

Implementation of R134a Thermophysical Properties for MARS Application

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1. Introduction

MARS is a multi-dimensional thermal-hydraulic system analysis code based on RELAP5 developed by US-NRC [1]. Initially aimed for analyzing two-phase transients of nuclear power plant, various functions of this system code enabled to simulate other features such as thermal-hydraulic experiments. MARS requires 3 files for analysis: executable MARS file, input, and thermodynamic property file (tpf) for target fluids like light water or heavy water. Most experiments and scenarios were interested in behavior of water so original tpf's were sufficient enough for analysis.

As MARS application became wider, needs for other fluid properties rose since MARS do not have extra function to interpret foreign materials that does not have tpf. One way of solving this problem is to generate external tpf file and if successfully implemented, this methodology could widen the application of MARS to other fields of engineering. Previous study shows application of RELAP5 code to solar energy facility with molten salt (60% NaNO₃ and 40% KNO₃) as working fluid [2]. Based on external experimental correlations, thermodynamic properties of molten salt were evaluated as a function of pressure and temperature and those equations were used to generate tpf. Not all database was available for essential parts such as vapor phase properties so physical laws and approximations were applied. To validate external tpf, experimental values were compared with RELAP5 analysis. In nuclear field, simulation of other fluid is also important since many thermo-hydraulic experiments utilize other fluids like FC-72, R123, and R134a. These refrigerants are convenient than water for certain boiling experiments because they have low boiling point and could easily simulate high pressure environment of nuclear power plants. Experimental data is converted to water's case by applying dimensionless numbers originated from Pi theorem.

Thus, this study aims for tpf generation of R134a. The reasons for its selection is because R134a is currently used in refrigerator and frequently used in flow boiling experiment related with heat transfer coefficient and CHF measurement. The paper overviews composition of tpf, conventional tpfh2o

generation method, and new program structures and methods for generating tpf134a.

2. Methods for tpf Generation

This section reviews conventional method of generating tpfh2o. Other method of fitting was applied with R134a properties from NIST (national institute of standards and technology) standard reference data [3]. Fitted equations and their original data were compared with coefficient of determination. Execution file was also modified for application.

2.1 tpfh2o Generation with Gibbs function

FORTRAN program stgh2o generates tpf in binary format for given input file that consists of temperatures and pressures. Table I summarizes files required to compile the main program. The main process is recording six fundamental properties required to tpf (specific volume, internal energy, thermal expansion coefficient, isothermal compressibility, specific heat, and entropy) with Gibbs free energy value calculated from astem.f90 subroutines. Gibbs function is characterized as array of 'g' and each component is partial derivatives of Gibbs function according to pressure or temperature. Equation (1) to (6) shows Gibbs function array values and equations (7) to (12) indicate processes to calculate thermophysical properties with array values.

Gibbs function array 'g'

$$g(1) = G = U + PV - TS \quad (1)$$

$$g(2) = G_p = V \quad (2)$$

$$g(3) = G_{pp} = \left(\frac{\partial V}{\partial T} \right)_T \quad (3)$$

$$g(4) = G_T = -S \quad (4)$$

$$g(5) = G_{pT} = \left(\frac{\partial V}{\partial T} \right)_p \quad (5)$$

$$g(6) = G_{TT} = - \left(\frac{\partial S}{\partial T} \right)_p \quad (6)$$

Specific volume (V)
 $V = g(2)$ (7)

Internal energy (U)
 $U = G + TS - PV = g(1) - T \times g(4) - P \times g(2)$ (8)

Thermal expansion coefficient (β)
 $\beta = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P = g(5) / g(2)$ (9)

Isothermal compressibility (κ)
 $\kappa = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T = -g(3) / g(2)$ (10)

Specific heat (C_p)
 $C_p = T \left(\frac{\partial S}{\partial T} \right) = -T \times g(6)$ (11)

Entropy (S)
 $S = -g(4)$ (12)

Table I: FORTRAN files that compiles stgh2o.exe

	Functions
stgh2o.f90	Main program.
astem.f90	Calculates Gibbs function.
pastpd.f90	Calculates saturation properties.
fabend.f90	Execution abortion.
edate.f90	Date record.
eclock.f90	Time record.

Apart from binary tpf, additional file is generated in .pr format that records the contents of tpf in recognizable format. The 3 thermophysical property tables corresponds to 3 subroutines table3, table4, and table5 in stgh2o.f90 file.

File name, date and time, displays input values								
-Temperature: T_1, T_2, \dots, T_n								
-Pressure: P_1, P_2, \dots, P_n								
Fluid triple point, critical point								
Boundary: maximum/minimum value of temperature/pressure								
Saturation property Table based on input temperature (both phase)								
$T_1 \sim T_n$	Saturation pressure of T_1 to T_n	V	U	β	κ	C_p	S	
Saturation property Table based on input pressure (both phase)								
$P_1 \sim P_n$	Saturation temperature of P_1 to P_n	V	U	β	κ	C_p	S	
Table based on input pressure and temperature set (single phase)								
P_1	$T_1 \sim T_n$	Phase	V	U	β	κ	C_p	S
P_2	$T_1 \sim T_n$	Phase	V	U	β	κ	C_p	S
...								
P_n	$T_1 \sim T_n$	Phase	V	U	β	κ	C_p	S

Fig. 1. Structure of tpf shown in .pr format file.

2.2 Fitting Equations with R134a Database

Unfortunately, the coefficients used to calculate water's Gibbs energy are defined by experimental values and very complex to modify for other applications. Thus the six properties cannot be calculated with conventional method. Instead, external database was applied to form fitted equation that is function of pressure and temperature. The thermophysical property values for liquid and vapor differ greatly so the equations were separated with phase. Fitting was done with MATLAB's curve fitting tool. Units for temperature and pressure are K and Pa. ($220 < T < 373, 1.0E+5 < P < 4.0E+6$)

Specific volume [m^3/kg], $R^2=0.9924, 0.9917$
 $V(liq) = (2.649 \times 10^{-10})T^3 - (2.111 \times 10^{-7})T^2$ (13)
 $+ (5.763 \times 10^{-5})T - (3.169 \times 10^{-12})P + 0.004612$

$V(vap) = 0.0002423T + 27510P^{-1} - 0.08782$ (14)

Internal energy [J/kg], $R^2=0.9969, 0.9951$
 $U(liq) = 1403T - (2.037 \times 10^{-4})P - 182500$ (15)
 $U(vap) = 1.32T^2 - (1.04 \times 10^{-9})P^2$ (16)
 $- 0.009169P + 282400$

Specific heat [J/kg-K], $R^2=0.9969, 0.9954$
 $C_p(liq) = -4.679 \times 10^5 + 8644T - 0.02148P$
 $- 63.55T^2 + 0.0003203TP + 0.233T^3$
 $- (1.785 \times 10^{-6})T^2P - 0.000426T^4$ (17)
 $+ (4.401 \times 10^{-9})T^3P + (3.109 \times 10^{-7})T^5$
 $- (4.057 \times 10^{-12})T^4P$
 $C_p(vap) = 4447 - 25.33T - 0.01609P + 0.04383T^2$
 $+ 0.0001112TP + (1.619 \times 10^{-8})P^2$
 $- (1.872 \times 10^{-7})T^2P - (1.141 \times 10^{-10})TP^2$ (18)
 $+ (3.081 \times 10^{-15})P^3 + (1.97 \times 10^{-13})T^2P^2$
 $- (9.612 \times 10^{-18})TP^3 + (8.235 \times 10^{-23})P^4$

Entropy [J/Kg-K], $R^2=0.9996, 0.9953$
 $S(liq) = 4.866T - (2.373 \times 10^{-6})P - 331.4$ (19)
 $S(vap) = 619.1 + 8.017T - 0.002006P$
 $- 0.01913T^2 + (1.0 \times 10^{-5})TP - (2.683 \times 10^{-11})P^2$ (20)
 $+ (2.207 \times 10^{-5})T^3 - (1.447 \times 10^{-8})T^2P$
 $+ (3.638 \times 10^{-13})TP^2 - (1.699 \times 10^{-17})P^3$

Fitted equations were compared with original data with coefficient of determination (R^2) calculated. All data set showed R^2 value larger than 0.99.

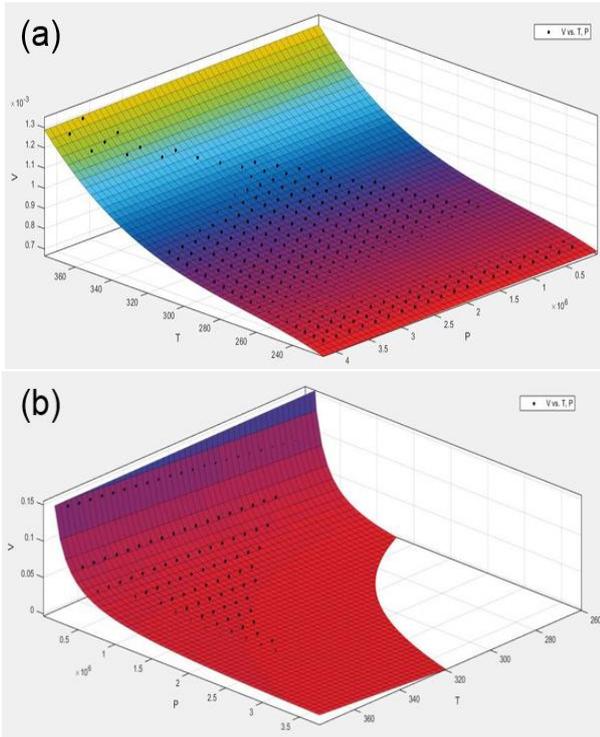


Fig. 2. Specific volume of (a) liquid with $R^2=0.9924$, (b) vapor with $R^2=0.9917$

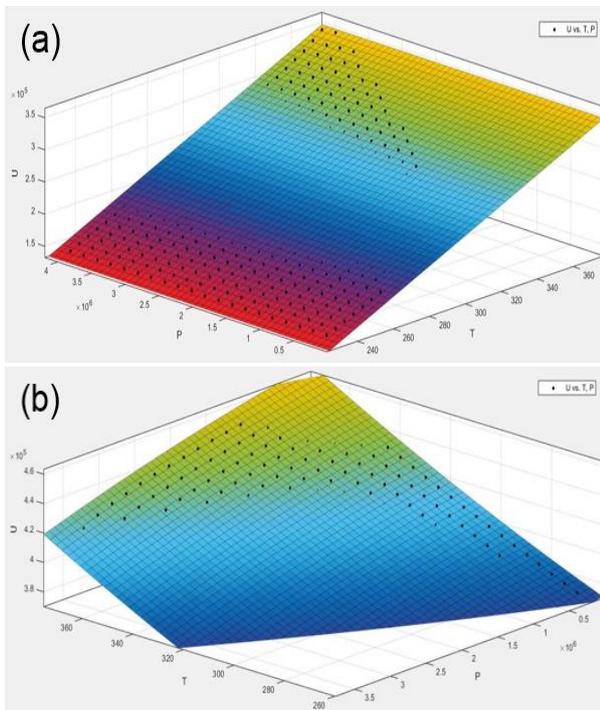


Fig.3. Internal energy of (a) liquid with $R^2=0.9969$, (b) vapor with $R^2=0.9951$

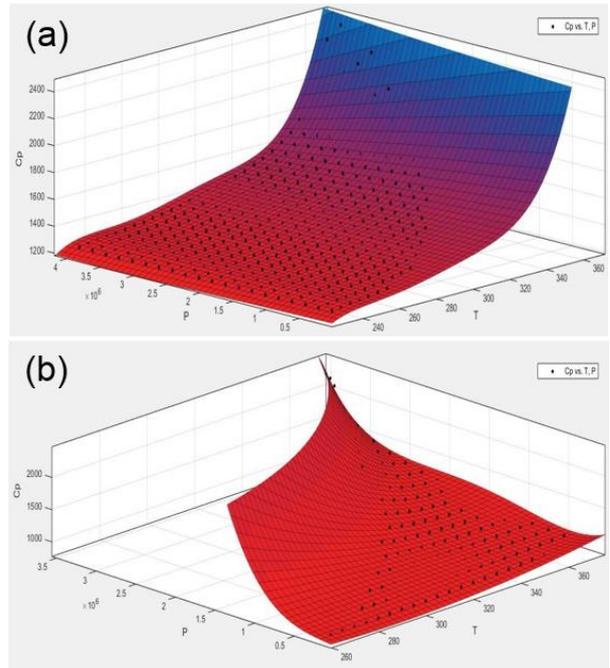


Fig.4. Specific heat of (a) liquid with $R^2=0.9969$, (b) vapor with $R^2=0.9954$

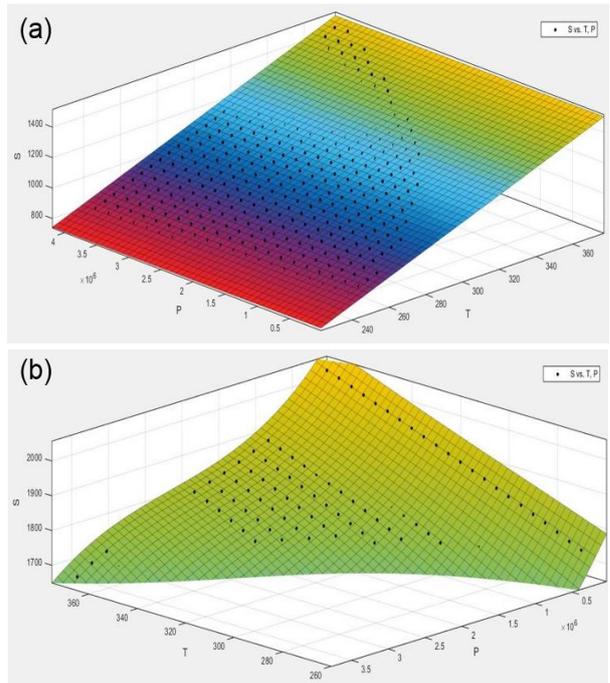


Fig. 5. Entropy of (a) liquid with $R^2=0.9996$, (b) vapor with $R^2=0.9953$

Database for thermal expansion coefficient and isothermal compressibility were unavailable. From definitions of equation (9) and (10), those properties could be calculated by partial derivative of specific volume. Thus, equation (13) and (14) were used to calculate thermal expansion coefficient and isothermal compressibility.

Thermal expansion coefficient [1/K]

$$\beta(liq) = \frac{(7.947 \times 10^{-10})T^2 - (4.222 \times 10^{-7})T + 5.763 \times 10^{-5}}{V(liq)} \quad (21)$$

$$\beta(vap) = \frac{0.0002423}{V(vap)} \quad (22)$$

Isothermal compressibility [1/Pa]

$$\kappa(liq) = \frac{3.169 \times 10^{-12}}{V(liq)} \quad (23)$$

$$\kappa(vap) = \frac{(2.751 \times 10^4)P^{-2}}{V(vap)} \quad (24)$$

Saturation curve is crucial for phase determination and saturation temperature or pressure calculation. Simplified form of Clausius-Clapeyron equation was used to form saturation curve of R134a (equation (25)). Phase determination was done by a simple algorithm. For a given temperature and pressure, if the saturation pressure is larger than given pressure, the phase was determined as vapor. Otherwise, it was determined as liquid.

$$P_{sat} = e^{\left(-\frac{2650}{T} + 22.29\right)} \quad (25)$$

$$T_{Sat} = \frac{2650}{22.29 - \ln P} \quad (26)$$

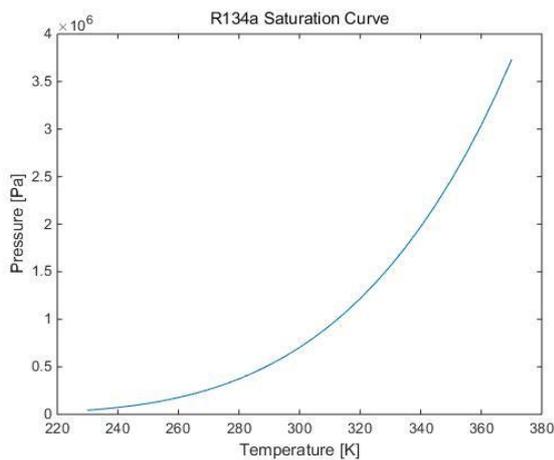


Fig. 6. Saturation curve of R134a.

2.3 Program modification to stgr134a

The fitted equations were directly implemented in the subroutines of stgh2o where table values of Fig. 1 are calculated, and saturation equation were also directly implemented in the phase determination subroutine. Further simplification made it possible to

generate tpr134a using only stgr134a.f90 (modified version of stgh2o), edate.f90, and eclock.f90.

Besides from tpr134a generation, external fluid registration procedure must be applied to the source code of execution file. Thermal conductivity, viscosity, and surface tension properties were also required to implement R134a in execution file so the equations were made with similar methods. Current study is in the phase of successful recognition of tpr134a by modified MARS execution file.

3. Conclusions

Generation methods of tpf were discussed. Conventional tpfh2o utilized Gibbs function to calculate the properties. However, since that method could not be applied to other fluids, fitting equation with temperature and pressure variables were applied from R134a property database. Direct implementation of these equations simplified the structure of main program. Further assessment is required to check whether the thermodynamic properties for R134a is valid, so that it may be implemented to analyze real case of thermal-hydraulic experiment.

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