

Fluid Properties for MOOSE

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Introduction

The Multiphysics Object-Oriented Simulation Environment (MOOSE) enables a wide range of advanced nuclear reactor simulations. Under the guidance of MOOSE's Finite Volume Team, we worked on the fluid properties module. Significant contributions include enabling Tabulated Fluid Properties (TFP) for systems thermal hydraulics analysis, Temperature and Pressure functionalized Fluid Properties, and Lead & Lead-Bismuth properties. Along with improving the capabilities of the fluid properties module, we also improved the documentation to allow for future users and developers to understand how the module works.

New capabilities will be **published** in the Journal of Open Source Science

Use of Fluid Properties

- Pronghorn: finite volume coarse mesh CFD code for core / plenum analysis
- Subchannel: lattice-based reactor core thermal hydraulics
- Thermal Hydraulics Module (THM) & RELAP-7: 1D simulation of the coolant flow through the reactor heat exchanger, pump, etc.

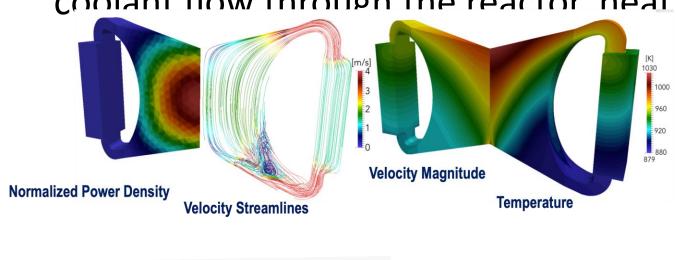
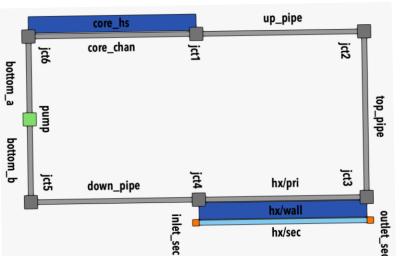


Figure 1: Temperature profile in an assembly generated using Subchannel [4] (bottom right image)

Figure 2: A primary loop with circulating Helium made with THM [6] (bottom left image)

Figure 3: Molten Salt Fast Reactor simulations using the Navier Stokes module [7] (top image)



Assessment of the Fluid Properties

- All fluids properties in the module were tested using Pronghorn, Subchannel and the Thermal Hydraulics Module.
- Issues identified: missing formulations (v, e), missing automatic differentiation implementations, missing properties, missing derivatives of properties with regards to state variables
- Seven properties extended to work across all nuclear simulation codes

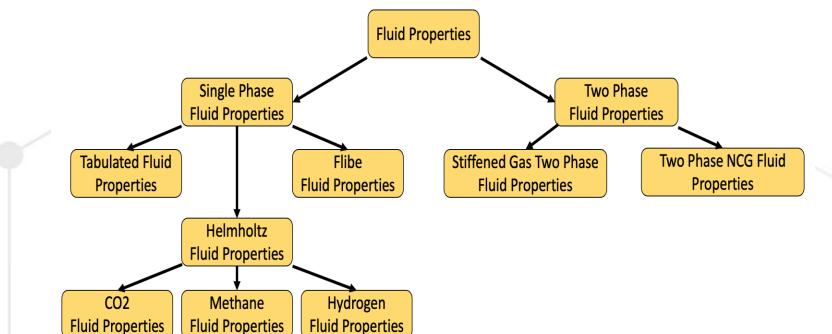


Figure 4: Inheritance diagram of Fluid Properties module. Different fluid property files inherit from different "base" classes

Fluid Properties and Definitions

- Different variable sets have better numerical solver properties
 - Pressure, temperature (p, T)
 - Specific volume, specific internal energy (v, e)
- Fluid properties can be challenging to obtain with (v, e)
- (p, h) and (v, h) formulations used in parts of the codes
- Initialization with isentropic transformations even requires (h, s) and (T, s) formulations
- p ≡ Pressure (Pa)
- $T \equiv Temperature (K)$
- $v \equiv Specific Volume (m³/kg)$
- e ≡ Specific Internal Energy (J/kg)
- h ≡ Specific Enthalpy (J/kg)
- $s \equiv Specific Entropy (J/K \cdot kg)$
- g ≡ Gibbs Free Energy (J)
- cp ≡ Specific Heat Capacity at Constant Pressure (J/K·kg)
- cv ≡ Specific Heat Capacity at Constant Volume (J/K·kg)
- $\rho \equiv Density (kg/m^3)$
- c ≡ Speed of Sound in fluid (m/s)
- mu ≡ Dynamic Viscosity (Pa·s)
- $k \equiv Thermal Conductivity (W/m·K)$

Tabulated Fluid Properties (TFP)

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- Tabulated data is a common way of inputting fluid properties
- Previously, only (pressure, temperature) was available
- Inversion from (v, e) variables, used in RELAP-7/THM, was implemented using Newton's Method
- C++ templated was used to enable both bicubic and bilinear Interpolation
- TFP will be used by NASA to test Nuclear Thermal Propulsion (NTP) engine systems with parahydrogen
- NTP engine fluid properties drastically vary throughout system, TFP provides the necessary flexibility

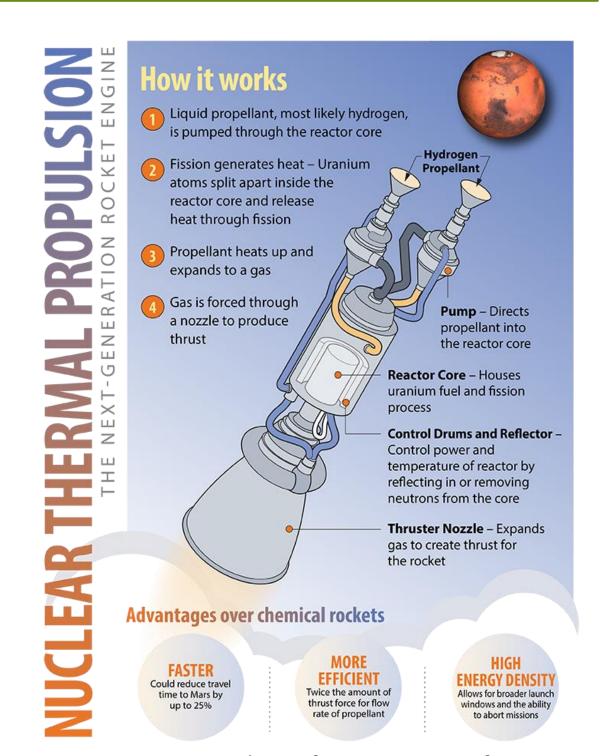
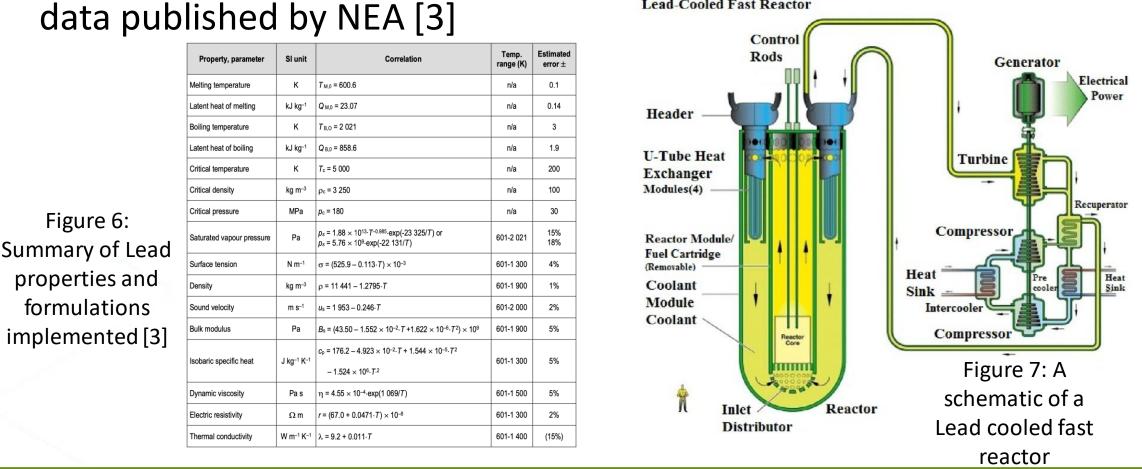


Figure 5: Graphic of NTP engine from Department of Energy³

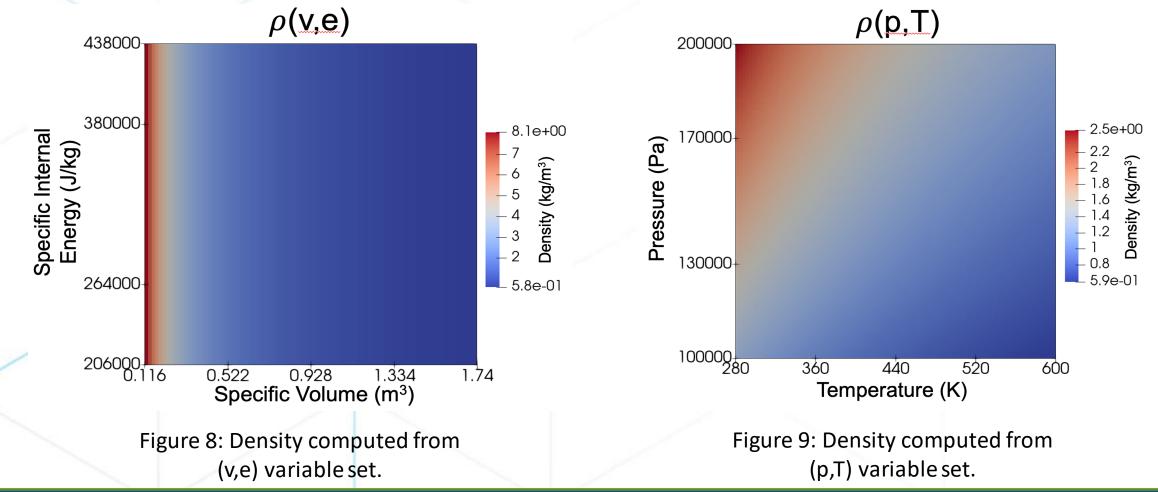
Pb & Pb-Bismuth Fluid Properties

- Lead and Lead-Bismuth are **high-density metallic coolants**, with low neutron absorption and very high thermal conductivity, making them prime candidates for advanced reactor coolants
- In support of modeling efforts at Argonne National Laboratory, we added these fluid properties to MOOSE, from open-source



Variable Sets

- Properties are usually known in terms of pressure and temperature
- Depending on the application, properties may be computed using (v,e), (v,h), (h,s), (p,h), (p, ρ), for both numerical and physical modeling reasons
- Newton's Method is leveraged for fast and flexible conversions between sets
- Capability enabled for ALL fluid properties



Bibliography

¹ .Cody J. Permann and Derek R. Gaston and David Andrs and Robert W. Carlsen and Fande

Kong and Alexander D. Lindsay and Jason M. Miller and John W. Peterson and Andrew E. Slaughter and Roy H. Stogner and Richard C. Martineau. {MOOSE}: Enabling massively parallel multiphysics simulation,

2022, SoftwareX, http://www.sciencedirect.com/science/article/pii/S2352711019302973

² . Fazio, et al., I.S. (2015). Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal-hydraulics and Technologies- 2015 Edition (NEA--7268). Nuclear Energy Agency of the OECD (NEA)

³ "Infographic: How Does Nuclear Thermal Propulsion Work?" Energy.gov, https://www.energy.gov/ne/downloads/infographic-

how-does-nuclear-thermal-propulsion-work.

⁴ Figure made by Mauricio Tano using the MOOSE Navier Stokes module

⁵ Pioro, Igor, Mokry, Sarah. "Thermophysical Properties at Critical and Supercritical Pressures". Heat Transfer - Theoretical Analysis, Experimental Investigations and Industrial Systems, edited by Aziz Belmiloudi, IntechOpen, 2011. 10.5772/13790.

6 RELAP-7 Theory Manual, INL/EXT-14-31366 (Revision 2)

7 Development of a Subchannel Capability for Liquid-Metal Fast Reactors in Pronghorn, Tano et al., INL/EXT-22 (in processing)

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