phasic axial velocity [m/s]

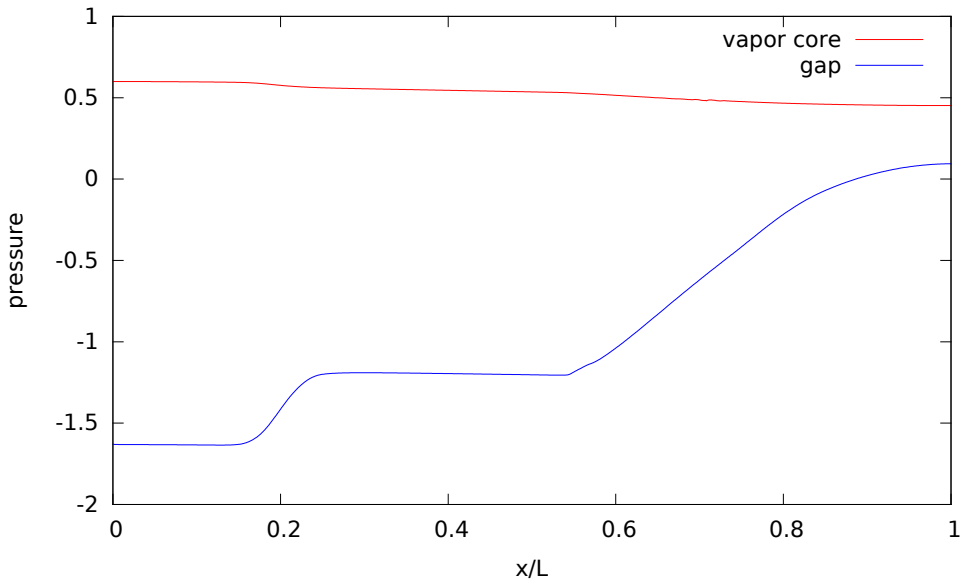


Figure 7: Normalized pressure distributions along the gap region and the vapor core

and vapor have practically the same velocities. These show the significant difference in the velocities predicted in the vapor core compared to the gap between the wick and the outer wall. The flow of liquid can be considered negligible compared to the vapor. This result can be confirmed using a simple mass balance to estimate the flow rates. It can be shown that to a first approximation, the ratio between the liquid and vapor flow rates is roughly equal to the density ratio. For this result, this explains the two orders of magnitude difference that is seen. Further, at the nominal density ratio, this difference would be greatly amplified.

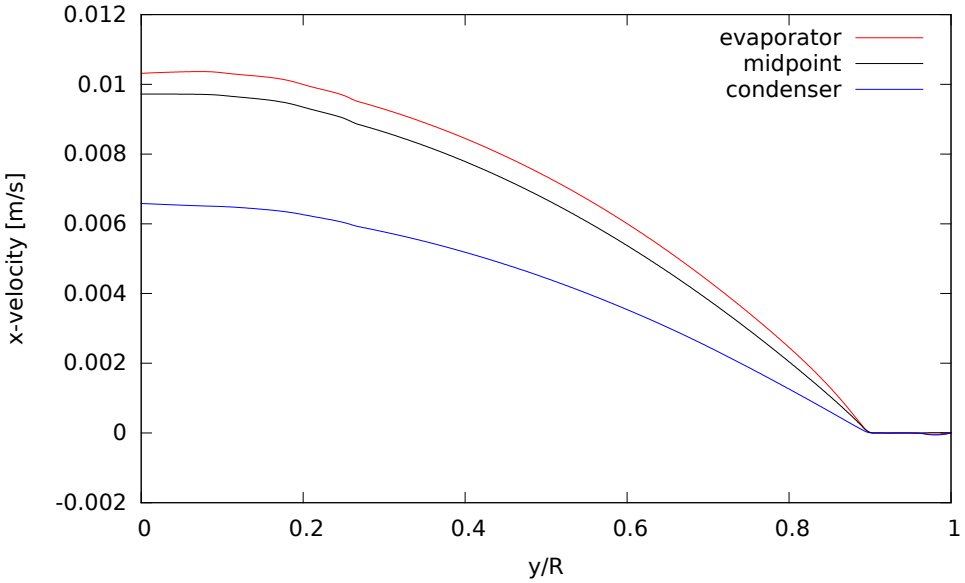


Figure 8: Radial distributions of axial velocity in the evaporator, condenser, and at the midpoint of the heat pipe

4 Summary and Future Work

Initial simulations of heat pipes have been performed with the Nek-2P code. These simulations are able to qualitatively match the expected results for heat pipes. This indicates that Nek-2P is a viable tool for more in-depth model development.

Significant challenges have been identified as a result of these simulations. As a consequence of the required net balance in mass transfer rates, severe restrictions are placed on the time step size Additionally, the thermal boundary conditions must be prescribed with a balance in heat flux into the evaporator and out of the condenser. Ideally, the heat flux would be prescribed into the evaporator and the condenser would be exposed to a constant temperature boundary. However, this would require simulating a variable thermodynamic state for the overall heat pipe. It is possible this can be addressed by including a globally variable vapor density and the possibility of including this capability is under investigation.

Future work will be focused on closing the gap between the modeled conditions and the target

conditions for a high temperature sodium heat pipe. Once this has been achieved, operational limits can be investigated, such as liquid entrainment from the wick or choked flow of the vapor. Investigations of these operational limits will be used to produce phenomenological based models for Sockeye.

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Nuclear Science and Engineering Division
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 208
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