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Implementation of the Pure and Mixture Gases Properties in MARS-GCR

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1. Introduction

High temperature heat applications using nuclear energy become highlighted as a countermeasure to cope with dwindling fossil fuels. Advanced Generation IV reactors produce heats higher than conventional nuclear reactors. They are high temperature gas-cooled reactors (HTGRs), gas-cooled fast reactors (GFRs) and liquid metal-cooled fast reactors (LMFRs). High temperature nuclear heat can be used not only to replace the fossil fuel now used to supply industrial process heat but also to produce massive amount of hydrogen and synthetic fuel, while contributing high-efficiency electricity generation. A HTGR that produces heat up to 950^{o}C is a promising candidate in conventional and emerging process heat and electricity markets [1].

A high temperature nuclear system introduces an intermediate gas loop which transports nuclear heat to heat application systems or a high-efficiency electricity generation system by helium brayton or supercritical carbon-dioxide (CO_2) cycles. Various coolant options such as helium (He), CO_2, nitrogen (N_2) and gas mixtures are considered for them. In addition, argon (Ar), N_2 and H_2 have been widely used in high temperature industrial processes. This necessitates a need to model accurately the thermo-fluid performance of these pure and mixture gases systems.

In this study, a program, GasProp [2] has been developed to generate the thermodynamic and transport properties of the pure and mixture gases. And, the generated properties have been incorporated in the MARS-GCR code [3], a KAERI developed system thermal-hydraulics code, and the MARS-GCR modeling capability has been demonstrated.

2. Program GasProp

In 2010, US National Institute of Standards and Technology (NIST) released REFPROP [4] routines that calculates the thermodynamic and transport properties of industrially important fluid and their mixtures based on the most up-to-date pure fluid and mixture models. Thermodynamic properties of pure fluids are calculated by Helmholtz equation of state. Mixture properties are modeled using mixing rules to the Helmholtz energy of consisting mixture components. Transport properties are modeled with either fluid-specific correlations or friction theory method.

Using REFPROP routines, a program GasProp has been developed to generate the thermodynamic and transport properties of the pure fluids, CO_2, He, N_2, H_2, Ar and O_2, and the new fluid mixtures consisting of these pure fluids. Among various NIST modeling options, we used the NIST recommended models for pure fluids, which are known to generate the most accurate properties. For new mixtures, we applied Kunz and Wagner model as a mixing rule [5].

Program GasProp is designed to automatically setup the temperature and pressure ranges of a given fluid for property generation covering a range from the triple point to a supercritical state. Fine interval is provided near critical point to model the discontinuity in properties. Users can select a pure fluid or a mixture composition of concern in mole fraction, the upper limit of the temperature and pressure ranges and output format. It generates gas properties in a table form, an interactive form or a binary format that can be read and used by the MARS-GCR code.

Fig. 1 compares the properties of CO_2 gas generated by GasProp (open symbols) with those of REFPROP (closed symbols), where temperatures range from triple point to 2000K at critical pressure. It is shown that GasProp can reproduce almost the same properties as REFPROP. This applies to the other pure fluids.

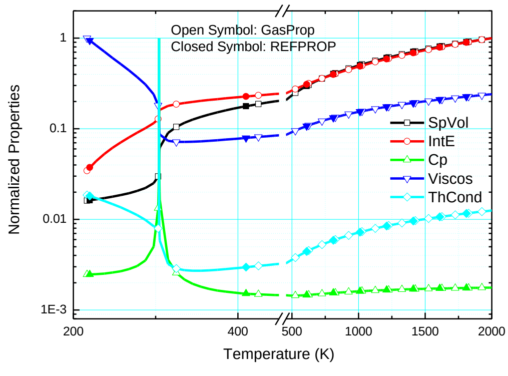

Fig. 1 Properties of CO_2 gas by GasProp and REFPROP

Due to pitfalls in the REFPROP models, some properties near triple point and for the mixture fluids containing either hydrogen or helium may result in negative or unexpected values. GasProp automatically detects and recalculates them by linear interpolation method. Uncertainties involved in user models can vary the results especially for the mixture gases. This causes some deviations in the GasProp properties from those of

REFPROP. Fig. 2 shows the deviation of the calculated properties by GasProp and REFPROP for He-CO_2 mixture gas having respective mole fractions of 0.2 and 0.8. Temperatures range from 300K to 1500K and pressures range from 0.5 to 15MPa. There are relatively large deviations in the thermal conductivity. Deviation increases when the temperature gets closer to 300K due to large modeling uncertainties involved near critical point, but still within 7%. Deviations in the other transport and thermodynamic properties are negligible.

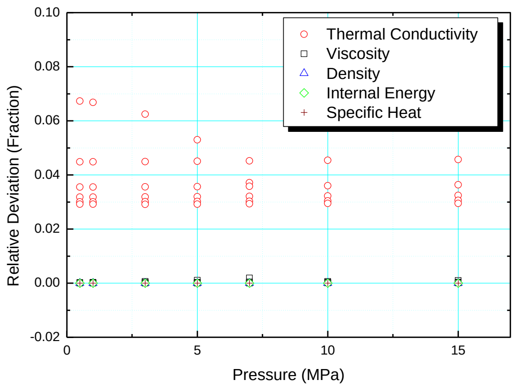

Fig. 2 Deviation of Transport Properties of He-CO_2 mixture gas by GasProp and REFPROP

3. Implementation of Gas Properties in MARS-GCR

MARS-GCR is an extended version of the MARS code [6], a multi-dimensional thermal-hydraulics system analysis code for water reactors. MARS-GCR V1 (hereinafter MARS-GCR) was developed in 2005 for application to HTGRs and GFRs. Improved models of the MARS-GCR code are those for the He and CO_2 properties as main system fluids, the gas convection heat transfer package, the radiation heat transfer and the contact heat transfer [3], which enabled a transient thermo-fluid analysis of the HTGRs and GFRs.

In order to enhance modeling capability for general gas-cooled systems, we implemented and updated the property models of the pure and mixture gases in the MARS-GCR code as main system fluids. MARS-GCR was modified to recognize these gases as main system fluids, then to read and interpolate the thermodynamic and transport property tables generated by the GasProp program. For the implementation of the property models, 36 routines of MARS-GCR were modified.

Modeling capability of the improved MARS-GCR was verified and validated by comparing the calculated properties by MARS-GCR with those of GasProp at corresponding states. Fig. 3 shows the deviations in the calculated parameters for the He-CO_2 mixture gas (20:80 mole fractions), where temperatures range from 500K to 1500K and pressures range from 0.5 to 15MPa. Both parameters, the multiplication of density, internal energy and specific heat (ρuCp) and the Prandtl number (Cpμ/κ), represent the modeling accuracy of MARS-GCR in thermodynamic and transport properties respectively. It is shown that the relative fractional deviation is below 5.e-4 within interpolation error and that the property models are well implemented in MARS-GCR.

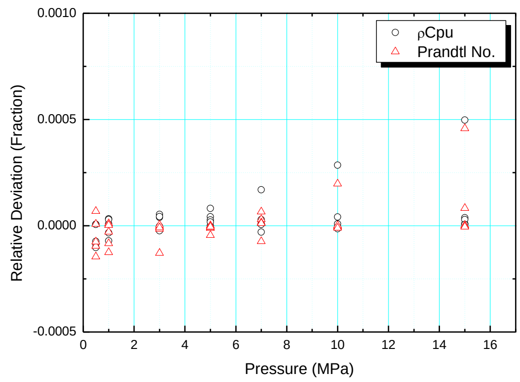

Fig. 3 Deviation of Thermodynamic and Transport Properties of He-CO_2 mixture gas by MARS-GCR and GasProp

4. Conclusions

The capability of the MARS-GCR code has been extended for application to the thermo-fluid analysis of general gas-cooled systems. The program GasProp was developed to generate the thermodynamic and transport property tables of various pure gases and gas mixtures of concern. Then, the MARS-GCR code was improved to read and interpolate these property tables.

With this improvement, MARS-GCR becomes capable of modeling not only the light and heavy water systems but also the gas-cooled systems with He, CO_2, H_2, O_2, N_2, Ar, He-N_2 mixture, He-CO_2 mixture or other user-defined gas mixtures as main system fluids.

As a future work, we will improve the accuracy of the property models near triple, saturated and critical states.

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