INL/MIS-21-61344-Revision-0

Sockeye Accomplishments - NEAMS TH Deep Dive FY20

January 2021

Changing the World's Energy Future

Joshua E Hansel

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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Sockeye

Sockeye FY20 Accomplishments

NEAMS Thermal-Hydraulics Area Deep Dive

Joshua Hansel
Computational Scientist
Idaho National Laboratory

Lander Ibarra
Principal Nuclear Engineer
Argonne National Laboratory

Justin Thomas
Principal Nuclear Engineer
Argonne National Laboratory

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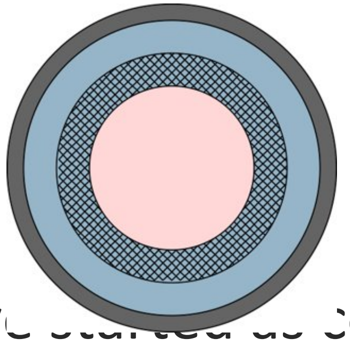
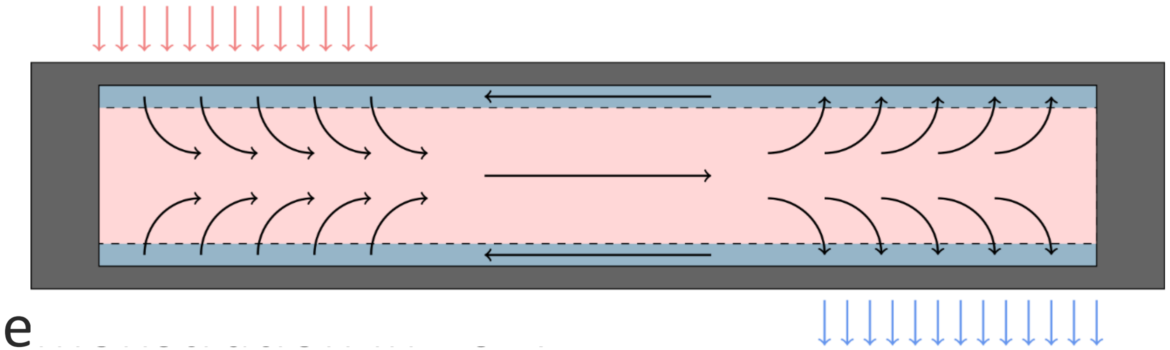
Presentation Overview

- Activities Overview
- Development Updates
- V&V Plan
- Microreactor Application Driver
- Multiphysics Modeling

Introduction

- Sockeye created to model heat pipes
  - Many microreactor designs utilize heat pipes due to their compactness, efficiency, and reliability





- Sockeye started as coupling de
  - Implemented lumped capacitance scheme (~5 DOFs)
- Started new model based on 1-D, two-phase flow model of RELAP-7 in 2019
  - Added capillary pressure in pressure relaxation term, based on estimate of interface curvature from local void fraction solution
  - Changed flow regime maps to reflect flow in heat pipe
  - Added sodium and potassium properties

Team

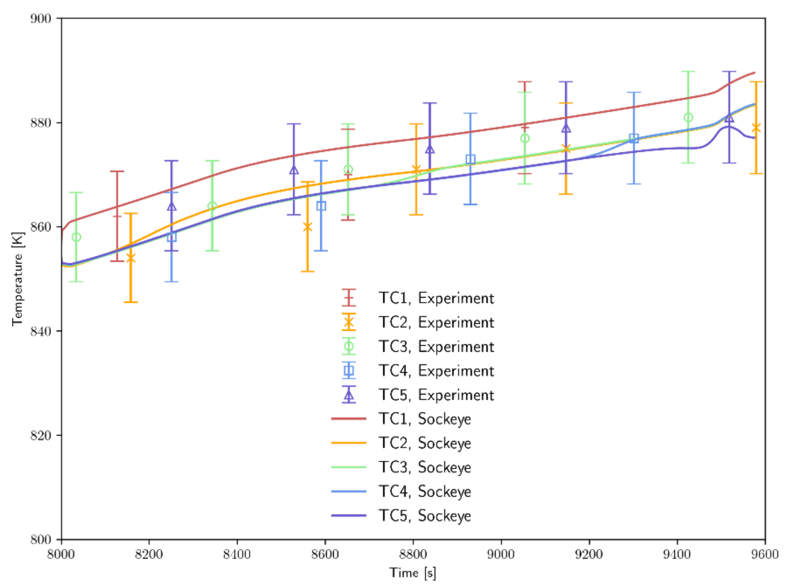
- Team:
  - INL:
    - Joshua Hansel: Lead developer
    - David Andrs: THM lead developer
    - Lise Charlot: Developer and member of eVinci Design Team
  - ANL:
    - Lander Ibarra: V&V plan
    - Justin Thomas: NEAMS microreactor application driver
    - Dave Grabaskas: Model support
  - LANL:
    - Topher Matthews: Multiphysics coupling using DireWolf
    - Bob Reid: Consultation on heat pipe physics, models, and validation
  - WEC: Provided input on development and list of functional requirements
- With the exception of Joshua and David, all contributors are new in FY20!

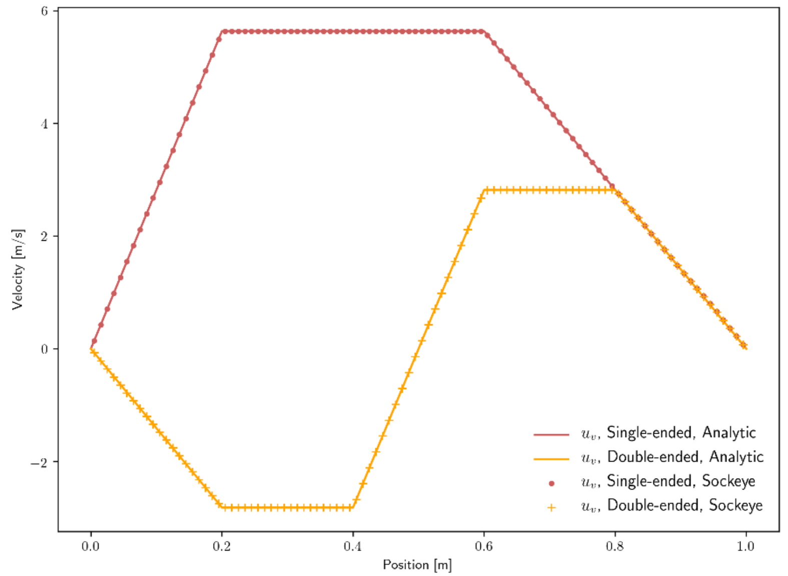
Activities Overview

- NEAMS Milestone (July 2020): Add the ability to melt/freeze the working fluid
- Development and documentation supporting WEC functional requirements
- NEAMS microreactor application driver
- V&V plan
- Articles in MOOSE special volume of *Nuclear Technology*

Publications

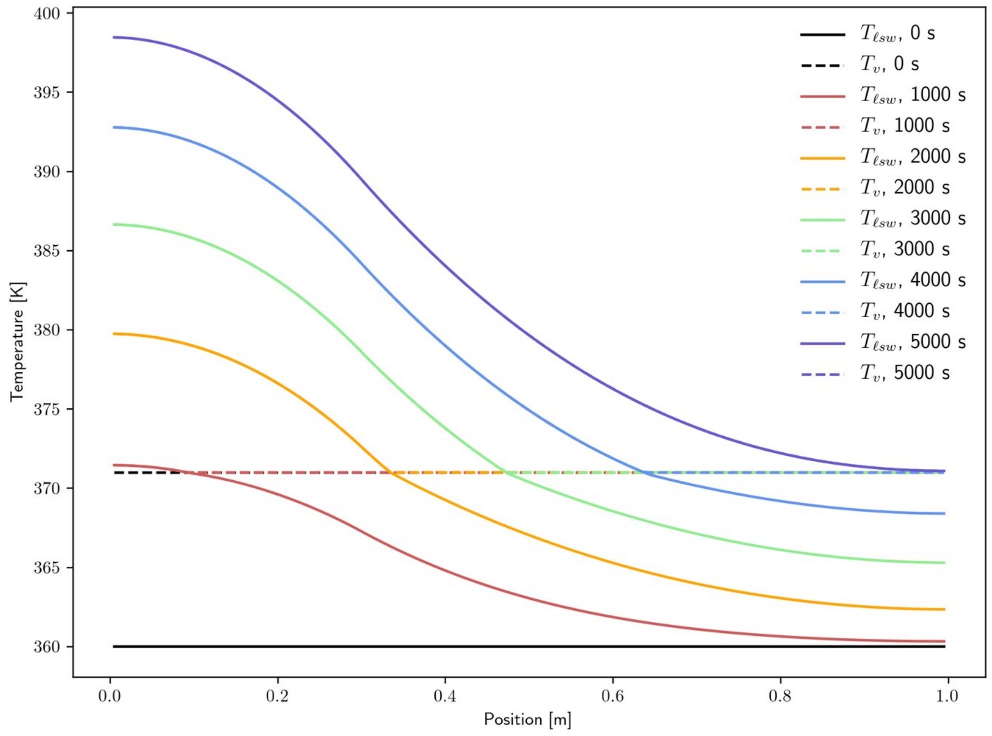
- NEAMS Milestone reports:
  - INL/EXT-20-59174: J.E. Hansel, R.A. Berry. *Three-Phase Modeling in Sockeye*. July 2020. Idaho National Laboratory.
- Journal articles:
  - J.E. Hansel, R.A. Berry, D. Andrs, M.S. Kunick, R.C. Martineau. *Sockeye: A 1-D, Two-Phase, Compressible Flow Heat Pipe Application*. Nuclear Technology. 2020. Accepted.
  - C. Matthews, V. Laboure, M. DeHart, J. Hansel, D. Andrs, Y. Wang, J. Ortensi, R.C. Martineau. *Coupled Multiphysics Simulations of Heat Pipe Microreactors Using DireWolf*. Nuclear Technology. 2020. Accepted.

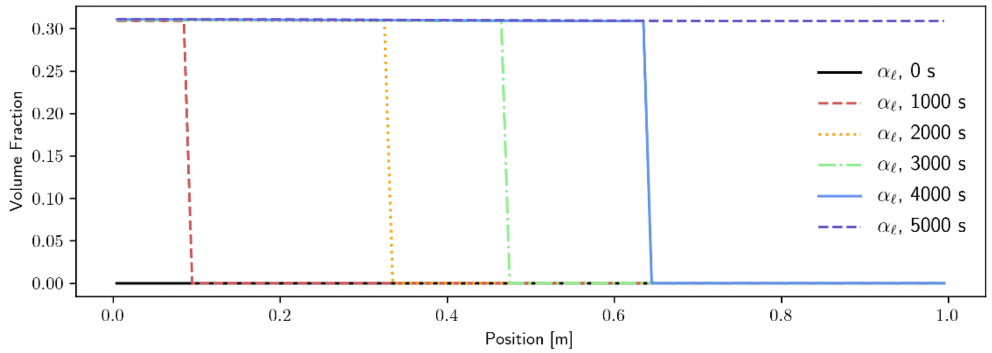




Development: Melt Capabilities

- Completed NEAMS Milestone to implement melt/freeze capability.
- Reformulated flow model to include solid phase.
  - Assumed thermal equilibrium between liquid and solid phases.
  - Determined mixture of liquid vs. solid based on mapping of internal energy including latent heat of fusion.
- Disabled certain terms until a "startup completion" condition was met.
- Accurately and robustly modeling startup will require more work.



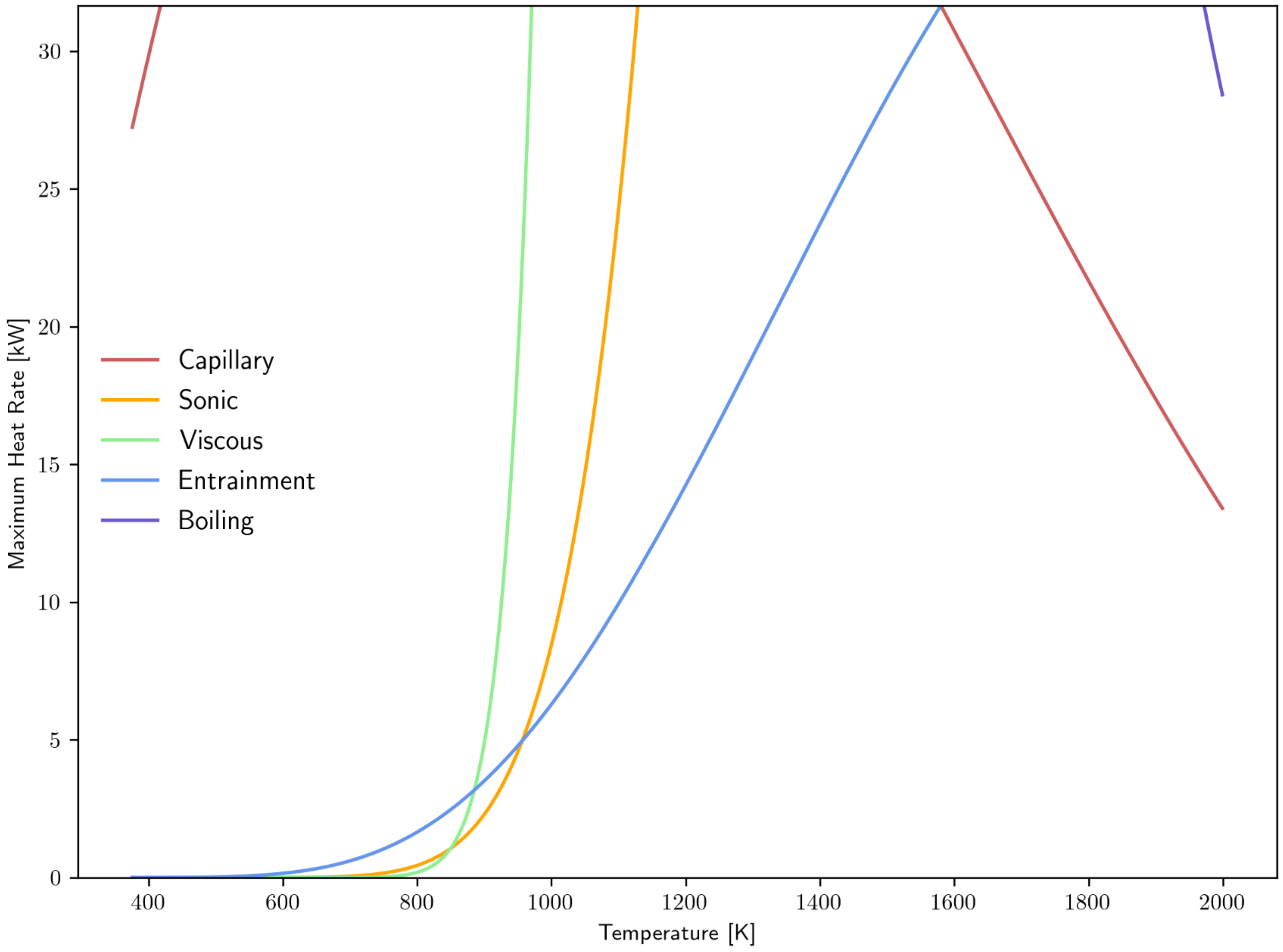


Development: Miscellaneous Model Improvements

- Extended model to allow full range of void fractions
  - Before, only void fractions corresponding to perfectly saturated wick.
  - This change also allowed IC to have a specified working fluid mass or wick fill level.
- Robustness improvements to flow regime switching
  - Smoothed discontinuities in various closures to alleviate convergence difficulties
- Added porous pressure loss term for liquid traveling through wick
- Implemented vapor friction factor closure
- Implemented custom-closure ability
- Changed closures to not allow convex curvature, thus eliminating negative capillary pressures

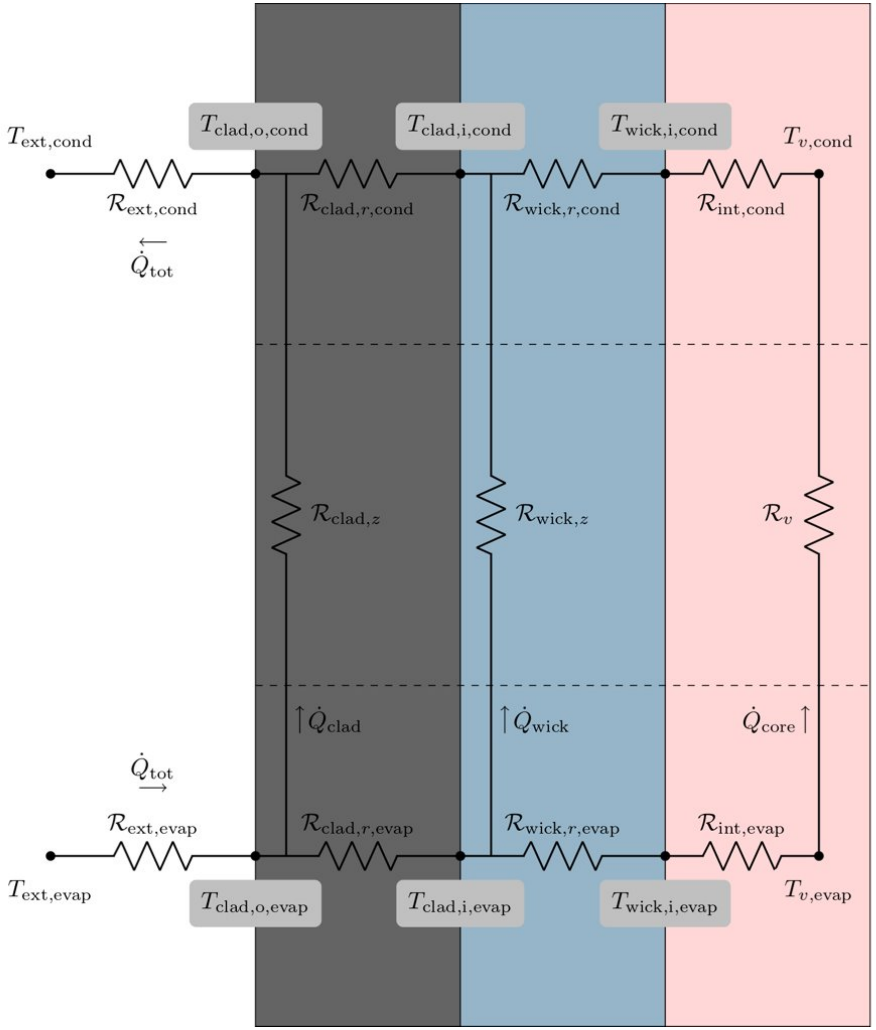
Development: Analytic Limits

- Implemented analytic expressions for operational limits as a function of temperature.
- This can be used to show the operating envelope (see right).
- These limits can be used as a standalone utility or be used to limit boundary conditions.



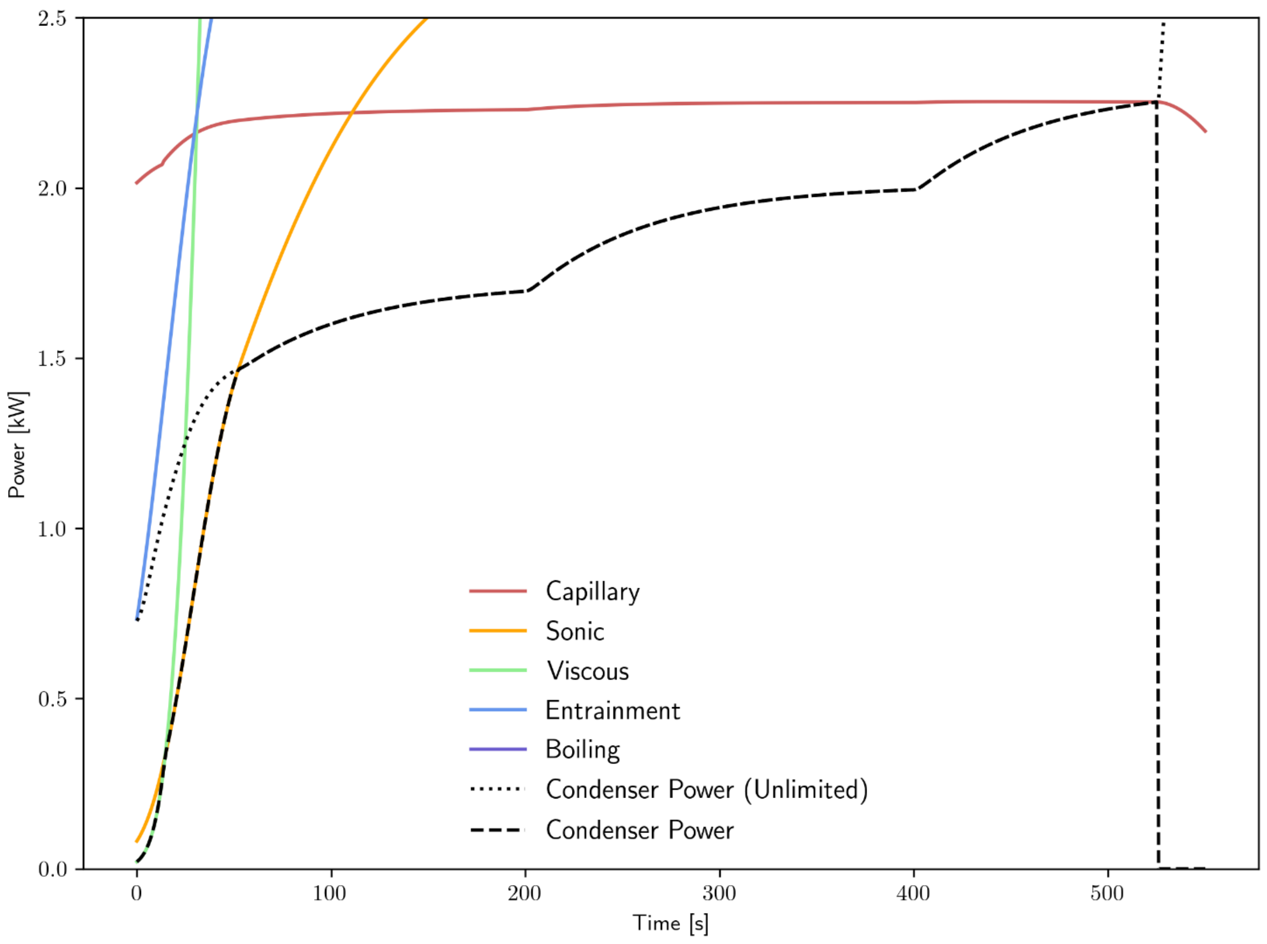
Development: Conduction Model

- Developed an alternate heat pipe model based on effective heat conduction
  - In most cases, more robust but less accurate.
  - Useful in cases where accurate modeling of operational limits is not important, such as normal operation.
- Uses arbitrarily high thermal conductivity in vapor core region to mimic the effective heat transfer in a heat pipe.
- Analytic limits are used to renormalize BC on evaporator or condenser side to satisfy limits.



Development: Conduction Model Example - Cascading Failure

- **Problem Description:**
  - For 200 s, heat at rate Q.
  - At 200 s, increase heat rate by Q/6 due to failure of adjacent heat pipe.
  - At 400 s, increase heat rate by another Q/6 due to failure of another adjacent heat pipe.
- **Results:**
  - In beginning of transient, heat rate is limited by viscous and sonic limits until it heats up enough.
  - Heat pipe handles one adjacent failure, but not two - the capillary limit is reached.
  - Unlike viscous and sonic limits, capillary limit leads to dryout, making heat pipe ineffective for heat removal.



V&V Plan: Overview

- Goals
- Scope
- Gap Analysis
- V&V Report and Plan
- Status FY20

V&V Plan: Objectives

- The main objective of the Sockeye Verification and Validation effort is to:
  - Demonstrate that the code fulfills the functional and performance requirements for its use as an engineering tool for design and safety analysis of microreactors.

- This effort entails four high level activities:
  - 1. Software requirements identification.
  - 2. Software assessment base development.
  - 3. Determination of acceptance.
  - 4. Gap closure.

- The V&V methodology adopted needs to be:
  - Flexible enough to accommodate active Sockeye development,
  - Robust enough for rigorous code capability testing and thorough code coverage,
  - Well documented with usage of an appropriate quality assurance (QA) standard.

V&V Plan: Methodology

- The Sockeye V&V methodology has been derived
  - from the evaluation model development and assessment process (EMDAP) in Regulatory Guide 1.203.
  - EMDAP only used for laying out the methodology structure.

- Methodology and implementation are described in a V&V gap analysis and plan report. Draft shared with
  - Microreactor Campaign.
  - eVinci design team at WEC.

- Top-down:
  Model-driven Code Verification

Software Specification

Model Implementation

Model Evaluation

Gap Identification

V&V Plan: Software Requirements Identification

- Identification of Sockeye's application scope
    - code functional and performance requirements can be established.
- High level functional requirements are aligned with the objectives of the heat pipe modeling component of NEAMS to provide an engineering tool for design and safety analysis of microreactors that must:
    - Be usable within a multi-physics application (BlueCRAB, DireWolf);
    - Be fast-running and robust;
    - Evaluate transients including behavior during startup and shutdown;
    - Evaluate operational limits.
- Functional and performance requirements complemented by heat pipe designers/code users:
    - Industry involvement is paramount to capture nuclear vendor needs and prioritize code development, verification and validation;
    - Flexibility in the V&V methodology and early industry engagement to maximize application and robustness of Sockeye.

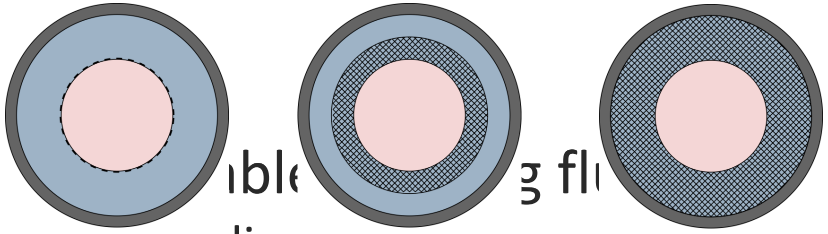
V&V Plan: Industry Involvement

Task No.	Task Description	Priority	Comment	Needed For
1	Develop V&V Plan	High		Documentation
2	Identify V&V Gaps	High		Documentation
3	**Develop theory necessary to model three phase (solid, liquid, gas) heat pipes for start-up, steady state, and**	High		Normal Ops
4	**Perform code implementation of three phase heat pipe model**	High		Normal Ops
5	Develop capability to compute heat pipe operational limits	High	Standalone python utility implemented that computes heat pipe limits based on analytical relations.	Normal Ops
6	Compute the thermal hydraulic conditions of heat pipe and output to a text file	High	Sockeye is able to output variables throughout transient to a text file as well as exodus file format which can be post-processed in Paraview or post-processing software of choice (e.g. MATLAB or python)	Normal Ops
7	Simulate standalone heat pipe coupled with core and heat exchanger	High	Coupling is performed by temperature or heat flux to external application (such as heat exchanger or core).	Normal Ops
8	Simulate multiple heat pipes coupled with core and heat exchanger	High	**Heat exchanger modelling & coupling require additional time/work (e.g. Bryton Cycle flow over tube array).**	Normal Ops

V&V Plan: Requirements Identification Example

Scope

- Wick type is annular region of any thickness.
  - No grooved or arterial wicks.



- …ble … g fl…
  - sodium
  - potassium
- No non-condensable gases.

Models

- 1-D, 2-phase, compressible flow.
- Well-posed system of 7 PDEs:
  - Volume fraction balance
  - Liquid/vapor mass conservation
  - Liquid/vapor momentum balance
  - Liquid/vapor energy conservation
- Finite volume discretization.
- Closures:
  - Capillary pressure
  - Interfacial area density
  - Interfacial heat transfer coefficients
  - Wall heat transfer coefficients
  - Wick permeability
  - Vapor friction
  - Interfacial friction

V&V Plan: Plan Development

- The V&V plan is the result of the overall V&V assessment work.
  - It prioritizes and categorizes the closure of any remaining gaps in the V&V Test Matrix,
  - software documentation, or
  - software capabilities where possible.

- Addressing test matrix gaps:
  - **Includes** additional testing of the software to confirm suitable implementation of the described models;
  - **Excludes** the implementation of new models that close phenomenological gaps.
- Assess Impacts of Test Matrix Gaps:
  - Impact of these gaps should be assessed for their anticipated effect on Sockeye heat pipes safety analyses (e.g. increased uncertainties, larger safety margin, etc.)
    - Gaps will be prioritized at a high level in accordance with their importance to heat pipes systems level safety analysis
  - Additional needs for validation are being identified and documented to address any gaps that can exist in data and/or benchmarks.

V&V Plan: Test Matrix Extract

	Validation Dataset							
	SAFE-30 [6]	SAFE-100 [7]	SAFE-100a [8]	KRUSTY [11]	Faghri [9] [10]	SPR [13]	TAMU [12]	CFD [4]
Material Properties								
Working Fluid Properties			X					
Wick Characteristics							X	
Wall Properties		X	X					X
Physical Phenomena								
Capillary Pressure								
Liquid Pressure Drop		X					X	
Vapor Pressure Drop					X		X	
Wall Convective Heat Transfer	X	X	X	X				
Wall Conduction Heat Transfer	X	X	X	X				
Interfacial Mass Transfer								
Interfacial Heat Transfer								
Experimental Data								
Vapor Temperature Distribution			X		X		X	
Liquid Temperature Distribution		X	X	X				
Phase Distribution						X	X	
Friction Factors							X	X
Operational Limits								
Capillary Limit					X			
Boiling Limit								
Sonic Limit	X	X		X	X			
Entrainment Limit					X			
Viscous Limit		X		X				

V&V Plan: Status FY20

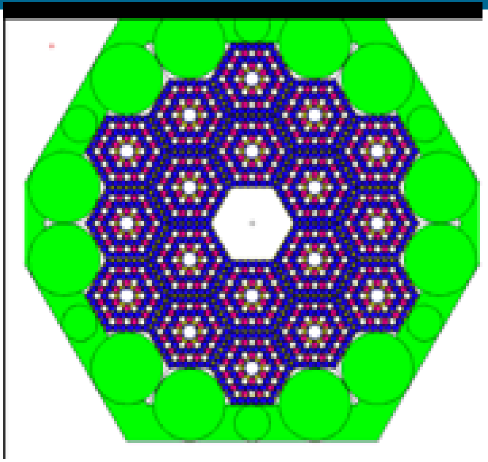
- The V&V methodology has been reviewed and by members of the NEAMS MR campaign to help guide the experimental campaign and members of the industry (eVinci WEC)

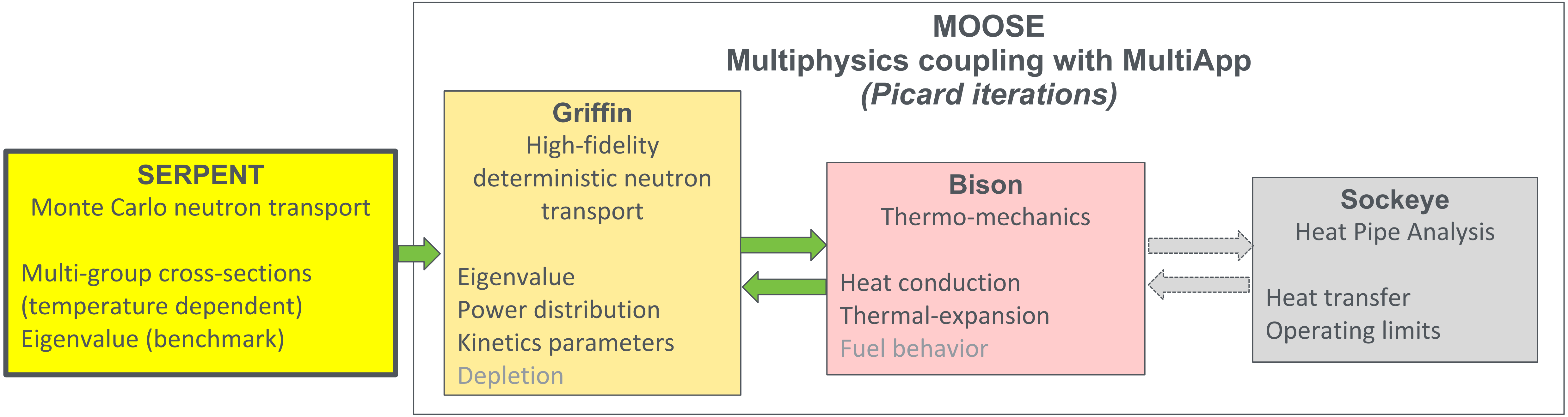
- Sockeye V&V report Draft issued and reviewed. Comments addressed and Validation database being expanded.

- Verification and Validation efforts are continuing for Sockeye

NEAMS Microreactor App Drivers (FY20)

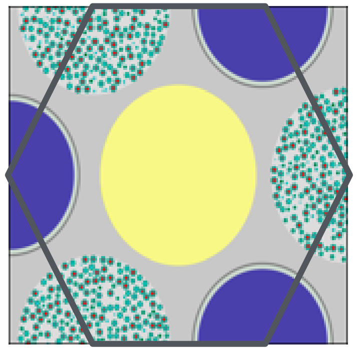
- Microreactor App Driver Effort led by Nicolas Stauff (ANL)
  - Develop internal experience within the national labs with the NEAMS codes
  - Provide user feedback to developers and NEAMS program
  - Apply NEAMS tools to solve MR problems of interest to the industry
- Based on EMPIRE concept heat-pipe 2MWth, thermal spectrum microreactor design
  - ➢ Start from reference EMPIRE inputs developed by LANL MEITNER Resource Team
- Multi-physics problem of interest: Heat-pipe temperature increase (load following)





App Driver: Modeling Exercises

- **Unit-cell (1.8 kWt)**



Refl. BC

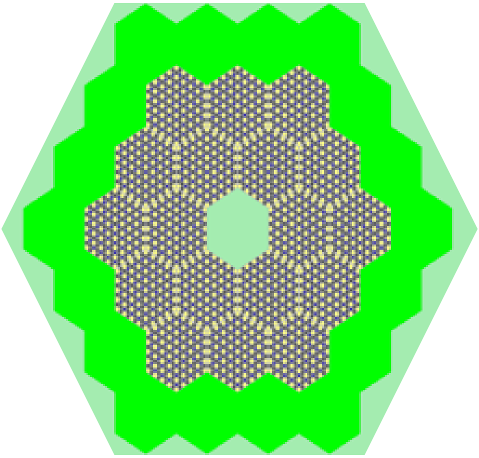
Heat pipe

Fuel block (40% packing fraction TRISO/UCO)

Graphite matrix

YH_2 Moderator with SS316 envelope

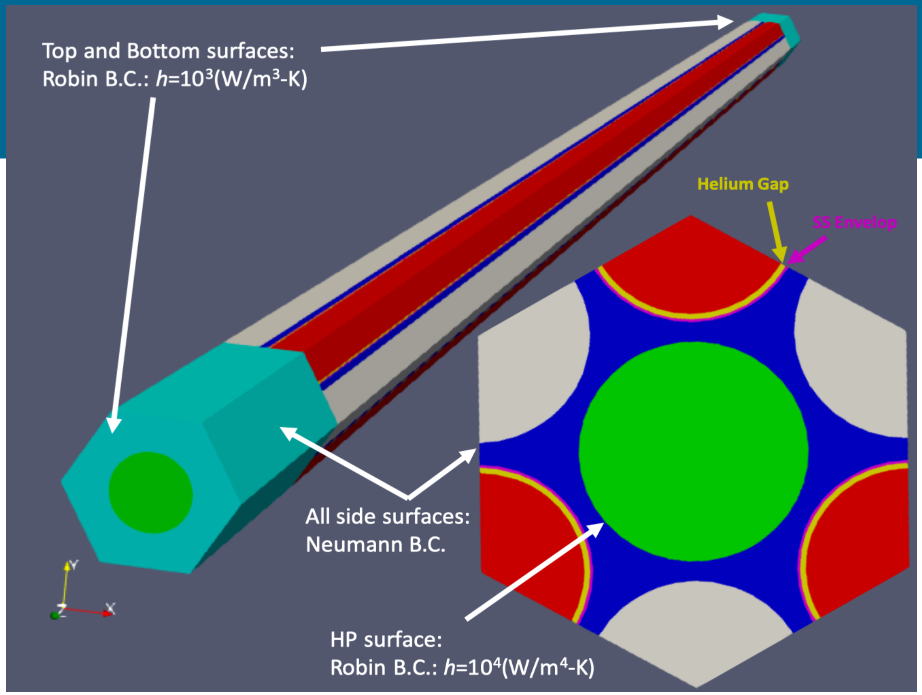
- **Full-core (2 MWt) (includes design simplifications)**

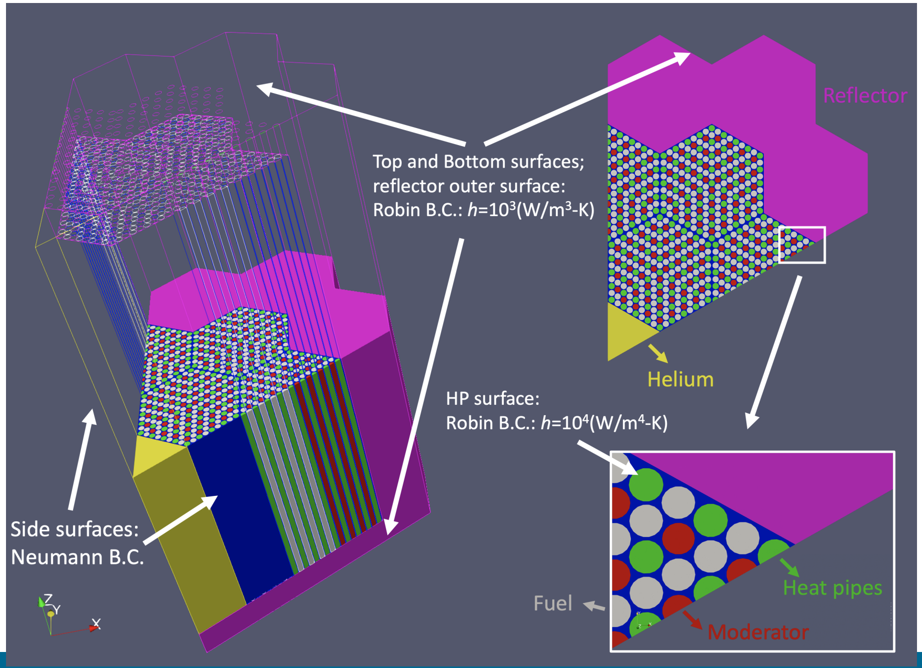


Air

Beryllium reflector

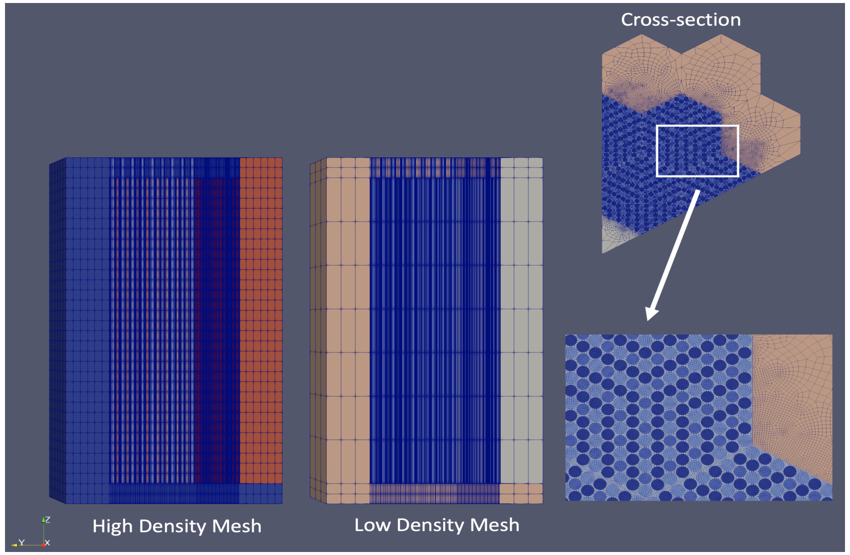
Fuel assembly

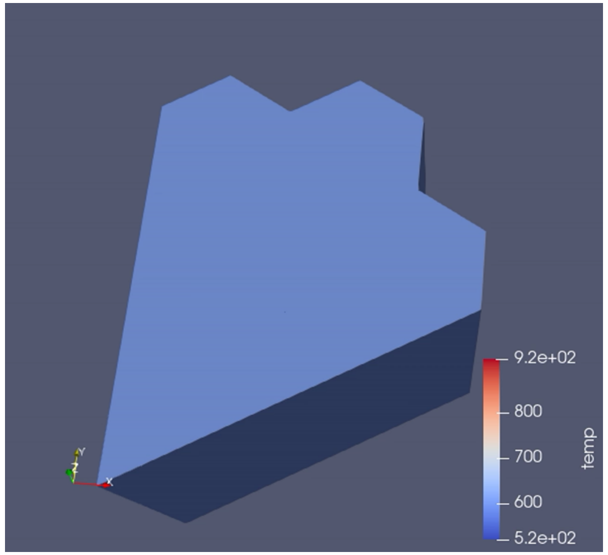




App Driver: Full-Core Analysis

- **Griffin**: Relatively good agreement on K-eff and temperature coefficient with het. diffusion - *future work will investigate transport SN and diffusion with SPH treatment*
- **Sockeye**: Gained experience for Heat-Pipe modeling
- **Griffin/Bison**: coupled Multiphysics (Neutronic/Thermo/Mecha) simulations :
  - Investigated tradeoff between computation time and accuracy on the density of the mesh
  - Transient simulations completed on a full-core model, while running within one day with a small ANL cluster
  - Acquired experience with multi-physics simulation (input/mesh consistency, etc.)



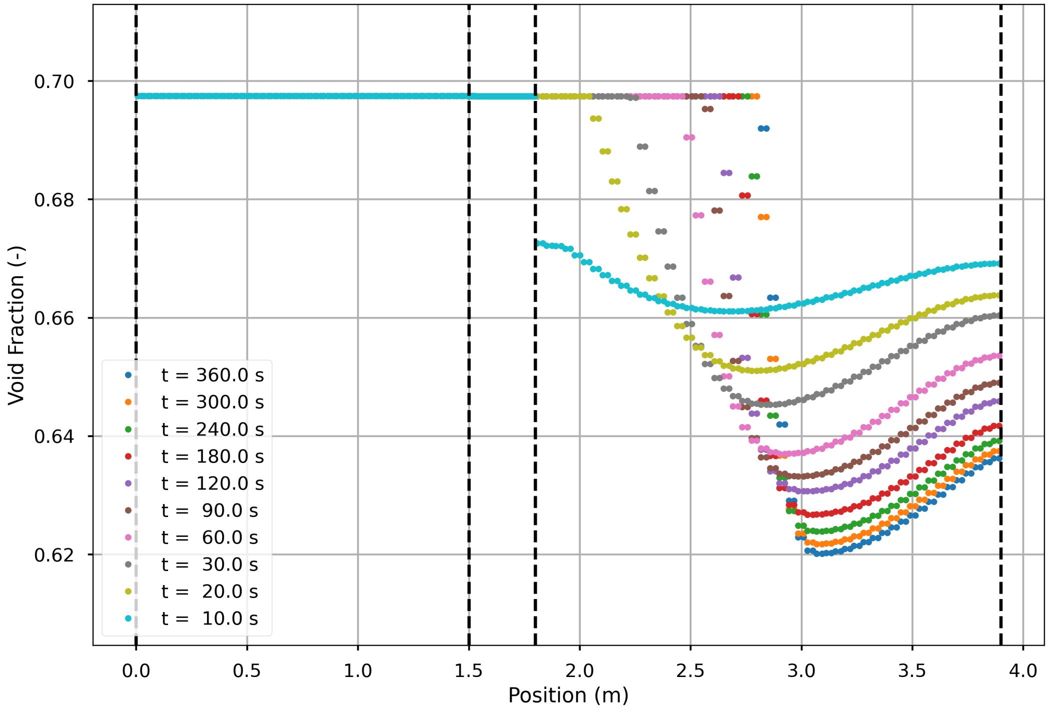


App Driver: Heat Pipe Performance Modeling (FY20)

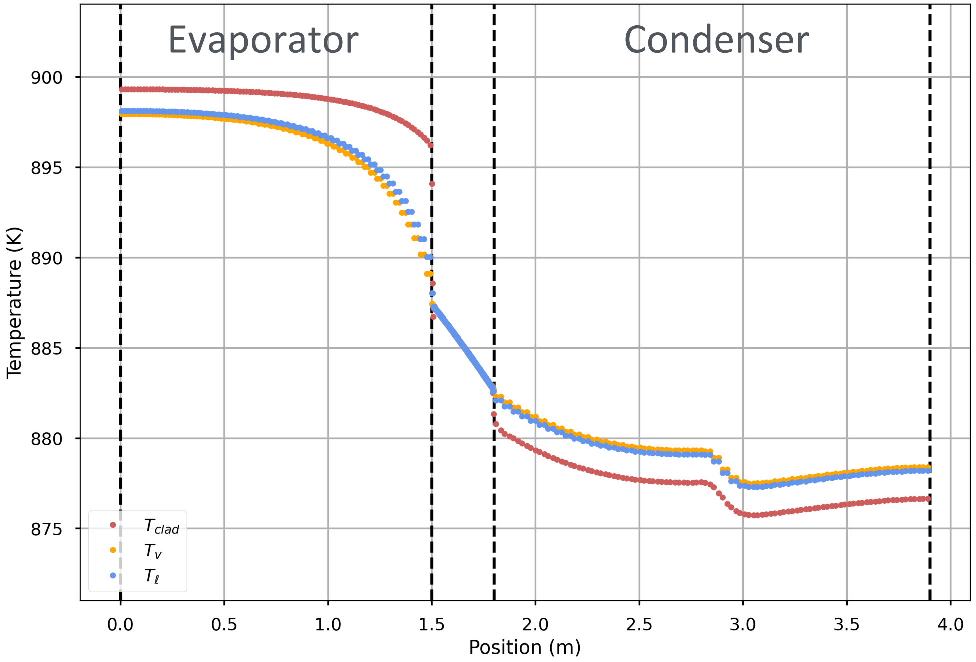
- Experienced Sockeye for Heat-Pipe modeling
- Model of Heat-Pipe with potassium, based on INL/EXT-17-43212 Rev 1
- Identified temperature range of operation in the heat-pipe
- Sockeye 2-fluid model employed to reach steady-state condition

Void Fraction

E



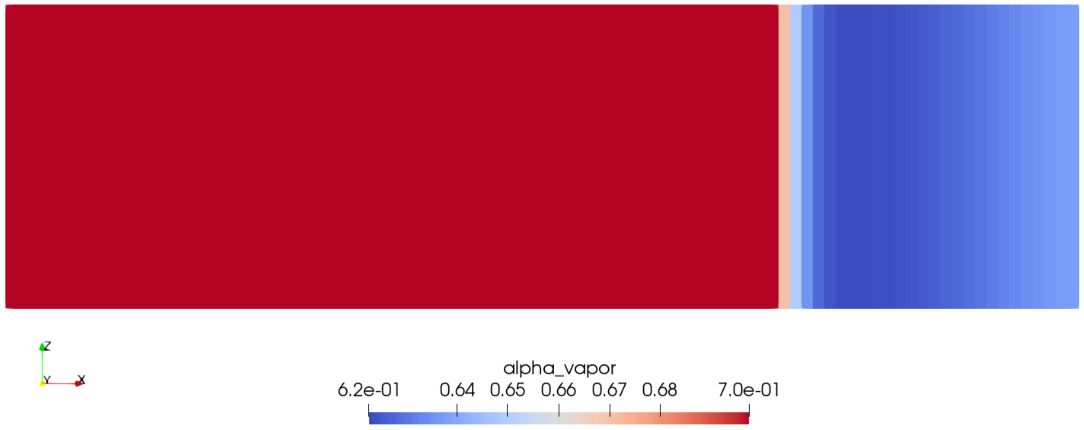
Steady-State Temperature Profile in Heat Pipe



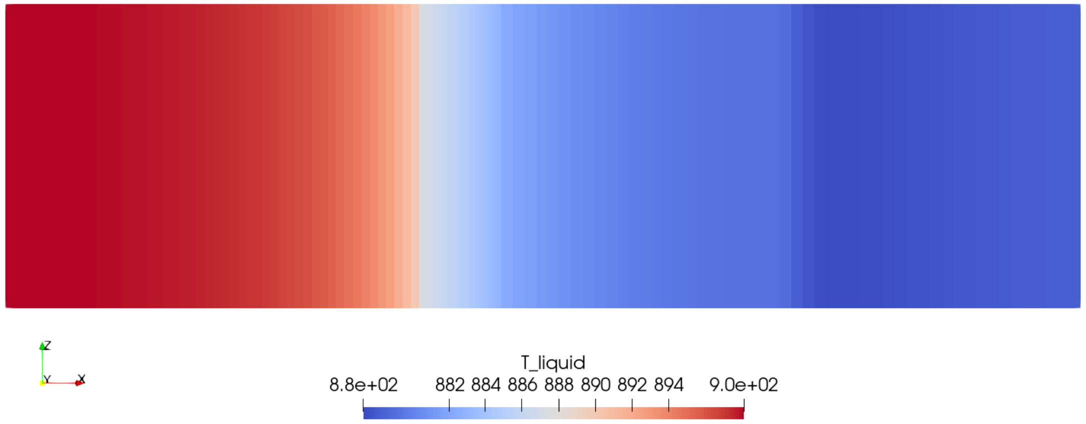
App Driver: Heat Pipe Performance Modeling (Ongoing)

- Moving to *effective conductivity* model based on experience of MEITNER team
  - Reduced computational expense
  - Maintains awareness of heat pipe performance limits
- Setting effective thermal conductivity to match the thermal predictions of the two-phase model
  - Working with development team to address apparent convergence issues in transient solver

Void Fraction Distribution at Steady-State Conditions



Liquid Temperature Distribution at Steady-State Conditions

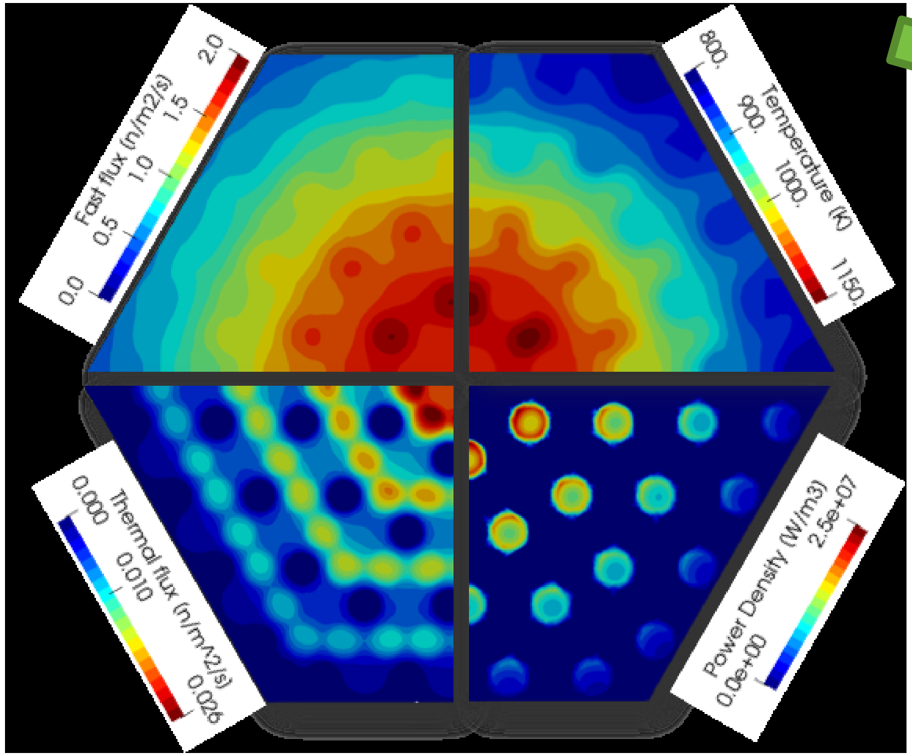


App Driver: Status FY20

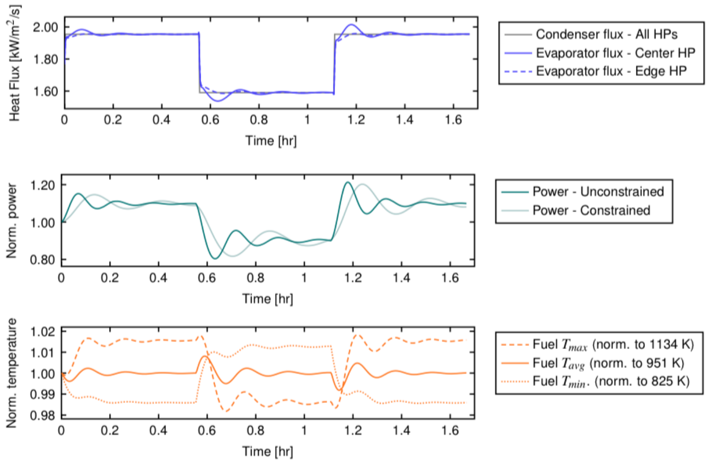
- In FY20, we built a team of lab experts to:
  - Gain user experience with NEAMS codes Bison, Griffin, Sockeye
  - Develop Sockeye heat pipe performance models using the two-phase models
  - Provided feedback to the development team
    - User experience
    - Identified bugs and potential of improvements
  - Demonstrate codes capability by solving microreactor multiphysics simulation with Bison + Griffin

Next Steps: Multiphysics Simulations

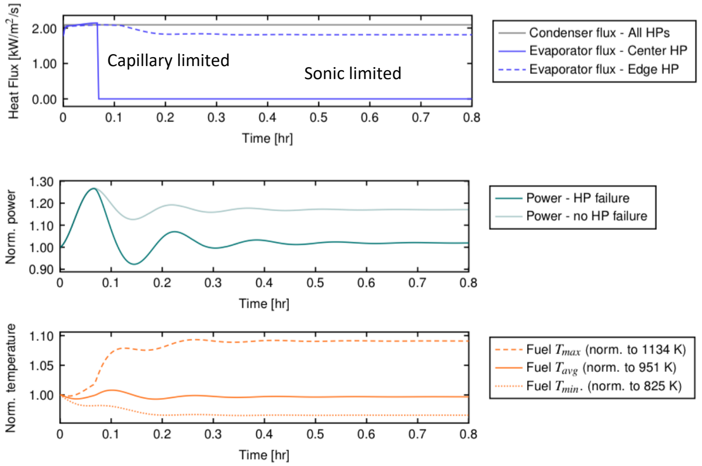
Leverage DireWolf simulations started under ARPA-E MEITNER



Power Transients



Cascading HP Failure



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