Consistent Fluids Study

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A study is performed to determine if RELAP5-3D would perform better (lower mass error) if the fluid properties were calculated in a manner more consistent with the numerical solution scheme.

Background on RELAP5-3D Fluids

Properties of fluids have been studied and tabulated by the National Bureau of Standards (NBS) [1] and its successor the National Institute of Standards and Technology (NIST) [2], the American Society of Mechanical Engineers (ASME) [3], and the Nuclear Regulatory Commission (NRC) [2] to name a few. The studies have created exhaustive, detailed tables and produced complex mathematical functions of many variables. These functions are called property generators and they are used to calculate the fluid properties at a given fluid state.

From the outset of RELAP5 (and many of its predecessor RELAP codes), fluid properties have been obtained from a simplified table lookup [4] rather than by evaluating a computationally intensive fluid property generator. Given the small size of computer and disk storage in the 1970s, and the speed of computers, the small table size made it possible to load default water properties into the code at compile time and table lookup ran much faster than the property generator. However, this simplification introduced an approximation error into the calculation of the fluid properties at a fluid state.

The first tables were constructed for light water using the 1967 ASME Steam Tables calculated using the 1967 International Formulation Committee (IFC) Formulation for Industrial Use known as IFC-67 [3]. These tables tabulated saturation properties as a function of temperature, saturation properties as a function of pressure, and single-phase properties as a function of pressure and temperature. The properties and derivatives produced are saturation pressure (P_S), saturation temperature (T^S), specific volume (v), specific internal energy (U), specific entropy (s), and three derivatives: isobaric thermal expansion coefficient (β); isothermal compressibility (κ); and the specific heat at constant pressure (C_P). The pressure and temperature grid points, sparse in comparison with the IFC, were selected so that calculations would be in reasonably good agreement with data in typical light water reactor operating conditions and accident scenarios of interest.

As the range of reactor conditions increased, improved water property data was developed. A table for water property based on a 1984 standard produced by U. S. National Bureau of Standards and the National Research Council of Canada (NBS/NRC) Steam Tables [2] was added as external file tpfh2on. It can be read into RELAP5 if specified by user input. The file contains a table based on pressure and specific internal energy in addition to the pressure and temperature based table. Another Thermal Fluid

Property (TPF) file, tpfh2o95, based on the 1995 Steam Tables from the International Association for the Properties of Water and Steam (IAPWS), IAPWS-95 [3] was built and can be accessed through user input.

In the 1980s, a variation of RELAP5, the Advanced Thermal Hydraulic Energy Network Analyzer (ATHENA) [5], was created to analyze fusion reactors. Naturally, it used hydrogen and helium fluids properties. Opportunities to analyze different types of reactors involving alternate fluids increased, and the fluids necessary to analyze them were added to ATHENA. In 1999, its fluid properties and other capabilities were merged into the DOE version of RELAP5, which already had 3D modeling ability, to create RELAP5-3D. Included among these fluids are molten salts, liquid metals, gasses for HTGRs, refrigerants, fluids for modeling experimental facilities, and even human blood [6].

Mass Error Reduction

The improved water property tables were incorporated to improve code calculation by having more accurate data (less error) in a wider variety of fluid states. Other ways of improving calculations involve reducing various kinds of errors (such as approximation, truncation, and roundoff) that are inherent in computer programming. Of particular interest is mass error.

Reducing mass error has become increasingly important for all reactor calculations. One means to reduce mass (and other) errors is to reduce the approximation error in the calculation of the fluid properties for a given fluid state. According to Sec. 3.2 of Vol. 1 [6], "The accuracy of these thermo-dynamic tables can be improved (under the penalty of increased storage requirements) by increasing the number of pressure and temperature points in the input data to the thermodynamic table generation subroutine. This can sometimes improve code performance by reducing mass error."

In 2010, a study was made of where best to increase the number of points based on accuracy needs for the range of operational and accident fluid conditions at that time [7]. The improvements to the grids of pressure and temperature or pressure and specific internal energy points, along with other improvements to the fluid property tables, have been adopted in the most recent code versions.

Another concept for reducing mass error is consistency between certain fluid property derivatives and the RELAP5-3D solution scheme. The code uses Taylor polynomials to replace derivatives of density and pressure in the finite difference form of the governing partial differential equations. The coefficients of these polynomials, E.G. $\partial T^S/\partial P$, are obtained from analytical formulas from the equation of state that are functions of temperature, pressure, and derivative quantities β, κ, and C_P. However, the solution scheme itself is linear; therefore, a linearized approximation of the derivative terms would be more consistent and might reduce mass error.

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A follow-on study [8] developed and tested a methodology to improve the consistency between the fluid property derivatives used in the numerical solution scheme and those in the linearized solution scheme itself. For a simple test case with the 1984 water property file, mass error was reduced when linear approximations to the derivatives of the Taylor polynomial coefficients were used.

A new study was performed with the H2ON water properties. For any fluid state point (U, P), the bounding rectangle is first located. Then linear interpolants for both the fluid property values and their derivatives are calculated from the values at the four corners.

Thereafter, a weighted average of the corresponding table lookup derivative value and the linear finite difference value is formed. A fixed weighting factor, ω, of 1.0 produces the pure derivative from the analytical formula. A fixed weighting factor of ω = 0.0 yields the pure linear approximant. Any fixed value between 0.0 and 1.0 is allowable, and in addition, two options that vary the weighting factor as a function of the location within the bounding rectangle were also programmed. Options ω = 1.0 and 0.0 have been verified to produce the same calculation as before the introduction of weighted averaging.

Comparisons were made among five choices of ω: 0.0, 0.5, 1.0, and the two variable options. To assess the impact of these options on mass error, the code was run with numerous test cases. These included two simple two-volume test cases that inject or extract fluid from a volume to vary the fluid state, the Edwards' pipe [9] blowdown, the standard typical PWR [10] test case, and others. The code performed well with all of the choices. Among the choices of ω, the options of ω = 0.0 and one of the variable options generally produced lower mass error than the others.

Consistent Fluid Capability

This capability has been submitted for inclusion in a future release of RELAP5-3D. The default value for the weighting remains ω = 1.0; thus it will have no effect on legacy calculations. The user will be able to optionally select a different weighting value by adding an extra word to the 120 - 129 hydrodynamic system cards as will be specified in Appendix A of Volume 2 of the manuals for that version of the code.

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