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Development Of A Fast Method For Retrieving Thermodynamic Properties To Accelerate Transient Vapor Compression Cycle Simulation

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Development of a fast method for retrieving thermodynamic properties to accelerate transient vapor compression cycle simulation

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ABSTRACT

The most significant computational requirements for simulating vapor compression system models are associated with evaluation of thermodynamic properties. Reducing the computation time is particularly important for transient models because a number of properties and derivatives of properties need to be evaluated at each simulation time step. The typical approach for evaluating thermodynamic properties involves the use of complicated equations of state (EOS), which are utilized in standard software tools like RefProp and CoolProp. Overall computation speed can be significantly enhanced using fast property evaluation methods. This paper presents an improved method to quickly and accurately retrieve refrigerant properties which combines thermodynamic property relations, classical regression methods, and artificial neural networks (ANNs) in order to obtain simpler model structures. Since the proposed approach has an explicit functional form, it is able to avoid the computation time to find nearest points in a thermodynamic database. Speed and accuracy comparisons between the proposed method, RefProp, CoolProp, and popular interpolation schemes are provided for a wide range of pressures and enthalpies. Then, performance comparisons between the proposed and baseline methods for a transient heat exchanger simulation are provided.

1. INTRODUCTION

Dynamic modeling of vapor compression cycles (VCC) are particularly important for designing and evaluating controls and fault detection and diagnosis (FDD) algorithms. It is acknowledged that the computation time for evaluating refrigerant thermodynamic properties has a dominant effect on the overall simulation time for transient VCC models (Aute and Radermacher, 2014). For example, when a heat exchanger is modeled using a finite volume method, density and its partial derivatives with respect to pressure and enthalpy have to be calculated for all control volumes of a refrigerant and for each time step. The NIST RefProp database (Lemmon *et al*., 2002) and CoolProp (Bell *et al*., 2013), which is an open-source thermodynamic and transport properties library, are widely used tools for the evaluation of refrigerant properties. However, due to the nature of solving Equations of State (EOS) which requires numerical iterations, the computational time for a dynamic VCC simulation with direct use of RefProp or CoolProp can be very significant. Therefore, it is beneficial to develop a fast property calculation method for reducing the computational cost.

Various approaches have been developed and tested in the literature. Ding *et al*. (2005, 2007) proposed an implicit curving-fitting method for the calculation of pure and mixed refrigerant properties and tested it with R22 and R407C. Calculation speed was reported to be 100-1000 times faster than RefProp with a negligible error (less than 0.02%). Laughman *et al*. (2012) developed an interpolation-based method, which uses bi-cubic functions to interpolate the Helmholtz energy surface as a function of temperature and density. All other properties except for temperature and density were calculated based on the Helmholtz energy with high speed and accuracy. Kunick *et al*. (2008) described a spline interpolation method to calculate thermodynamic properties of liquid water and steam. A significant

computing time reduction was achieved with high accuracy. Aute and Radermacher (2014) utilized a regression method with polynomial forms to approximate thermophysical properties of a refrigerant. It was reported that the proposed curve fits are more than two orders of magnitude faster than RefProp based on P-h flash calculation. Sozen *et al.* (2007) applied artificial neural networks (ANN) to predict thermodynamic properties of R508b for two-phase and superheated region. Sencan and Kalogirou (2005) adopted ANNs to predict several thermophysical properties of mixed refrigerants. The number of hidden neurons was selected based on a parametric study.

From the literature, interpolation methods are numerically sensitive to the resolution of a thermodynamic property table due to the computation time to search nearest points in the thermodynamic database. ANNs are a potential alternative approach to avoid the searching time. Another benefit of applying ANNs is that partial derivatives of properties, which are necessary for a dynamic VCC simulation, can be calculated explicitly from an ANN model structure without including a numerical method such as the forward difference scheme. Existing studies have successfully demonstrated the performance of ANNs in predicting refrigerant properties by comparing ANN approaches with tools that utilized EOSs. However, for practical perspectives, it is more interesting to understand how ANN approaches perform compared with interpolation methods. In addition, it is important to demonstrate overall performance of different property evaluation methods when integrated within an overall VCC simulation.

This paper proposes a fast property evaluation method that combines thermodynamic relations, classical regression methods, and ANNs to retrieve density and its partial derivatives with respect to pressure and enthalpy in order to accelerate a transient VCC simulation where pressure and enthalpy are dynamic states. To obtain simpler model structures for numerical efficiency and accuracy, instead of obtaining ANN formulations covering the entire thermodynamic phase zones, ANN is only applied to the super-heated vapor region and is combined with simpler model structures for liquid and two-phase regions. The calculation speed of the proposed method is compared with baseline methods, i.e. Refprop and CoolProp that utilize EOSs, and CoolProp interpolation schemes. In addition, performance comparisons for a transient simulation of a heat exchanger are also provided.

2. METHODOLGY

This section describes a method for retrieving density and partial derivatives with respect to pressure and enthalpy. These property evaluations are needed in a dynamic model formulation for heat exchangers where the state variables are enthalpy and pressure. The domain of interest for a VCC simulation which uses R134a as a working fluid for case studies in this paper is shown in Figure 1. The upper and lower bounds of pressure are 1.2 MPa and 0.3 MPa, respectively. The values of 170 kJ/kg and 490 kJ/kg were selected as enthalpy bounds which correspond to 20 K subcooling and superheat temperatures. A separate model was developed for each zone to approximate density and partial derivatives. RefProp was used to collect data for model training.
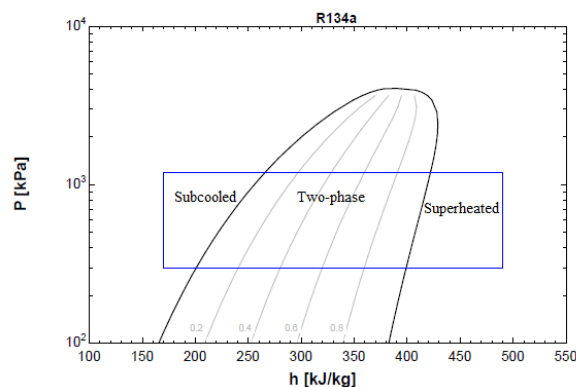

Figure 1: Property calculation region on P-h diagram

2.1 Functions for saturation lines
Density (kg/m^3) and enthalpy (J/kg) on the saturation lines can be described as functions of pressure (kPa). Saturation enthalpies are mapped for classifying the phase region associated with the dynamic state, i.e. pressure and enthalpy, of a transient VCC model. In addition, models for the saturation (liquid and vapor) densities are developed to calculate

density in the two-phase region as described in the next section. A non-linear regression model was capable of approximating those saturation properties with high efficiency and accuracy. The general non-linear function is represented in Equation (1).

$$f(t) = c_1 + \frac{c_2}{1 + e^{(c_3 t + c_4)}}$$

(1)

where, c_1, c_2, c_3, c_4 are coefficients to be estimated. Table 1 summarizes the coefficients for saturation density (kg/m³) and enthalpy (J/kg) of the refrigerant, i.e. R134a, within the pressure (kPa) bounds.

Table 1: Coefficients of logistic regression

Property, $f(P)$	c_1	c_2	c_3	c_4
h_f	3.0802E+05	-1.0576E+07	1.0212E-03	4.2825E+00
h_g	4.2891E+05	-1.0977E+07	1.5995E-03	5.4310E+00
ρ_f	9.6188E+02	2.7496E+04	8.1468E-04	4.1697E+00
ρ_g	6.6107E+02	-8.4183E+02	3.0976E-04	-1.2881E+00

2.2 Function in subcooled region

For the subcritical region, density in the subcooled zone mainly depends on temperature. That is, pressure dependency of density of liquid is negligible. Since enthalpy for liquid is primarily a linear function of temperature, density can be modeled with enthalpy only. We propose a linear affine model structure for modeling density for a subcooled liquid. Note that the partial derivative of the density with respect to enthalpy is a constant. The linear regression model of density (kg/m³) with enthalpy (J/kg) obtained for our case studies is $\rho = -0.002521 \times h + 1800$.

2.3 Functions in two-phase region

Density in the two-phase region changes dramatically near the saturated liquid line, which makes it hard to approximate using an empirical function. Although an ANN model structure could cover the two-phase region, the number of neurons would need to be large enough to capture the sudden change which makes a resulting model computationally inefficient. A more efficient method to retrieve density is to use simple thermodynamic relations.

Based on the definition of vapor quality, mass-based intensive properties, such as enthalpy (J/kg) and specific volume (m³/kg), can be calculated using combinations of saturated liquid and vapor properties as well as quality. Since density is the reciprocal of specific volume, it can be obtained by Equation (2) within the two-phase region:

$$\frac{1}{\rho} = \frac{1-x}{\rho_f} + \frac{x}{\rho_g}$$

(2)

where x is vapor quality, ρ_f and ρ_g are liquid and vapor saturation density, respectively. Quality is obtained from enthalpy and saturation enthalpies at a given pressure as follows:

$$h = h_f(1-x) + h_g x$$

(3)

where h_f, h_g are liquid and vapor saturation enthalpies, respectively. Since the saturation density and enthalpies are modeled with pressure as described in Section 2.1, density in the two-phase region can be readily calculated using Equations (2) and (3). In addition, note that exact formulas for partial derivatives can be derived from Equations (1) - (3).

2.4 Functions in superheated region

Unlike a subcooled liquid, the compressibility of a superheated vapor makes the density sensitive to a change of pressure. To approximate density in this region, a more complex function with respect to pressure and enthalpy is needed. In this work, an ANN model is built to map density (kg/m³) for the superheated vapor region. Three neurons

in the hidden layers was found to be appropriate for accuracy and computational speed. The Levenberg-Marquardt algorithm (LM) is used for training. The formulation is similar to that shown by Sozen *et al.* (2007). The resulting model for our case studies is represented in Equation (4):

$$\rho = \frac{84414.755}{1+e^{-C_1}} - \frac{174560.55}{1+e^{-C_2}} - \frac{147233.185}{1+e^{-C_3}} + 361626.961 \tag{4}$$

Where the C_i terms are functions of pressure and enthalpy as given in Table 2. Note that, since the obtained function is explicit with respect to pressure (kPa) and enthalpy (J/kg), exact formulas for partial derivatives can be derived.

Table 2: Coefficients of ANN function

$C_i = c_{1i}P + c_{2i}h + c_{3i}$			
Component (*i*)	c_{1i}	c_{2i}	c_{3i}
1	1.8088E-03	-5.1422E-06	8.9751E-01
2	-2.2093E-03	2.2892E-05	-5.1269E+00
3	-1.5584E-03	-6.7321E-06	1.1289E+00

3. CASE STUDY SETUP

3.1 Comparison of property call speeds
To demonstrate the computational benefit of the proposed method, it is compared with baseline methods, i.e. Refprop and CoolProp which solve EOSs, and an interpolation method. 10,000 samples from the bounded domain of P-h diagram were generated to test the accuracy and speed. The comparisons were carried out in the MATLAB environment.

CoolProp interpolation schemes, i.e. Tabular Taylor Series Extrapolation (TTSE) and Bicubic Interpolation, were selected as reference interpolation methods. For detailed descriptions of these methods, refer to Bell *et al.* (2013). It should be noted that the CoolProp tabular interpolation must be called in the low-level interface. The primary reason for the low-low level interface (in contrast to the high-level interface) is faster calculation speed enabled by avoidance of string operations which are computationally expensive. In this work, the CoolProp low-level interface was called in MATLAB through an access to a Dynamic-link library (DLL). Since both CoolProp high-level and low-level interfaces were used in this paper, to clarify the use of different methods, "CoolProp" in the following sections refers to the primary EOS-based high-level interface method.

In terms of accuracy, the absolute fraction of variance (R^2) was used to measure approximation errors, which is defined as follows:

$$R^2 = 1 - \left(\frac{\sum_j (t_j - o_j)^2}{\sum_j (o_j)^2} \right) \tag{5}$$

where *t* is the target value from RefProp and *o* is the output value from the proposed method.

3.2 Implementation in dynamic simulations
The primary goal of the proposed method is to speed up a dynamic VCC simulation. The proposed method and baseline methods were integrated with a dynamic condenser finite-volume model (Bendapudi *et al.*, 2008) for a chiller. The discretized refrigerant mass and energy balances of kth control volume are shown as below:

$$V_k \left(\frac{\partial \rho_k}{\partial P} \right)_{h_k} \frac{dP}{dt} + V_k \left(\frac{\partial \rho_k}{\partial h_k} \right)_P \frac{dh_k}{dt} = \dot{m}_{k-1} - \dot{m}_k \tag{6}$$

$$V_\mathrm{k}\left[h_k\left(\frac{\partial\rho_k}{\partial P}\right)_{h_k}-1\right]\frac{dP}{dt}+V_\mathrm{k}\left[h_k\left(\frac{\partial\rho_k}{\partial h_k}\right)_P+\rho_k\right]\frac{dh_k}{dt}=\dot{m}_{k-1}h_{k-1}-\dot{m}_k h_k-\dot{Q}_k \tag{7}$$

Where, V is the volume, $\dot{m}$ is the mass flow rate of the control volume interfaces, $\dot{Q}$ is the heat transfer between tube and the refrigerant.

Using 15 control volumes and the MATLAB ode45 solver, both a start-up and transient period due to a load change were simulated for comparisons of accuracy and speed. Comparisons to available measurements are also provided in the following section.

4. RESULTS

4.1 Property call comparison
Comparison of the predicted density for 10,000 samples between the proposed method and RefProp is shown in Figure 2. The R^2 value over the domain of interest is greater than 0.99. A comparison of computation speed for all of the different property evaluation methods is shown in Table 3.
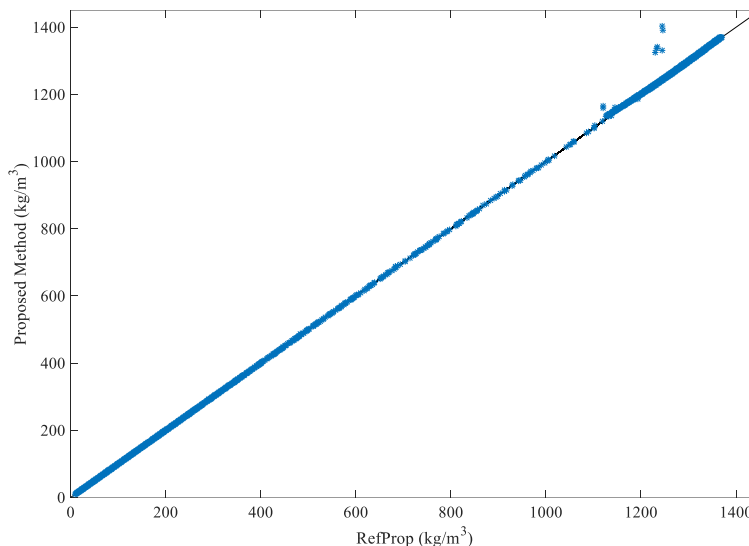

Figure 2: Comparison of predicted density between the proposed method and RefProp

Table 3: Speed comparison of density predictions for 10,000 P-h sample states

Methods	Computation time (s)	Computation time relative to proposed method (-)
Proposed method	0.007	1
CoolProp Bicubic	0.732	110.6
CoolProp TTSE	0.728	110.0
CoolProp EOS	1.499	226.5
RefProp	2.189	330.7

As expected, the proposed method to model density is much faster than RefProp, CoolProp and interpolation schemes, while maintaining high accuracy. Relatively high errors occurred in the subcooled region, where it is approximated by a linear function.

The partial derivatives of density with respect to pressure and density at sampled points are shown in Figures 3-4. The R^2 values for $\partial\rho/\partial P|h$ and $\partial\rho/\partial h|P$ are greater than 0.99 and 0.95, respectively.

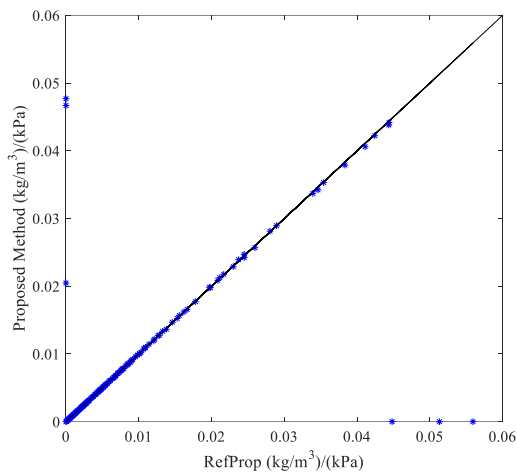17th International Refrigeration and Air Conditioning Conference at Purdue, July 9-12, 2018

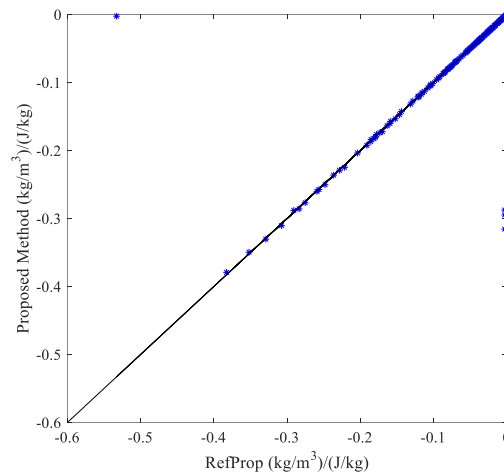**Figure 3:** Comparison of $\partial\rho/\partial P|h$

Figure 4: Comparison of $\partial\rho/\partial h|P$

Computational speed comparisons are listed in Table 4. It should be noted that when using RefProp, CoolProp, and interpolation schemes, partial derivatives of the two-phase region state are approximated by a central difference method. From the results, the proposed method shows much computational benefit. Relatively high errors occurred for partial derivatives in the subcooled region. This is because liquid density was approximated by a linear affine function of enthalpy such that the partial derivative with respect to pressure is always 0 and that with respect to enthalpy is always constant. On the other hand, the prediction error results from classification error. Due to curve fitting errors associated with mapping the enthalpy of saturated liquid, some states in the subcooled region may be classified as a two-phase condition which results in a higher value of partial derivative than that of RefProp.

It is interesting that in both cases, the CoolProp interpolation schemes are just 2 times faster than the EOS-based high-level interface. This is attributed to a different programming environment, MATLAB. If the interpolation method were called within Python or C++ environments, the speed would be expected to be much faster.

Table 4: Speed comparison of partial derivatives prediction

Methods	$\partial\rho/\partial P|h$		$\partial\rho/\partial h|P$	
	Computation time (s)	Computation time relative to proposed method (-)	Computation time (s)	Computation time relative to proposed method (-)
Proposed method	0.045	1	0.037	1
CoolProp Bicubic	1.713	38	1.701	46
CoolProp TTSE	1.719	38.1	1.714	46.3
CoolProp EOS	3.968	88	3.921	106
RefProp	6.983	154.8	7.026	189.9

4.2 Simulation results comparison
Dynamic simulations for a chiller shell-tube condenser were performed using the proposed and baseline methods. For the proposed method, other properties such as temperature and transport properties were retrieved using CoolProp. Figures 5-8 compare the simulation results of predicted condensing pressure and outlet condenser water temperature during start-up and load-change periods.

There are negligible differences in the model predictions when using property evaluations for the proposed and baseline methods. All simulation results are comparable with measurements which demonstrate the reliability of the tested dynamic heat exchanger model (Bendapudi et al., 2008). Speed comparisons are shown in Table 5. The dynamic model that employed the fast property evaluation method was more than 12 times faster than that using RefProp, 7 times faster than that using CoolProp, and more than 5 times faster than that using interpolation schemes. Although computation savings were not nearly as significant as the savings for just the property evaluations alone, they were still quite significant.

Table 5: Speed comparison of simulation

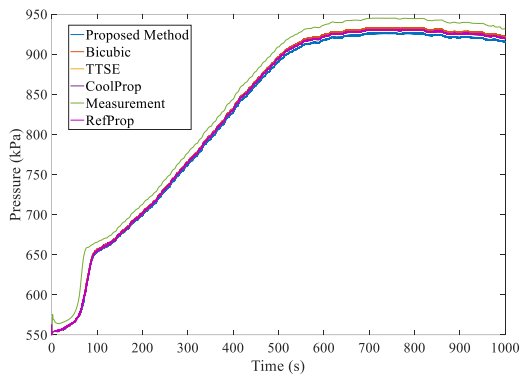| Methods	Start-up		Load change	
	Computation time (s)	Computation time relative to model employed proposed method (-)	Computation time (s)	Computation time relative to model employed proposed method (-)
Proposed method	303.7	1	170.5	1
CoolProp Bicubic	1581.6	5.2	962.8	5.6
CoolProp TTSE	1575.7	5.2	958.9	5.6
CoolProp EOS	2376.0	7.8	1508.5	8.8
RefProp	3784.9	12.5	2548.4	14.9

Figure 5: Validation of condensing pressure during a start-up period
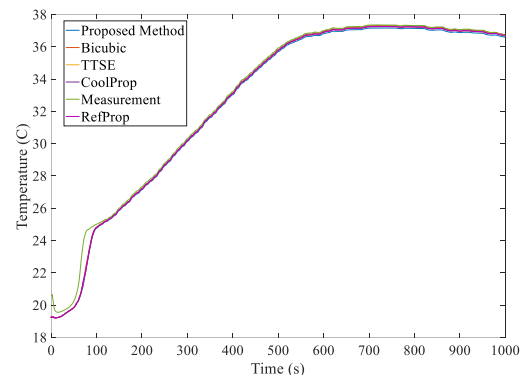

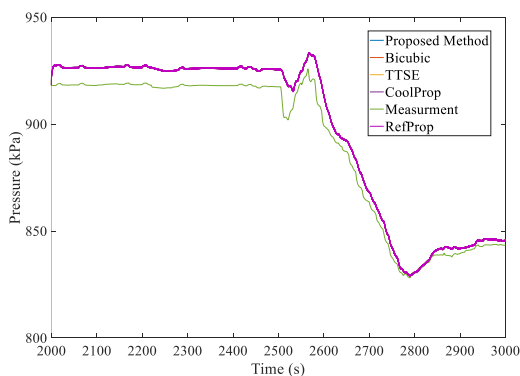**Figure 6:** Validation of water temperature during a start-up period

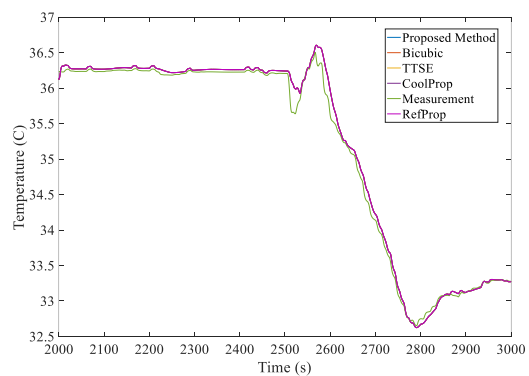**Figure 7:** Validation of condensing pressure during a load-change period

Figure 8: Validation of water temperature during a load-change period

5. CONCLUSIONS

This paper presents a fast method for calculating refrigerant density and its partial derivatives in order to accelerate a dynamic VCC simulation. The methodology combines thermodynamic relations, linear and non-linear regression equations, and ANNs in order to obtain simpler and hence computationally efficient models. Accuracy and speed were compared with popular refrigerant property libraries RefProp and CoolProp for R134a. Individual property calls were generally 100-300 times faster for predicting density, and 30-190 times faster for calculating partial derivatives. The presented method was integrated with a finite volume transient heat exchanger model to illustrate its computational benefits for an overall dynamic simulation. The speed up was greater than 5 times compared with CoolProp-based interpolation methods. The speed up could be further improved if other thermodynamic and transport properties are modeled.

NOMENCLATURE

C	Coefficient	(-)
h	Enthalpy	(J/kg)
$\dot{m}$	Mass flow rate	(kg/s)
P	Pressure	(kPa)
$\dot{Q}$	heat transfer	(W)
x	Quality	(-)
ρ	Density	(kg/m^3)
V	Volume	(m^3)

Subscript

f	Saturated liquid
g	Saturated vapor

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