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ABSTRACT

Version 2.3 of the RELAP5-3D computer program includes all features and models previously available only in the ATHENA version of the code. These include the addition of new working fluids (i.e., ammonia, blood, carbon dioxide, glycerol, helium, hydrogen, lead-bismuth, lithium, lithium-lead, nitrogen, potassium, sodium, and sodium-potassium) and a magnetohydrodynamic model that expands the capability of the code to model many more thermal-hydraulic systems. In addition to the new working fluids along with the standard working fluid water, one or more noncondensable gases (e.g., air, argon, carbon dioxide, carbon monoxide, helium, hydrogen, krypton, nitrogen, oxygen, sf6, xenon) can be specified as part of the vapor/gas phase of the working fluid. These noncondensable gases were in previous versions of RELAP5-3D. Recently four molten salts have been added as working fluids to RELAP5-3D Version 2.4, which has had limited release. These molten salts will be in RELAP5-3D Version 2.5, which will have a general release like RELAP5-3D Version 2.3. Applications that use these new features and models are discussed in this paper.

INTRODUCTION

The RELAP5 series of codes has been developed at the Idaho National Laboratory for over 25 years under sponsorship of the U. S. Department of Energy, the U. S. Nuclear Regulatory Commission, members of the International Code Assessment and Applications Program, members of the Code Applications and Maintenance Program, and members of the International RELAP5 Users Group. Specific world-wide applications of the code have included simulations of transients of light water reactor systems such as loss of coolant, anticipated transients without scram, and operational transients such as loss of feedwater, loss of offsite power, station blackout, and turbine trip. RELAP5-3D (Ref. 1), the latest in the series of RELAP5 codes, extends the applicability of earlier versions to include an integrated multidimensional thermal-hydraulic/neutronic capability. In addition to calculating the behavior of a reactor coolant system during a transient, it can be used for simulation of a wide variety of hydraulic and thermal transients in both nuclear and nonnuclear systems involving mixtures of vapor, liquid, noncondensable gases, and nonvolatile solute. The 3D capability in RELAP5-3D includes 3D hydrodynamics and 3D neutron kinetics [the 3D neutronics is based on the NESTLE code (Ref. 2)]. RELAP5-3D was

recently modified to include all the ATHENA (Ref. 3) features and models that were previously only available in the ATHENA configuration. The ATHENA features and models are currently used primarily in Generation IV reactor applications, space reactor applications, and nuclear fusion applications.

RELAP5-3D is also used in a SCDAP/RELAP5-3D (Ref. 4) configuration that is designed to calculate for severe accident situations the overall reactor coolant system thermal-hydraulic response, core damage progression, and reactor vessel heatup and damage. RELAP5-3D (also true of SCDAP/RELAP5-3D) is also used in an integrated code system configuration consisting of RELAP5-3D and other codes such as FLUENT, CFX, and CONTAIN. The coupling of the codes in this configuration is coordinated using an executive program (Ref. 5) in concert with the Parallel Virtual Machine (PVM) message passing software. The coupling can be done explicitly or semi-implicitly. For example, the FLUENT/RELAP5-3D (Ref. 6) coupling configuration is designed to perform detailed 3D analyses using FLUENT's capability while the boundary conditions required by the FLUENT calculation are provided by the balance-of-system model created using RELAP5-3D. The FLUENT/RELAP5-3D coupling configuration is currently used primarily in Generation IV reactor applications. RELAP5-3D is also used for the thermal-hydraulic module in the real-time nuclear plant simulation code RELAP5-R/T (Refs. 7, 8, 9), which is used in training simulators at nuclear power plants around the world. There is also a visualization system for the various RELAP5-3D configurations, which is called the RELAP5-3D Graphical User Interface (RGUI) (Ref. 10).

This paper discusses Version 2.3 of the RELAP5-3D computer program that now includes all features and models that were previously available in the ATHENA configuration version of the code. They are new working fluids and a magnetohydrodynamic model. This paper also discusses four molten salts that have been added as working fluids to RELAP5-3D Version 2.4, which has had limited release. These molten salts will be in RELAP5-3D Version 2.5, which will have a general release like RELAP5-3D Version 2.3. Applications that use these new features and models will be discussed in this paper.

WORKING FLUIDS

In the 1980's, various working fluids began to be added to the ATHENA configuration (Ref. 11, 12) of the RELAP5 code. When RELAP5-3D began in the 1990's to extend the capability of RELAP5, the ATHENA configuration (with its various working fluids) was continued and enhanced in the RELAP5-3D code.

The working fluids that were previously available in RELAP5-3D and are still available to RELAP5-3D Version 2.3 are as follows: light water (specified as h2o), heavy water (d2o), 1984 light water (h2on), and 1995 light water (h2o95). The additional working fluids now available to RELAP5-3D Version 2.3 that were previously available only in the ATHENA configuration are as follows: ammonia (nh3), blood (blood), carbon dioxide (co2), glycerol (glycerol), helium (he), hydrogen (h2), lead-bismuth (bipb), lithium (li), lithium-lead (lipb), nitrogen (n2), potassium (k), sodium (na), and sodium-potassium (nak).

Four molten salts [LiF-BeF_2 (0.66 – 0.34) (ms1), $NaBF_4$-NaF (0.92 – 0.08) (ms2), LiF-NaF-KF (0.465 – 0.115 – 0.42) (ms3), and NaF-ZrF_4 (0.50 – 0.50) (ms4)] have recently been added as working fluids to RELAP5-3D Version 2.4.

The basic properties for light water (specified as h2o) are calculated from default thermodynamic tables (Ref. 13, 14, 15) that tabulate 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. These tables are based on the 1967 ASME Steam Tables (Ref. 13), which are calculated using the 1967 International Formulation Committee (IFC) Formulation for Industrial Use and is known as IFC-67. The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are based on correlations from the 1967 ASME Steam Tables (Ref. 13) and Schmidt (Ref. 16).

The basic properties for heavy water (specified as d2o) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 17, 18, 19) that tabulate 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. These tables are based on the formulation from the Atomic Energy of Canada Limited (AECL) (Ref. 18) and the WASP program (Ref. 19) from the National Aeronautics and Space Administration (NASA). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are based on correlations from FLOWTRAN (Ref. 20) and TRAC (Ref. 21).

The basic properties for 1984 light water (specified as h2on) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 22) that tabulate saturation properties as a function of temperature, saturation properties as a function of pressure, and single-phase properties as a function of pressure and specific internal energy. These tables are based on the 1984 U. S. National Bureau of

Standards and the National Research Council of Canada (NBS/NRC) Steam Tables (Ref. 22). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, temperature, three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure), and transport properties (viscosity, thermal conductivity, and surface tension). The transport properties are based on correlations from the National Research Council of Canada (NBS/NRC) Steam Tables (Ref. 22).

The basic properties for 1995 light water (specified as h2o95) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 23) that tabulate 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. These tables are based on the 1995 Steam Tables from the International Association for the Properties of Water and Steam (IAPWS) (Ref. 23); it is known as IAPWS-95. IAPWS also released an industrial formation in 1997 (known as IAPWS-97), which is not as accurate, but more efficient than the 1995 formulation. Since the tables in RELAP5-3D are only built once (during installation), the code uses IAPWS-95 because it is more accurate. The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) use tables based on correlations from the IAPWS-95 Steam Tables (Ref 23).

The basic properties for ammonia (specified as nh3) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 25, 26, 27) that tabulate 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. These tables are based on the formulation from Reynolds (Ref. 26) and were found to be in reasonable agreement with data in Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties are from formulations based on least square fits to data from Vargaftik (Ref. 27) and the Handbook of Chemistry and Physics (Ref. 28). The date of Reference 28 is 1973, which is the actual date of handbook that was used in this work (References 26 and 27 are also dated in the 1970's). More recent editions of these references could be used to improve the properties.

The basic properties for blood (specified as blood) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 29, 30, 31) that tabulate 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. These tables are based on the formulation from Daubert and Danner (Ref. 30) as well as Cooney (Ref. 31). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations based on least square fits to data from Daubert and Danner (Ref. 30) as well as Cooney (Ref. 31).

The basic properties for carbon dioxide (specified as co2) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 32, 33) that tabulate 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. These tables are based on the formulation from National Institute of Standards and Technology (NIST) (Ref. 33). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are based on tables and correlations from NIST (Ref. 33), Hejzlar (Ref. 34), Dostal (Ref. 35), Vesovic et al. (Ref. 36), and Daubert et al. (Ref. 37).

The basic properties for glycerol (specified as glycerol) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 29, 30) that tabulate 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. These tables are based on the formulation from Daubert and Danner (Ref. 30). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations based on least square fits to data from Daubert and Danner (Ref. 30).

The basic properties for helium (specified as he) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27, 38, 39) that tabulate 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. These tables are based on the formulations and least square fits to data from Reynolds (Ref. 26) and Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure,

saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations based on least square fits to data from Vargaftik (Ref. 27) and the Handbook of Chemistry and Physics (Ref. 28).

The basic properties for hydrogen (specified as h2) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27) that tabulate 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. These tables are based on the formulations and least square fits to data from Reynolds (Ref. 26) and Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations based on least square fits to data from Vargaftik (Ref. 27) and the Handbook of Chemistry and Physics (Ref. 28).

The basic properties for lead-bismuth (specified as bipb) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 40, 41, 42, 43, 44, 45, 46) that tabulate 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. These tables are based on Young's soft sphere model formulation (Ref. 42) and the Clausius-Clapeyron formulation. The formulations used were based on least square fits to data from Hultgren et al. (Ref. 44), Kutateladze et al. (Ref. 45), and Nesmeyanov (Ref. 46). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations based on least square fits to data from Touloukian et al. (Ref. 47) and Lyon (Ref. 48).

The basic properties for lithium (specified as li) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27, 39, 42, 43, 49, 50) that tabulate 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. These tables are based on Young's soft sphere model formulation (Ref. 42) and Reynolds' formulation (Ref. 26). The formulations used were based on fits to data from Young (Ref. 42), Blink (Ref. 50), and Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations and least square fits to data from Vargaftik (Ref. 27), Maroni et al. (Ref. 51) and Smith et al. (Ref. 52).

The basic properties for lithium-lead (specified as lipb) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 42, 46, 50, 53) that tabulate 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. These tables are based on Young's soft sphere model formulation. The formulation used was based on fits to data from Young (Ref. 42), Blink (Ref. 50), and Nesmeyanov (Ref. 46). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations and least square fits to data from Vargaftik (Ref. 27) and the Handbook of Chemistry and Physics (Ref. 28).

The basic properties for nitrogen (specified as n2) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27, 38, 39, 53, 54) that tabulate 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. These tables are based on the formulations and least square fits to data from Reynolds (Ref. 26), Vargaftik (Ref. 27), and Angus et al. (Ref. 54). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations based on least square fits to data from Vargaftik (Ref. 27) and the National Bureau of Standards (Ref. 55).

The basic properties for potassium (specified as k) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27, 42, 49, 56) that tabulate 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. These tables are based on Young's soft sphere model formulation (Ref. 42, 56) and Reynolds' formulation (Ref. 26). The formulations used were based on fits to data from Young (Ref. 42, 56) and Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal

expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations and least square fits to data from Vargaftik (Ref. 27) and the Handbook of Chemistry and Physics (Ref. 28).

The basic properties for sodium (specified as na) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27, 38, 42, 57) that tabulate 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. These tables are based on Young's soft sphere model formulation (Ref. 42, 57) and Reynolds' formulation (Ref. 26). The formulations used were based on fits to data from Young (Ref. 42, 57) and Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations from Gierszewski et al. (Ref. 58) and least square fits to data from Vargaftik (Ref. 27).

The basic properties for sodium-potassium (specified as nak) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 24, 26, 27, 38, 42, 56, 57, 59) that tabulate 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. These tables are based on Young's soft sphere model formulation (Ref. 42) and Reynolds' formulation (Ref. 26). The formulations used were based on fits to data from Young (Ref. 42, 56, 57) and Vargaftik (Ref. 27). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, and three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure). The transport properties (viscosity, thermal conductivity, and surface tension) are from formulations from Gierszewski et al. (Ref. 58) and least square fits to data from Vargaftik (Ref. 27) and Handbook of Physics and Chemistry (Ref. 28).

The basic properties for molten salt 1 (specified as ms1), molten salt 2 (specified as ms2), molten salt 3 (specified as ms3), and molten salt 4 (specified as ms4) are calculated from optional (activated by the user in the input deck) thermodynamic tables (Ref. 60, 61, 62, 63, 64, 65, 66) that tabulate 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 four molten salts are LiF-BeF_2 (0.66 – 0.34) (ms1), $NaBF_4$-NaF (0.92 – 0.08) (ms2), LiF-NaF-KF (0.465 – 0.115 – 0.42) (ms3), and NaF-ZrF_4 (0.50 – 0.50) (ms4), where the mole fraction of each component is given in parentheses. Molten salts ms1 and ms3 are generally referred to as Flibe and Flinak, respectively. These tables are based on a simplified equation of state, which is similar to the one used by Sabharwall et al. (Ref. 61) in an older version of ATHENA, and it was extended to higher pressures and temperatures for RELAP5-3D. The simplified equation of state is based on formulations from Powers et al. (Ref. 62), Cantor et al. (Ref. 63), Cantor (Ref. 64), Chase (Ref. 65), and Knacke et al. (Ref. 66). The properties and derivatives in the tables are saturation pressure, saturation temperature, specific volume, specific internal energy, three derivatives (isobaric thermal expansion coefficient, isothermal compressibility, and specific heat at constant pressure), and transport properties (viscosity, thermal conductivity, and surface tension). The transport properties are from formulations from Powers et al. (Ref. 62); Cantor et al. (Ref. 63); Cantor (Ref. 64); Bird, Stewart, and Lightfoot (Ref. 67); and Williams (Ref. 68).

MAGNETOHYDRODYNAMIC MODEL

The magnetohydrodynamic (MHD) effect, occurring when a fluid of high electrical conductivity moves through a magnetic field, is a common phenomenon in fusion reactor systems. A liquid metal flowing through a duct enveloped in a magnetic field experiences induced electromotive forces due to the qv x B forces acting upon the electrons in the conduction band, giving rise to electric currents in the liquid (q = electric charge, v = liquid velocity, B = magnetic force). Because of this energy conversion, there is an effective energy loss from the fluid flow. The RELAP5-3D model modifies the viscous energy loss coefficient (i.e., the friction loss coefficient) to account for this loss. Application of this model in RELAP5-3D is limited to pipe/annulus/pressurizer components that contain the working fluids lithium, lithium-lead, or sodium-potassium as subcooled liquid.

The model used to calculate the MHD effect in RELAP5-3D was developed at the Idaho National Laboratory (Ref. 69, 70, 71), and it is based on the work from the University of California at Los Angeles and the Argonne National Laboratory. The model allows calculation of the pressure gradient resulting from the MHD effect. The model allows a circular duct and a rectangular duct. The model allows a uniform (constant non-fringe volume) magnetic field and a non-uniform (spatially varying fringe volume) magnetic field. A fringe volume is a volume at the edge of the magnetic field, where the field is non-uniform. The magnetic field is assumed perpendicular to the duct. The dimensionless Hartman number and the wall conduction ratio are used in the model.

APPLICATIONS

The fluids helium and nitrogen in the code have been recently used in the scoping transient analysis of the very high temperature reactor (VHTR) concept (Ref. 72). Low and high

pressure loss of forced convection cooling transients were simulated.

The fluid helium in the code has been recently been used to analyze the helium gas-cooled fast reactor (GFR) concept (Ref. 73). The analysis was done to examine the potential for laminarization in the GFR design.

The fluid carbon dioxide in the code has been recently been used to support the development of a supercritical carbon dioxide cycle in the GFR concept (Ref. 74). One of the applications has been in the verification of the new compressor model in RELAP5-3D (Ref. 75).

The fluid lead-bismuth in the code has been recently used in the design and analysis of lead-bismuth cooled reactors (Ref. 41). The code was used in the design of corrosion experiments at the INL.

Various fluids and the magnetohydrodynamic model in the code have been used to analyze fusion loss-of-cooling accidents (Ref. 76). The code was used in the International Thermonuclear Experimental Reactor (ITER) international fusion design study.

CONCLUSIONS

This paper has discussed Version 2.3 of the RELAP5-3D computer program that now includes all features and models that were previously available in the ATHENA configuration version of the code. They are new working fluids and a magnetohydrodynamic model. This paper also discussed four molten salts that have been added as working fluids to RELAP5-3D Version 2.4, which has had limited release. These molten salts will be in RELAP5-3D Version 2.5, which will have a general release like RELAP5-3D Version 2.3. Applications that use these new features and models were discussed in this paper.

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