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Latest developments in the MOOSE Fluid Properties Module

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INTRODUCTION

The fluid properties module in MOOSE [1] serves a variety of fluid simulation applications based on MOOSE, including the MOOSE Navier Stokes module [2], Pronghorn [3], SAM [4], the MOOSE thermal hydraulics module, RELAP-7 [5] and Pronghorn-subchannel [6]. It is used for coarse mesh multi-dimensional thermal-hydraulics [3], 1D systems analysis [4, 5] in nuclear reactor analysis, and porous flow simulations [7] for underground gas storage and water seepage. The use of consistent fluid properties across fluid flow applications facilitates coupled simulations [8].

The module offers a consistent set of interfaces that must be implemented to create a new fluid property. There are numerous fluid properties of interest in the entirety of all fields of fluid flow simulations, and this issue is exacerbated by the use of different variable sets depending on the compressibility of the fluid. For single-phase fluids, the following variable sets may be used to compute fluid properties: (pressure, temperature) and (specific volume, specific internal energy). Some properties may also be computed using the (pressure, density) or the (specific volume, specific enthalpy) variable sets. In order to reduce the challenge of adding a new fluid property, properties may be implemented partially.

FLUID PROPERTIES MODULE

The module follows the design principles of MOOSE. It leverages object-oriented programming, in particular inheritance and runtime polymorphism, so that fluid property function calls can be written with the base class and are naturally forwarded to the derived class. The inheritance structure of the module is shown in Fig. 1. Fluid properties are MOOSE `UserObjects` under the hood, though they have their own dedicated input file syntax, shown in listing 1.

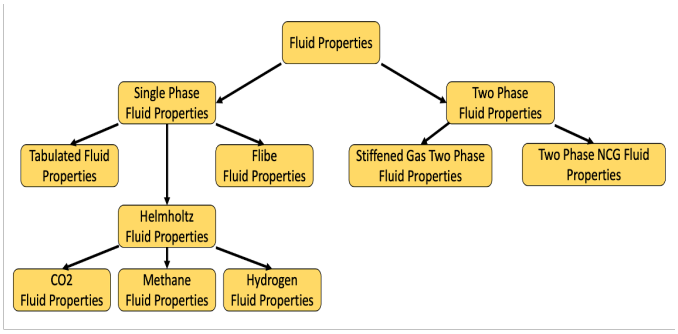

Fig. 1. Inheritance diagram for part of the fluid properties module.

Listing 1. Example of fluid properties input file syntax.

```
[FluidProperties]
  [lead]
    type = LeadFluidProperties
  []
[]
```

The following properties are provided for single phase fluids: density, thermal conductivity, specific heat, dynamic viscosity, isobaric heat capacity, specific internal energy, enthalpy, specific stagnation entropy, pressure and temperature (for variable set conversions), speed of sound in the fluid, volumetric thermal expansion coefficient, and Gibbs free energy. The units are usually S.I. units, but as in most of MOOSE, any unit set may be leveraged as long as the fluid properties producer and consumer code are consistent.

Table I summarizes the fluid properties available in the module, and for which variable set and applications they can be used. Many of the 'no' responses are simply due to missing implementations, rather than an impossibility to use them. Please contact the first author if you require one of these properties for a currently unsupported configuration.

NEWLY IMPLEMENTED ADVANCED REACTOR COOLANT PROPERTIES

The fluid properties of the sodium-potassium eutectic, lead and lead-bismuth eutectic were implemented in the module, following public Nuclear Energy Agency (NEA) reports [9, 10]. 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. The sodium-potassium eutectic is liquid at room temperature, does not corrode steel, and has a similarly high thermal conductivity. It was the coolant for the Experimental Breeder Reactor - I, the first nuclear reactor to produce electricity in 1951.

These three new fluid properties are weakly compressible; their density does not depend on pressure. As such, there is a relatively direct relationship between the specific volume and the specific internal energy of the fluid, which prevents us, to our knowledge, from using them with a conservative variable set. The definitions implemented however do suffice for their use with the Navier Stokes module, Pronghorn, SAM and subchannel.

NEW FUNCTIONALIZED FLUID PROPERTIES

While most fluid properties are implemented by users in `FluidProperties` objects in C++ in the module, it is often convenient to be able to specify the fluid properties directly in the input file. This enables rapid modifications of the sim-

TABLE I. Summary of single-phase fluid properties available in the module, variable sets implemented and general compatibility with a selection of downstream codes. An asterisk indicates a new development. All property names are suffixed with `FluidProperties`, which we do not include here.

Single phase fluid or object	(p,T)	(v,e)	Navier Stokes	Thermal Hydraulics	Subchannel	porous flow
Brine	yes	yes	no	no	N/A	yes
Air (ideal gas)	yes	yes	yes	yes	yes	yes
CO_2	yes	no	no	no	no	yes
StiffenedGas	yes	yes	yes	yes	yes	yes
CaloricallyImperfectGas	yes	yes	yes	yes	no	yes
Helium	yes	yes	yes	yes*	yes*	yes
Hydrogen	yes	no	no	no	no	yes
Methane	yes	no	no	no	no	yes
NaCl	yes	no	yes	no	no	no
Nitrogen	yes	no	no	no	no	yes
SodiumSaturation	yes	no	yes	no	no	N/A
Water IAPWS-IF97	yes*	yes	yes*	yes	no	yes
Simple (exponential density)	yes	yes	yes	yes*	yes*	yes
Linear (linear density in p,T)	yes	yes	yes	yes	no	no
Tabulated	yes	yes*	yes	yes*	no	yes
FLiBe salt	yes	no	yes	no	yes*	N/A
FLiNaK salt	yes	no	yes	no	yes*	N/A
Lead*	yes	no	yes	no	yes	N/A
Lead Bismuth*	yes	no	yes	no	yes	N/A
NaK eutectic*	yes	no	yes	no	yes	N/A

ulation parameters, for example for rapid prototyping of a simulation or for parametric studies. The `Function` system in MOOSE is leveraged to allow the users to provide density, dynamic viscosity and thermal conductivity as functions of temperature and pressure. Functions are usually dependent on x,y,z, and t, the spatial and temporal coordinates. Here we use them with $x = temperature$ and $y = pressure$. The isochoric specific heat is provided as a constant input by the user. All other properties are computed from these user-defined parameters.

In order to be able to perform variable set conversion with an arbitrary function for density which is, in other words, not always invertible analytically, new Newton solve utilities were added to the module. These inversion solve utilities, called `Newton1DSolve` and `Newton2DSolve` can solve the following types of problems:

$$\text{Find T such that: } \rho(T) = \rho_0 \tag{1}$$

$$\begin{aligned} \text{Find p, T such that: } \rho(p,T) &= \rho_0 \\ e(p,T) &= e_0 \end{aligned} \tag{2}$$

with p the pressure, T the temperature, ρ the density, and e the specific internal energy. The Newton solve utilities are written in a very general manner, and different single- and two-variable problems may be solved. User defined initial guesses for the variables to solve for (temperature and pressure in this example) can be provided to accelerate solves. These routines are compatible with properties of floating point and automatic differentiation types [11].

EXTENSION OF TABULATED FLUID PROPERTIES

Tabulated fluid properties are a general kind of fluid properties that may represent any fluid in existence as long as it is single phase and its properties are provided as a comma-separated-values (CSV) file. The properties are interpolated using bi-cubic polynomials in between the provided data points. This `FluidProperty` object previously only supported tabulations in pressure and temperature. It was expanded to support tabulations in specific volume and specific internal energy or specific enthalpy and to handle conversions from tabulations in pressure, temperature to tabulations in these alternative variable sets. This enables the use of the `TabulatedFluidProperties` in the thermal hydraulics module and RELAP-7 for single-phase gaseous fluids such as hydrogen.

Bilinear interpolation utilities in MOOSE were adapted to provide an alternative to the bicubic interpolations, which may not be monotonous. This particular implementation was not deployed and only the bicubic interpolation is available at this point. However, the non-monotonicity has not been reported as problematic by users to the authors' knowledge. The tabulated fluid properties also rely on Newton's method-based variable sets inversions described in section on functionalized fluid properties for a selected set of property definitions.

EXTENSION OF WATER FLUID PROPERTIES

Water fluid properties, based on the IAPWS industrial formulation 97 formulations, were implemented in the fluid properties module before this work. They were initially implemented for the pressure-temperature variable set. Recent work has enabled use of water fluid properties for a conserved variable set. It heavily relies on the Newton method described in the section on functionalized fluid properties, including the ability to propagate derivatives with automatic differentiation necessary for the thermal hydraulics module.

CONCLUSIONS

The capabilities of the fluid properties module were significantly expanded over the past year. Four additional fluid properties, including a highly flexible general function-based property, were added to the module. Almost a dozen other properties were extended to support two variable sets: pressure/temperature and specific volume/specific internal energy. The development of the module continues. Interfaces with international databases of fluid properties should be developed. Other expansion avenues may include multi-phase fluid properties and salt-fuel burnup-dependent properties.

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