2014

Standardized Polynomials for Fast Evaluation of Refrigerant Thermophysical Properties

Vikrant Aute
University of Maryland, United States of America, vikrant@umd.edu

Reinhard Radermacher
University of Maryland, United States of America, raderm@umd.edu

Standardized Polynomials for Fast Evaluation of Refrigerant Thermophysical Properties

Vikrant AUTE[1]*, Reinhard RADERMACHER[2]

[1]University of Maryland, Department of Mechanical Engineering,
College Park, MD, USA
Phone: +1 301 405 8726, Email: vikrant@umd.edu

[2]University of Maryland, Department of Mechanical Engineering,
College Park, MD, USA
Phone: + 1 301 405 5286, Email: raderm@umd.edu

* Corresponding Author

ABSTRACT

Steady state and dynamic simulation and optimization are a key step in the design of heating, ventilation, air-conditioning and refrigeration (HVAC&R) systems. It is well known that the computation time in such simulations is dominated by the refrigerant thermophysical property calculations. These calculations generally involve calculating all thermophysical properties given one or two independent parameters. Refrigerant thermophysical properties are typically calculated using some fundamental equations of state (EOS). The NIST REFPROP database is an industrially accepted standard for EOS implementation. Due to the iterative nature of the EOS calculations in REFPROP, the computation time is significant and sometimes not acceptable for optimization of HVAC&R systems. In this paper, a comprehensive approach for speeding up thermophysical property calculations is presented, including the functional forms as well as the implementation aspects. A set of polynomial functional forms are presented that allow for approximation of all the thermophysical properties in all the regions for a particular refrigerant (pure fluid or a blend) of interest. The polynomials can be easily scaled to make a judicious trade-off between computation time and accuracy. Analyses for refrigerants such as R1234yf, R32, R410A, R407C and R407F are presented. Using the proposed curve fits, the saturation properties for any refrigerant can be evaluated using less than 42 floating point operations (flops) and the flash calculations with less than 300 flops per property. The mean absolute error in predicted saturation properties is 0.001% and that of flash calculations is within 0.05%. Overall the individual property calculations are 100-5000 times faster than NIST REFPROP resulting in component and system simulation speed up factor of more than 100 for refrigerant blends. The use of two standardized and scalable functional forms for approximating all properties for all refrigerants of interest facilitates easy and robust implementation on a variety of steady state and transient simulation platforms as well as on hardware since limited data needs to be stored.

1. INTRODUCTION

The use of simulation based design and optimization methods is gaining grounds in the heating, ventilation, air-conditioning and refrigeration (HVAC&R) industry. This is especially true given the vast amount of computing power available on a mainstream desktop computer. Most design optimization tasks require iterative and repeated evaluation of different component and system models. The different components include heat exchangers, compressors, expansion devices and pipes. The systems can include single stage vapor compression systems, two-stage systems, etc. Each system level simulation for performance prediction requires numerous component model evaluations. It is well known that the computation time in such simulations is dominated by the refrigerant thermophysical property calculations. Thermophysical properties include thermodynamic and transport properties. These calculations generally involve calculating all thermophysical properties (e.g., density, quality, specific heat, etc.) and transport properties (e.g., viscosity, thermal conductivity), given one or two independent parameters such as pressure, pressure and enthalpy or temperature and density. The thermophysical properties are calculated using some fundamental equations

of state (EOS) and the NIST REFPROP database is a widely accepted standard for EOS implementation. Due to the iterative nature of the EOS calculations in REFPROP, the computation time is significant and sometimes not acceptable for repeated optimization. The required thermophysical properties can be categorized into various regions such as single phase liquid, two-phase, single phase vapor, saturation (dew and bubble) properties and the supercritical region.

This paper presents a comprehensive approach for fast evaluation of refrigerant thermophysical properties. The NIST REFPROP 9.1 (Lemmon et al., 2013) database, henceforth referred to as REFPROP, is considered as the standard for thermophysical property values. The goal of the proposed approach is to accurately reproduce REFPROP data while keeping the computational cost to a minimum. Whereas as fast evaluation of properties is beneficial in all fields that use refrigerant properties, the particular focus in this paper is on vapor compression systems and related components. The remainder of the paper is organized as follows: Section-2 gives some background on HVAC&R system simulation and summarizes the related literature, Section-3 explains the approach in detail and Section-4 provides some benchmarks followed by Conclusions in Section-5.

2. LITERATURE REVIEW

2.1 HVAC&R System Simulations

There are various methods for the simulation of generalized vapor compression system as summarized in Ding (2007) and Winkler et al. (2008). Based on the solution techniques for component-based simulations, majority of the methods involve the use of pressure, enthalpy and mass flow rate as the inlet state for each component model. Amongst all the component models, the heat exchanger models are responsible for a significant fraction of the total computation time due to a large number of property calculations. A typical finite volume heat exchanger simulation (Jiang et al., 2006) requires at least one flash calculation and two saturation line calculations for each segment (e.g., finite volume). Assuming that the heat exchanger models are based on a finite volume approach and the compressor is based on the ARI 10 coefficient map model, Table 1 provides a summary of the different thermophysical property calls required in a system simulation. Other components such as connecting pipes can be assumed to be a subset of heat exchangers.

Table 1: Types of thermophysical property calls in typical HVAC&R system simulation

Component Model	Property Calls	Comments
Compressor	$[T]_f = G(P)$ $[T]_g = H(P)$ $[T, \rho, x, Cp, s] = F(P, h)$ $[T, \rho, x, Cp, h] = S(P, s)$	$G(P)$, $H(P)$: calculate bubble and dew point temperature respectively, given pressure.
Heat Exchangers	$[T, \rho, x, Cp] = F(P, h)$ $[T, h, \rho, Cp, \mu, k]_f = G(P)$ $[T, h, \rho, Cp, \mu, k]_g = H(P)$	Includes both evaporator and condenser; Typically entropy values are not required unless second-law related analysis is carried out.
Expansion Device	$[T, \rho, x, Cp] = F(P, h)$	

As seen from Table 1, the most dominant property call is the P-h flash property call, followed by the saturation and transport properties. Numerical analysis using REFPROP also reveals that the P-h flash call (i.e., calculate properties given P and h) is the most computationally expensive calculation. The bubble and dew point properties are required for the evaluation of heat transfer, pressure drop and void fraction during two phase flow.

There are three key aspects to consider when approximating thermophysical property calculations, namely, (1) Speed, (2) accuracy and (3) consistency. In addition, there are various practical aspects that should be considered as well, such as (1) scalability, (2) development time, (3) implementation methods and (4) portability.

2.2 Literature Review

Refrigerant thermophysical properties can be fundamentally calculated using an appropriate Equation of State (EOS). There are various EOS presented in the literature for different refrigerants and some of these EOS are more computationally expensive to evaluate than others. The NIST REFROP Version 9.1 database is a widely accepted source for such EOS and refrigerant thermophysical properties calculation. It is also very well known that directly using EOS for property calculations incurs a huge penalty on the computation time of HVAC&R simulations. Over the last three decades, several researchers have proposed different methods for speeding up refrigerant thermophysical properties calculations. Based on the underlying mathematical technique, these methods can be categorized into the following groups: (a) simplified EOS, (b) implicit methods, (c) explicit methods, and (d) black-box methods.

The literature review presented here is limited to methods focusing on speeding refrigerant property calculations and does not cover methods based on simplified EOS. Black-box methods such as those using artificial neural networks are not discussed here, since they are more suitable for prediction of properties for new refrigerants and not for approximation.

One of the first published studies focusing on improving thermophysical properties calculation was conducted by Cleland (1986) and later extended in Cleland (1994). Cleland (1986) proposed the use of various polynomials forms for calculation of saturated liquid and vapor properties (mainly enthalpy, density and temperature) and for enthalpy and density as a function of saturation temperature and a given sub-cooling and superheat value. It is also one of the few papers that actually discuss the effect of using faster property routines on overall system simulation results. Their proposed forms are very easy to implement. It should be noted that some of their proposed equations are not purely polynomials and include exponential functions also which can be 20X more expensive to evaluate compared to polynomial terms.

Martin-Dominguez and McDonald (1993) proposed another explicit method for calculating saturated thermodynamic properties or R22. They propose the use of various polynomials forms that include logarithmic and exponential terms as well. In some cases, piecewise fits are developed. The reported prediction accuracy for most of the properties is 1% or better. There is no mention about the time comparison or computational complexity of their method.

Ding et al. (2005, 2007 and 2009) presented an implicit method for calculation of refrigeration thermodynamic properties and demonstrated application to R22 and R407C. The speed up ranged from 100 to 1000 compared to REFPROP. They make certain assumptions on the degree of sub-cooling for single phase calculations. Ding (2007) summarizes the requirements on refrigeration property calculations for reliable vapor compression system simulations. Various aspects such as speed, stability, reversibility (also referred to as consistency) and continuity are emphasized. The advantages and disadvantages of methods such as look-up tables, explicit regression and implicit formulations are discussed.

Kunick et al. (2008, 2009) presented a method based on spline interpolation which is significantly faster than REFPROP, while maintaining high accuracy and consistency. They reported speed up factor of 225 for $T(P,h)$.

Sieres et al. (2012) presented a hybrid approach for fast properties evaluation. The approach is referred to as Hybrid, because it is based on a combination of the implicit formulation developed by Ding et al. (2005, 2007) and their proposed explicit formulations for some of the derived properties. The reported extensively on the accuracies in terms of maximum and mean percentage deviation but there was no mention of the computational complexity or speed comparison for the approach. The reported mean percent deviation for the calculation of bubble temperature as a function of pressure for R1234yf and for R407C were 1E-04 and 7E-03 respectively.

Laughman et al. (2012) presented an interpolation based method for fast calculation of refrigerant properties. The method is based on the use of bi-cubic functions to interpolate Helmholtz energy as a function of temperature and density. Their proposed approach place particular emphasis on the consistency aspect. Sample results for superheated R134a property calculations demonstrated a speed up factor of 65, compared to conventional EOS method.

Based on the literature review, it can be concluded that the existing methods provide a speed up of at most 1000 compared to REFPROP database. There are very few studies that report the computational complexity, the accuracy and the effect on overall simulation results. This lack of information makes it challenging to conduct a comparative

evaluation existing methods on a fair basis. Further, typical REFPROP functions output multiple thermodynamic properties. There is no mention in the literature about how the comparison with REFPROP was carried out.

3. PROPOSED APPROACH

3.1 Overview

In the following sections, the proposed interpolation-based approach is described in more detail. The functions used to calculate properties along the saturation lines as a function of pressure are referred to as 1D functions, due to the single input. The functions that require two independent parameters (e.g., Pressure and enthalpy, pressure and entropy, etc.) are referred to as 2D functions. It is shown that all of the 1D functions can be approximated with very high accuracy using a single functional form. The same is true for all of the 2D functions as well. The proposed approach is an explicit interpolation based approach and uses a combination of curve fits and REFPROP.

The curve fits are developed for the most commonly used range of application based on a *P-h* diagram. As shown in Figure 1, the entire P-h domain is divided into four regions and different curve fits are developed for properties within each of these regions. In addition to these regions, there are two sets of curve fits for all the properties at the saturated liquid (e.g., bubble point) and the saturated vapor (e.g., dew point) state. Region-IV may be applicable to some refrigerants such as CO_2. The top boundary for Regions I, II and III is set at a pressure level such that the corresponding dew point is 3K below the critical point. The high and low enthalpy values are chosen such that 50K subcooling and 50K superheat is covered for the entire pressure range.

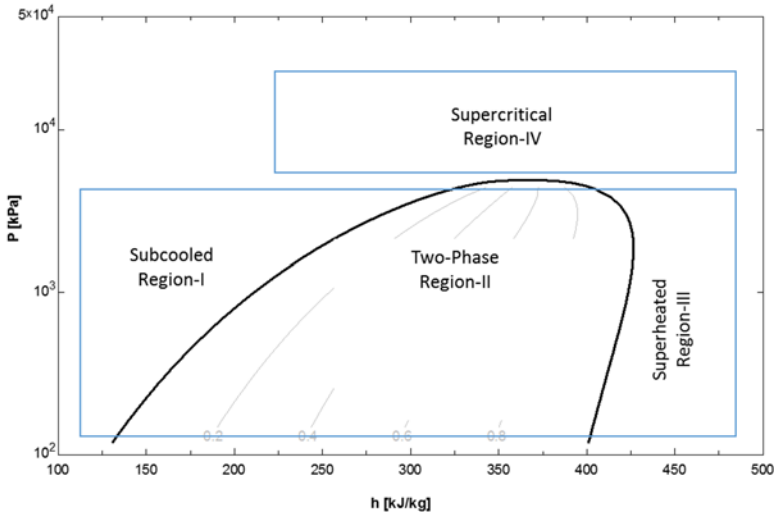

Figure 1: P-h plot for R410A, representing the various property approximation regions

3.2 Approximation of 1D Functions

In this section, the approximation of all the 1D functions, namely the calculation of thermophysical properties along the saturation lines as a function of Pressure, is discussed.

It can be easily shown that almost all of the thermophysical properties along the saturation lines can be easily approximated using a rational polynomial that is a function of Pressure. Rational polynomials and their properties have been extensively studied in the literature. In particular, Press et al. (2007) discuss their application for interpolation and extrapolation.

A generalized rational polynomial is represented in Equation 1.

$$f(x) = \frac{\sum_{i=0}^{m} a_i x^i}{1 + \sum_{j=1}^{n} b_i x^i} \tag{1}$$

where, x is Pressure, i and j are integers. During regression, using Equation 1, a family of curves can be generated by varying the values of m and n, applying transformations and by eliminating the denominator (i.e., setting it to 1). Rational polynomials are capable of representing more complex function behavior than just polynomials. As with polynomials, they are also easy to evaluate taking at most 2n floating point operations for a polynomial of order n in the numerator and denominator.

3.2 Approximation of 2D Functions

Thermophysical property functions in two dimensions are obviously more complex to approximate and it is a challenge to develop a single functional form that represents all the properties of interest. After a systematic analysis of various functional forms and numerical trials, the authors propose the use of Chebyshev Rational Polynomials (Abramowitz and Stegun, 1964) to approximate these functions. Chebyshev polynomials, named after the Russian mathematician Pafnuty Chebyshev, have been extensively studied in the literature. For example, Boehm (1964) and related references prove that for any continuous function on a given interval, there exists a Chebyshev polynomial that can approximate the said function. For a more recent reference on the use of Chebyshev polynomials for function approximations, the reader is referred to Press et al. (2007).

A generic Chebyshev function of one variable is shown in Equation 2.

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad T_0(x) = 1 \ , \ T_1(x) = x \tag{2}$$

There are several interesting aspects of the above function. Firstly, the equation is always defined on the interval [-1, 1]. So when using the above equation for interpolation, the input value x used in the source data for regression and in forward calculation should be mapped onto the interval [-1, 1].

Similarly, a Chebyshev function of two variables can be represented as shown in Equation 3.

$$f(x,y) = a_0 + a_1T_1(x) + b_1T_1(y) + a_2T_2(x) + c_1T_1(x)T_1(y) + a_2T_2(y) \tag{3}$$

In the above equation, a_i, b_i and c_i are coefficients and the order of the equation is said to be 2.

Correspondingly, a Chebyshev rational polynomial in two variables can be represented as:

$$f(x,y) = \frac{a_0 + a_1T_1(x) + b_1T_1(y)}{1 + a_1T_1(x) + b_1T_1(y) + a_2T_2(x) + a_2T_2(y)} \tag{4}$$

3.3 Key Characteristics of the Proposed Approach

The proposed approach has the following characteristics:

a. Standardized functional forms allow for easy implementation in hardware and software.
b. The resulting regression based on the proposed equations is a linear regression, thus avoiding any challenges associated with nonlinear regression.
c. Constant time calculations irrespective of whether the fluid is a pure fluid or a blend.
d. Closed form expressions for derivatives can be easily implemented, either through analytical derivation or automatic-differentiation. Derivatives are generally used in transient simulations.
e. Scalability – Various speed vs. accuracy trade-offs can be made changing the order of the polynomials.
f. Multiple property calculations can be parallelized.

g. In the worst case scenario, for the regions not covered by the proposed curve fits, the saturation fits can be used to determine the phase and then phase-specific codes from REFPROP can be invoked to gain roughly 4X speed improvement, compared to non-phase specific calls.
h. The worst case computational complexity for the 1D functions is 42 flops (floating point operations) and that for the 2D functions is 300 flops.

As with any other explicit interpolation based approach, the proposed approach has no provision built-in to guarantee consistency in property calculations. However, numerically it can be shown that the calculations are reasonably consistent for steady state and dynamic simulations of HVAC&R systems, given the very high prediction accuracy.

3.4 Implementation Aspects

The entire approach is implemented as a computer code and facilitates quick generation of curve fits for any new fluid or a user-defined blend. The prerequisite is that such a fluid or a blend must be supported by REFPROP. The source data for regression is generated using REFPROP for a given range of Pressure and Enthalpy values, or just pressure values for saturation properties. The number of initial points is chosen iteratively, starting with several thousand. Multiple curve fits based on varying polynomial order and transformations are generated for each thermophysical property of interest and their accuracy is evaluated by comparing the various regression metrics. The best curve fit is chosen for implementation after comprehensive error analyses. As shown in the literature (Reynolds, 2010), Horner's Rule is still the best method for implementing polynomials in a high level programming language.

4. ANALYSES & DISCUSSION

The accuracy and efficiency of the proposed approach is verified by comparing the predicted property values to REFPROP. Several refrigerants are chosen for the analyses, viz. R1234yf, R32, R410A, R407C and R407F. Table 2 shows the range of input values for which the interpolation polynomials used in the present analysis were generated. For brevity, the detailed functional forms and regression coefficients are not listed here. The r^2 value for all the 1D regressions was greater than 0.9999999 and that for 2D regressions was better than 0.99999. Representative functional forms and their complexities for R410A are listed in Table 3 for saturation properties and Table 4 for P-h flash calculations. The overall speed up compared to REFPROP is also listed in Table 2.

4.1 Individual Property Call Comparison

It should be noted that in a given component simulation, such as a heat exchanger, the refrigerant undergoes phase change and as such the required properties may fall in more than one of the four regions discussed in Section-3. Thus, for speed and accuracy comparisons, the entire P-h domain should be considered. The speed up is expected to be significantly higher when only individual regions are considered for comparison against REFPROP. For 1D functions, 10,000 points were chosen sequentially from the lower pressure value to the high pressure value. A similar matrix was created for 2D functions by choosing 1000 points in each dimension, giving a total of 1.0 Million points, spanning over a 50K subcooled state to 50K superheat state for each pressure level. The property calls are grouped as saturation property calls and a P-h flash calls. The calculated properties are those used in the heat exchanger model (Jiang et al., 2006) used for analysis in Section 4.2. For the P-h flash calls, multiple properties are evaluated at once, since REFPROP does the same.

Three key error metrics are used in the analysis, viz. (1) Maximum absolute error (MAE), (2) Maximum absolute percent error (MAPE) and (3) Mean or average absolute percent error (AAPE). The MAE metric gives the worst case accuracy and is relevant for quantities like Temperature, which are generally not compared on a percentage basis. The MAPE metric represents the worst case error as a percent of the true value. The AAPE metric indicates the spread of the absolute percentage errors over the entire domain. The MAPE and AAPE metrics together provide a good representation of the distribution of the errors.

Detailed error analyses was conducted for all the previously mentioned refrigerants, but for brevity, only the best and worst cases in terms of speed and accuracy are presented in Table 2. It is observed that for calculating the saturation properties of refrigerant blends, the speed up ranges from 1000 to 6000. The speed up for the P-h flash calculation ranges from 200 to 290. For the P-h flash calculations, relatively high errors occur very near to the saturated liquid line. This is because at qualities less than 0.05, the properties such as density change drastically. The curve fits

generated for this analyses are valid over the entire operating envelope for a given refrigerant for all applications. Application specific curve fits, such as saturation temperature between 0°C and 50°C for an air-conditioning only simulation can be developed to improve the accuracy and speed.

4.2 Comparison of Simulation Results

The proposed approach is implemented in a set of sub-routines that are then used in a heat exchanger simulation. A finite volume heat exchanger model (Jiang et al., 2006) is chosen for component speed up evaluation. Different types of heat exchangers are chosen for analyses. The simulations are conducted using the proposed approach for property calculations as well as with REFPROP. The deviation in the various predicted performance metrics are highlighted in Table 7. The refrigerant charge, pressure drop (DP) and the heat transfer coefficient (HTC) calculations generally require all the thermophysical properties and hence are a good metric to characterize the local deviations as well as any accumulated errors.

Table 2: Range of Applicability and Speed up over REFPROP 9.1

Refrigerant / Parameter	Pressure Range (kPa)	Enthalpy Range (kJ/kg)	Saturated Liquid Properties Speed Up	Saturated Vapor Properties Speed Up	Ph-Flash Speed Up
R1234yf	15-3200	16-445	279	107	27
R32	300-5500	140-560	292	252	64
R410A	400-4000	200-450	2269	1194	294
R407C	130-4000	150-470	6368	2681	219
R407F	160-4300	160-470	5998	3985	292

Table 3: Functional forms used for approximating R410A saturation properties

Property, $F(P)$	Functional Form (Numerator order / Denominator order)	Transformation	Approximate Complexity FLOPS
Cp_f, Cp_g, k_g, h_g, mu_g, ρ_f	20 / 0	-	41
h_f	5/6	-	24
k_f	8/8	-	34
mu_f	6/6	-	26
ρ_g	18 / 0	-	37
T_f	4/4	$ln(P)$	28
T_g	4/5	$ln(P)$	30

Table 4: Functional forms used for R410A *P-h* flash calculations

Property, $F(P,h)$	Functional Form (Numerator order / Denominator order)	Transformation	Approximate Complexity FLOPS
Region-I *: T, rho*	10 / 0	-	270
Region-I*: Cp*	9/10	-	110
Region-II*: T*	5/6	ln(P)	65
Region-II*: rho*	10/11	ln(P), ln(h)	125
Region-II*: x*	10/11	-	110
Region-III*: T, rho*	10 / 0	-	267
Region-III*: Cp*	10 / 0	$ln(h)$	275
Region-III*: s*	8 / 0	$ln(P)$, $ln(h)$	200

As observed from Table 7, there is practically no difference between the predicted simulation results obtained using the curve-fits versus those from REFPROP. As with previous analyses, the observed speed up is much higher for refrigerant blends as compared to pure fluids. It should be noted that the speed up is much less than the one observed

in Section 4.1 for individual property call comparisons. This is because the heat exchanger model invokes various other REFPROP routines that are not optimized for fast calculation. In the presented analyses, the most complex (e.g., highest order polynomials) functional forms were used to evaluate the best possible accuracies. Depending upon the application and the refrigerant of interest, various trade-offs can be made to arrive at a set of curve fits offering the most speed up.

Table 5: Accuracy of predicted saturation properties compared to REFPROP

Refrigerant / Property	Max. Abs. Error	Max. Abs. Percent Error	Abs. Mean Percent Error
R32 – Saturated Liquid			
T	2.88E-07	1.16E-07	2.5E-09
h	2.58E-03	1.68E-06	2.02E-08
ρ	1.69E-05	1.46E-06	1.28E-07
μ	0	2.89E-06	2.67E-07
k	4.2E-09	3.93E-06	1.60E-07
R32 – Saturated Vapor			
T	2.88E-07	1.16E-07	2.50E-09
h	6.84E-04	1.35E-07	1.90E-09
ρ	7.99E-08	4.02E-07	1.07E-08
μ	0	4.16E-07	1.62E-08
k	8.12E-08	1.33E-4	2.87E-05
R407F – Saturated Liquid			
T	1.55E-04	4.45E-05	3.04E-06
h	3.00E-01	1.93E-04	8.60E-06
P	6.91E-03	7.12E-04	4.79E-05
μ	2.35E-08	7.70E-03	2.08E-03
K	1.59E-05	2.54E-02	3.77E-03
R407F – Saturated Vapor			
T	2.85E-04	1.15E-04	6.55E-06
h	1.38E+00	3.44E-04	1.97E-05
P	4.2E-03	1.95E-02	6.71E-04
μ	1.12E-08	8.85E-02	6.93E-03
K	1.17E-06	3.14E-03	6.17E-04

Table 6: Accuracy of P-h flash calculation compared to REFPROP

Refrigerant	Max. Abs. Error	Max. Abs. Percent Error	Abs. Mean Percent Error
R32			
T	6.79E-04	2.68E-04	1.14E-05
x	7.3E-08	3.06E-04	5.87E-08
P	4.22E-02	5.14E-03	2.09E-04
Cp	9.93E+00	9.82E-01	2.08E-03
R407F			
T	3.49E-03	9.99E-04	4.83E-05
x	4.31E-04	6.02E+00	1.07E-02
ρ	1.00E+00	1.73E-01	2.8E-03
Cp	6.6E+01	3.28E+00	3.42E-03

Table 7: Heat Exchanger simulation comparison, REFPROP vs. proposed polynomials

HX Type	R1234yf Evap.	R32 Cond.	R32 Evap.	R404A Evap.	R407C Evap.	R407F Evap.	R410A Cond.	R410A Evap.
Speed Up Factor	65	10	105	646	119	109	100	105
Heat Capacity (%)	4.7E-05	1.9E-05	1.2E-05	1.1E-03	3.9E-04	1.5E-05	3.7E-03	1.7E-04
Sensible Capacity (%)	5.1E-05	1.9E-05	7.5E-06	1.2E-03	2.8E-04	2.8E-04	3.7E-03	1.7E-04
Ref. DP (%)	1.1E-04	2.4E-03	1.2E-05	6.3E-03	1.9E-03	1.0E-03	9.8E-01	3.7E-03
Ref. Outlet T Diff. (K)	6.0E-05	2.9E-05	5.4E-05	7.5E-04	9.2E-04	3.3E-05	4.4E-03	2.5E-04
Ref. Charge (%)	8.5E-05	7.5E-05	2.8E-06	5.1E-02	3.6E-04	3.4E-03	5.1E-02	7.0E-03
Ref. Two-ph. Charge (%)	1.6E-06	1.0E-04	1.2E-06	5.4E-02	2.3E-03	8.0E-03	7.3E-02	7.8E-03
Ref. Vapor Charge (%)	1.8E-04	4.1E-06	2.7E-05	4.4E-03	2.8E-03	7.5E-04	6.8E-05	2.6E-04
Ref. Two phase HTC (%)	3.5E-06	4.0E-04	7.9E-07	1.2E-02	6.6E-04	6.1E-03	3.0E-01	5.0E-03
Ref. Vapor HTC (%)	2.7E-05	4.0E-06	6.5E-05	9.9E-02	5.8E-03	6.2E-04	6.6E-05	1.8E-02

5. CONCLUSIONS

Accurate, fast and robust refrigerant thermophysical property calculations are the key to success in simulation and optimization of HVAC&R systems. In such simulations, majority of the computation time is dominated by the property calculation codes. An interpolation based approach to speed up property calculations was presented. A rational polynomial functional form was proposed to represent all the thermophysical properties as a function of saturation pressure. A similar standardized equation based on Chebyshev polynomials was proposed for calculating properties as a function of pressure and enthalpy. Both functional forms result in a linear regression and facilitate easy implementation. Based on the numerical analyses, it is observed that the proposed curve fits are more than two orders of magnitude faster than REFPROP and are two orders of magnitude more accurate than other speed up methods reported in the literature. The examples presented in this paper were based on P-h flash calculations, but the same functional forms can be used for other independent properties, their partial derivatives as well as other refrigerants including CO_2.

NOMENCLATURE

Cp	Specific heat	(J/kg K)
h	Enthalpy	(J/kg)
k	Thermal conductivity	(W/mK)
P	Pressure	Pa
s	Entropy	(J/kg K)
T	Temperature	K
x	Quality	(–)
ρ	Density	(kg/m³)
μ	Dynamic viscosity	(Pa.s)

Subscripts

f	Saturated liquid
g	Saturated vapor

REFERENCES

Abramowitz, M., Stegun, I. A., eds., 1964, Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables, National Bureau of Standards, Applied Mathematics Series 55.

Boehm, B., 1964, Functions whose best rational Chebyshev approximations are polynomials, *Numerische Mathematik*, Vol. 6, No. 1, pp. 235-242.

Cleland, A.C., 1986, Computer subroutines for rapid evaluation of refrigerant thermodynamic properties, *International Journal of Refrigeration*, Vol. 9 (8), pp. 346–351.

Cleland, A.C., 1994, Polynomial curve-fits for refrigerant thermodynamic properties: extension to include R134a, *International Journal of Refrigeration* Vol. 17 (4) (1994) 245–249.

Ding, G., 2007, Review: Recent developments in simulation techniques for vapor-compression refrigeration systems, *International Journal of Refrigeration*, Vol. 30, pp. 1119-1133.

Ding, G., Wu, Z., Liu, J., Inagaki, T., Wang, K., and Fukaya, M., 2005, An implicit curve-fitting method for fast calculation of thermal properties of pure and mixed refrigerants, *International Journal of Refrigeration*, Vol. 28, No. 6, pp. 921-932.

Ding, G., Zhao, D., Wu, Z. and Han, W., 2009, Extension of the implicit curve-fitting method for fast calculation of thermodynamic properties of subcooled refrigerants, HVAC&R Research Journal, Vol. 15, pp. 875-888.

Jiang, H., Aute, V., Radermacher, R., 2006, CoilDesigner: A general-purpose simulation and design tool for air-to-refrigerant heat exchangers, International Journal of Refrigeration, Vol. 29, pp. 601-610.

Kunick, M., Kretzschmar, H. J., and Gampe, U., 2009, Fast calculation of thermodynamic properties in process modeling using spline-interpolation, *17th Symposium on Thermophysical Properties*, Boulder.

Laughman, C., Zhao, Y., Nikovski, D., 2012, Fast Refrigerant Property Calculations Using Interpolation-Based Methods, *International Refrigeration and Air Conditioning Conference at Purdue*, July 16-19, 2012, Purdue, Indiana.

Lemmon, E.W., Huber, M.L., McLinden, M.O. 2013, NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.1, National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg.

Martin-Dominguez, I. R., McDonald, T. W., 1993, Correlations for some saturated thermodynamic and transport properties of refrigerant R-22, *ASHRAE Transactions* 99 (1) (1993), pp. 344-348.

Press, W. H., Teukolsky, S.A., Vetterling, W. T., Flannery, B. P. (2007), "Section 3.4. Rational Function Interpolation and Extrapolation", *Numerical Recipes: The Art of Scientific Computing (3rd ed.)*, New York: Cambridge University Press, ISBN 978-0-521-88068-8

Reynolds, G., 2010, Investigation of different methods of fast polynomial evaluation, *MS Dissertation*, The University of Edinburgh.

Sieres, J., Varas, F., Martinez-Suarez, A., 2012, A hybrid formulation for fast explicit calculation of thermodynamic properties of refrigerants, *International Journal. of Refrigeration*, Vol. 35, pp. 1021-1034.

Winkler, J., Aute, V., Radermacher, R., 2008, Comprehensive investigation of numerical methods in simulating a steady-state vapor compression system, *International Journal of Refrigeration*, Vol. 31, pp. 930-942.

Zhao, D., Ding, G., Wu, Z., 2009, Extension of implicit curve-fitting method for fast calculation of thermodynamic properties of refrigerants in supercritical region", *International Journal of Refrigeration*, Vol. 32, pp.1615-1625.

ACKNOWLEDGEMENT

The research presented in this manuscript was supported by the Integrated Systems Optimization Consortium at the University of Maryland.