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TR2026-109 July 14, 2026

Abstract

Continuing efforts to improve the energy efficiency and reduce the environmental impact of air-conditioning systems based on vapor-compression cycles have motivated the expanding use of zeotropic refrigerant mixtures. These mixtures exhibit temperature glide and phase-dependent composition variation, which must be accounted for in system-level modeling and dynamic simulation during equipment design and performance analysis processes. This work analyzes interpolation-based thermophysical property models for cycles with these zeotropic refrigerant mixtures that are designed to balance accuracy and computational cost. We examine the standard formulation of governing equations in pressure/specific enthalpy coordinates and identify associated limitations for mixture behavior, and then propose a framework using pressure/vapor quality as an alternative set of coordinates. We describe the accompanying changes to the conservation equations used to describe the system behavior to improve numerical efficiency and robustness in dynamic simulations of vapor-compression cycles using zeotropic refrigerants, and demonstrate the efficacy of these approaches in the simulation of both the standalone refrigerant properties and the overall cycle dynamics.

Purdue Air-Conditioning and Refrigeration Conference 2026

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ABSTRACT

Continuing efforts to improve the energy efficiency and reduce the environmental impact of air-conditioning systems based on vapor-compression cycles have motivated the expanding use of zeotropic refrigerant mixtures. These mixtures exhibit temperature glide and phase-dependent composition variation, which must be accounted for in system-level modeling and dynamic simulation during equipment design and performance analysis processes. This work analyzes interpolation-based thermophysical property models for cycles with these zeotropic refrigerant mixtures that are designed to balance accuracy and computational cost. We examine the standard formulation of governing equations in pressure/specific enthalpy coordinates and identify associated limitations for mixture behavior, and then propose a framework using pressure/vapor quality as an alternative set of coordinates. We describe the accompanying changes to the conservation equations used to describe the system behavior to improve numerical efficiency and robustness in dynamic simulations of vapor-compression cycles using zeotropic refrigerants, and demonstrate the efficacy of these approaches in the simulation of both the standalone refrigerant properties and the overall cycle dynamics.

1. INTRODUCTION

Refrigerant property models constitute the basis of vapor compression cycle models, which are increasingly employed in the design and optimization of HVAC equipment. The growing adoption of these modeling approaches has been driven by increasing system complexity, as advanced architectures are required to achieve higher efficiencies and reduce environmental impact (McLinden & Huber, 2020). Among the various model components, thermophysical refrigerant property models are particularly critical, as they provide important structure for the governing equations and account for a significant portion of the computational burden. These property calls represent more than 70% of the computational effort of a dynamic model (Aute & Radermacher, 2014), and recent results suggest that a single simulation of 5 minutes of system operation can make as many as 500 million property calls. Since the objective of these simulations is to resolve the time evolution of the underlying differential-algebraic equations (DAEs) describing the system over extended operating periods (e.g., 24 hours or longer), computational efficiency becomes a key challenge.

A key aspect of contemporary vapor compression system design, driven by efforts to mitigate their environmental impact, is the increasing use of low global warming potential (GWP) zeotropic refrigerant blends. These mixtures are attractive because they can significantly reduce the equivalent greenhouse gas emissions associated with system operation. However, zeotropic mixtures exhibit thermodynamic behavior that differs fundamentally from that of pure fluids or azeotropic blends. In particular, they are characterized by temperature glide during phase change and by composition variation between liquid and vapor phases within the two-phase region. These phenomena influence overall cycle performance by altering heat transfer characteristics and the distribution of refrigerant mass throughout the system. As such, there is a need for thermodynamic property models capable of accurately representing mixture behavior.

The growing importance of these zeotropic refrigerant mixtures has motivated extensive research into the development of high-accuracy thermophysical property models for system-level applications. While REFPROP (National Institute of Standards and Technology (NIST), 2018) is widely regarded as the standard tool for evaluating the thermophysical properties of refrigerant mixtures, its design objectives differ from those of the property models employed in this work. Specifically, REFPROP emphasizes predictive capabilities based on fundamental, physics-based formulations

for a broad range of fluid mixtures, without a primary emphasis on computational efficiency. In contrast, refrigerant mixtures used in commercial HVAC equipment are typically well-characterized, and system-level simulations require property models that achieve both high accuracy and computational efficiency. A comprehensive overview of the system-level implications of refrigerant mixtures in vapor-compression cycles is provided by Radermacher & Hwang (2005), while more recent work by Wang et al. (2024) investigates the integration of such mixtures into organic Rankine cycles, which share similar thermodynamic foundations with the vapor-compression systems considered here.

A substantial body of work has thus focused on the development of interpolatory models for refrigerant properties to support dynamic simulation. For example, Li (2021) describes the use of quadratic spline-based approaches for modeling the thermophysical properties of pure fluids and azeotropic mixtures, while work by Ma et al. (2018) presents a neural network-based framework for pure and azeotropic refrigerant property prediction in comparable applications. The present work builds upon the methodologies introduced in (Laughman & Qiao, 2021) and (Laughman et al., 2024) by extending them to the treatment of zeotropic mixtures within a similar computational framework as that presented in the 2021 paper. In addition, the data-cleaning architecture developed in (Laughman et al., 2024) is adopted to ensure the quality and consistency of the underlying thermophysical data.

While previous work is focused primarily on the development of computationally efficient and accurate interpolatory methods for pure fluids and azeotropic refrigerant mixtures, the present work is centered squarely upon the topic of characterizing zeotropic refrigerant mixtures in vapor-compression cycles. Models used for pure fluids are not directly applicable in this setting because they are not able to describe the effects of varying composition in the two-phase region. The present work approaches this problem by studying the coordinates used to describe the thermophysical refrigerant properties, and determining that the use of pressure and vapor quality have distinct advantages over the more traditional coordinates of pressure and specific enthalpy. We also follow the implications of this coordinate change upon the formulation of the physics-based conservation equations, and demonstrate that these modifications can result in effective dynamic cycle simulations with high-glide fluids.

This work develops thermophysical property models of the refrigerant R454C, which is composed of 21.5% R32 and 78.5% R1234yf by weight, as it is a high-glide mixture that has applications in a variety of commercial applications, and also applies this refrigerant model to a vapor-compression cycle. In Section 2, we describe the theoretical background of vapor-liquid equilibrium for both pure fluids and mixtures, and motivate the change of thermodynamic coordinates for interpolatory numerical methods. In Section 3, we illustrate the different formulation of the dynamic model required for these changes of coordinates, and then demonstrate the efficacy of these models at capturing the refrigerant property characteristics and describing the dynamic behavior of a cycle with this refrigerant in Section 4. We conclude the paper with a brief review of results in Section 5.

2. REFRIGERANT MIXTURE MODELS

In the development of interpolation-based refrigerant property models, it is necessary to consider both the intended application and the trade-off between model accuracy and the number of required coefficients. Physics-based models of vapor-compression cycles must capture fluid behavior in both single-phase and two-phase regions when formulating the governing conservation equations. Pressure P and specific enthalpy h are commonly selected as state variables for this purpose, as key performance metrics such as cooling capacity and compressor work are naturally expressed in these coordinates. Additionally, the use of (P, h) state variables avoids numerical difficulties associated with saturation boundaries that arise from the nonlinear relationship between pressure and temperature.

These governing equations are typically expressed as a system of differential-algebraic equations (DAEs), in which the conservation of mass, momentum, and energy is formulated in terms of the time derivatives of P and h, which serve as the primary model states. A wealth of literature demonstrates that models formulated in these coordinates can achieve high fidelity with respect to experimental measurements of vapor-compression system performance. To understand the common use of these coordinates for cycle models, as well as the accompanying limitations when describing zeotropic refrigerant mixtures, it is helpful to consider the fundamental approaches used to model two-phase fluids.

The (P, h) coordinates are convenient for modeling pure fluids, as can be seen by considering the characteristics of vapor-liquid equilibrium (VLE). VLE is achieved by minimizing the Gibbs free energy of the fluid, defined as

$$G = H - TS, \tag{1}$$

where G is the extensive Gibbs free energy, H is the extensive enthalpy, T is the temperature, and S is the extensive entropy of the fluid. The differential dG can be used to formulate the VLE conditions, since $dG = 0$ at a minimum for a given set of conditions. This differential can be expressed as

$$dG = -SdT + VdP + \sum_i \mu_i dN_i, \tag{2}$$

where V is the size of the control volume, μ_i is the chemical potential of the i^{th} component of the fluid, and N_i is the number of moles of component i, and is derived by using the fundamental thermodynamic identity for dU (Smith et al., 2005). This relation indicates that G can be parametrized as a function $G(P, T, \{N_i\})$, and that the chemical potential μ_i is defined for component i as

$$\mu = \left(\frac{dG}{dN}\right)_{T,P}. \tag{3}$$

For a single-phase pure fluid at thermodynamic equilibrium, the pressure P and temperature T are uniform, and the molar Gibbs free energy g is equal to the chemical potential μ. In extending this to a two-phase system with a mixture of coexisting liquid and vapor phases, the equilibrium condition $dG = 0$ requires that the chemical potentials of the two phases be equal, i.e., $\mu^l(P, T) = \mu^v(P, T)$. As the chemical potential of each phase is a function solely of temperature and pressure, this equality constrains the system such that there exists a unique temperature at which phase equilibrium is satisfied for a given pressure. Consequently, the thermodynamic state of the system along the coexistence curve can be expressed as a function of pressure alone.

This pressure-only dependence applies both to the bubble saturation curve, which represents the intersection of the liquid region and the two-phase region, as well as to the dew saturation curve, which represents the intersection of the vapor region and the two-phase region. We can therefore represent the properties along these curves, such as the specific enthalpy, as $h_{bub}(P)$ and $h_{dew}(P)$. As the equality of the chemical potentials μ^l and μ^v constrains the behavior of the bulk fluid in the two-phase state to be dependent only upon the states of the liquid and vapor components for a pure fluid, which are determined by the pressure alone, the bulk specific enthalpy in the two-phase region can be written as the molar-weighted combination of the two phases by using the vapor quality q, i.e.,

$$q = \frac{N^v}{N^l + N^v} \tag{4}$$

$$h = qh_{dew}(P) + (1 - q)h_{bub}(P), \tag{5}$$

and other properties in the two-phase region (e.g., specific entropy, specific volume) can be represented similarly.

While the conditions of VLE for pure fluids are relatively simple, the component-wise interactions for refrigerant mixtures make the calculation of VLE more complex. As the state of the mixture moves from single-phase regions to the two-phase region, the differences in volatility of the components result in changes in the phasic composition with respect to the bulk composition. Adopting the terminology used by the REFPROP documentation, we refer to the mole fraction of liquid for component i as x_i and the mole fraction of vapor for component i as y_i. The presence of multiple components thus necessitates the use of an array of liquid mole fractions $\{x_i\}$ as well as an array of vapor mole fractions $\{y_i\}$.

The conditions for VLE for mixtures are identical to those of a pure fluid and are provided in Equation 2 for which $dG = 0$, but the inclusion of multiple components commensurately increases the number of constraints that must be satisfied. In considering the constraints implied by this equation, thermodynamic equilibrium necessitates that the pressure and temperature for all components must be equal (thus forcing dT and dP to be zero), and also that the phasic chemical potentials for each component μ_i^l and μ_i^v must be equal. If this condition is not met, the transfer of a small amount of energy from liquid to vapor would result in an energy change of $dG = \mu_i^{(v)}\delta n_i + \mu_i^{(l)}(-\delta n_i) = (\mu_i^{(v)} - \mu_i^{(l)})\delta n_i > 0$, which cannot be the case at VLE.

The material balances for each component and the bulk fluid impose a range of constraints on VLE conditions that affect the fluid behavior. These constraints can be written as

$$\sum_{i=1}^{N_c} z_i = 1 \qquad \sum_{i=1}^{N_c} x_i = 1 \qquad \sum_{i=1}^{N_c} y_i = 1 \tag{6}$$

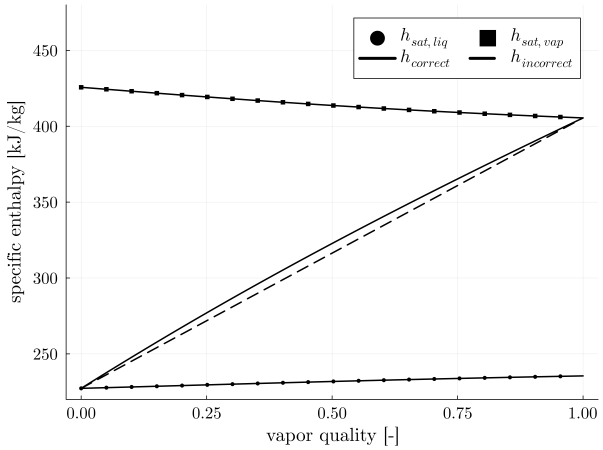

Figure 1: Saturated liquid and vapor enthalpies for R454C at 1 MPa, as well as the bulk enthalpy computed correctly (Equation 12) and under the incorrect assumption of quality independence (Equation 5).

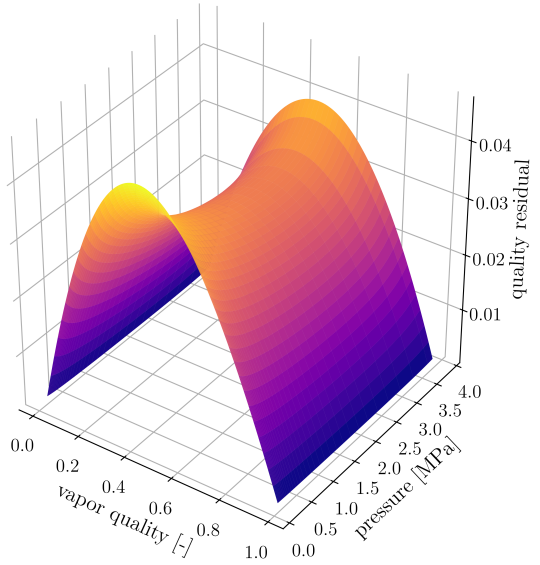

Figure 2: Deviation $q_{mix}(P,q) - q_{pure}(P)$ over the two-phase region for R454C over a range of pressures, demonstrating the need to correctly compute vapor quality.

where the phasic molar fractions vary throughout the two-phase region. These constraints imply that

$$\sum_{i}^{Nc}(y_i - x_i) = 0 \tag{7}$$

By writing the equilibrium ratio of a substance, defined as

$$K_i = \frac{y_i}{x_i}, \tag{8}$$

we can express the material balances for component i in the two-phase region under the assumption of a constant bulk composition of the fluid in a closed volume as

$$z_i = (qK_i + (1-q))x_i, \tag{9}$$

which can be reformulated as

$$x_i = \frac{z_i}{(1-q) + qK_i}. \tag{10}$$

Using the material balance constraint from Equation 7, we can re-express that as

$$\sum_{i=1}^{Nc} \frac{z_i(K_i - 1)}{1 + q(K_i - 1)} = 0. \tag{11}$$

This constraint on the material balances was first published by Rachford & Rice (1952), and must be enforced at VLE for mixtures. This implies that the vapor quality for every component i in a mixture is the same under the given assumptions; while the individual x_i and y_i for each component varies, the value of q for every component is identical.

These varying compositions mean that the bubble and dew specific enthalpies are also a function of the composition, rather than just the pressure. As a result, a flash computation for a fixed bulk composition $\{z_i\}$ can compute the saturated liquid enthalpy $h^l(P,T,\{x_i\})$ and the saturated vapor enthalpy $h^v(P,T,\{y_i\})$ at VLE. These material balances can be used to reformulate these enthalpy expressions by using the vapor quality q to express $h^l(P,q)$ and $h^v(P,q)$ and thereby compute the mixture enthalpy, i.e.,

$$h = qh^v(P,q) + (1-q)h^l(P,q). \tag{12}$$

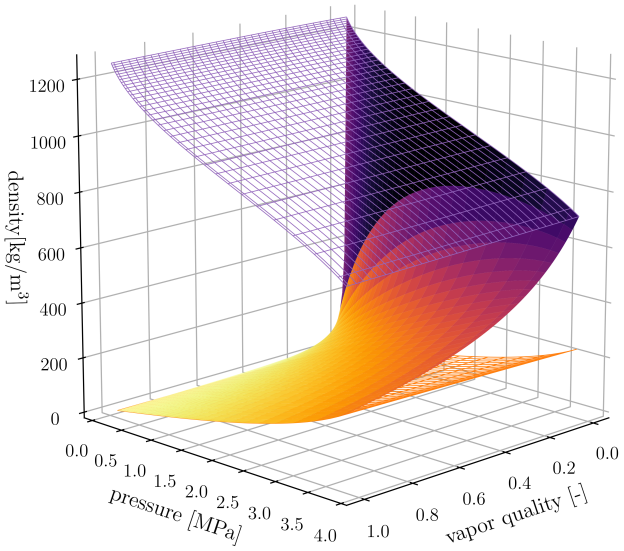

Figure 3: The refrigerant density function for R454C in the two-phase region, with the saturated liquid density function above and the saturated vapor density function below.

Figure 1 illustrates the importance of accounting for the dependence of properties on vapor quality. This figure plots the variation of both the saturated liquid enthalpy $h^l(P,q)$ and the saturated vapor enthalpy $h^v(P,q)$ for a constant pressure of 1 MPa through the two-phase region. While these lines would be horizontal for a pure fluid, their dependence on quality implies that the calculation of the bulk quality via Equation 12 will be different than the calculation under the assumption of quality independence (Equation 5). There is thus significant deviation between the actual bulk enthalpy, shown by the solid curve, and the incorrectly calculated bulk enthalpy, shown by the dashed curve.

The extent of this deviation over the entire two-phase region for R454C is illustrated in Figure 2. This plot of the pointwise difference between the vapor quality as computed from Equation 5 and the actual quality shows that the two qualities are the same at $q = 0$ and $q = 1$, but that the deviation between the two qualities peaks around a quality of 0.5, and is more pronounced at low and high pressures. This observation reinforces the importance of using the correct quality calculations for refrigerant mixtures.

In addition, the calculation of vapor quality from pressure and specific enthalpy is more computationally expensive for a mixture than for a pure fluid. The definition of vapor quality in terms of the specific enthalpies is given by

$$q = \frac{h - h_{bub}(P,q)}{h_{dew}(P,q) - h_{bub}(P,q)}, \tag{13}$$

which requires nonlinear iterations to calculate q given values of pressure and specific enthalpy. While Newton's method is often effective at solving such problems, the large number of refrigerant property calls that require the use of these iterations in the case where P and h are the states of the model can cause these models to be computationally slow, thus motivating the use of alternate state variables for the system. In comparison, the use of P and q as state variables eliminates these iterations, making their choice quite appealing.

Practical considerations relating to the numerical characteristics of the interpolated property functions also motivate the study of the underlying functions from which the properties are calculated, as can be explained through Figure 3. This figure shows the density of R454C in the two-phase region over a wide range of pressures and vapor qualities in the middle blue surface, as well as the saturated liquid density over the same region as a transparent grid above the density surface, and the saturated vapor density over the same region as a transparent grid below the density surface. As the density function has large derivatives in the two-phase region, a large number of coefficients will need to be stored to directly characterize this function to a high degree of accuracy throughout the two-phase domain. In comparison, the saturated liquid and vapor density functions have much smaller derivatives in the two-phase region,

and we expect that an interpolating function for these properties will require a much smaller number of coefficients to achieve a comparable level of accuracy. The use of these saturated liquid and vapor properties to describe the refrigerant mixture characteristics thus has tangible benefits when building a numerically parsimonious representation of refrigerant properties in the two-phase region.

This analysis suggests that the choice of P and h for thermodynamic coordinates, and consequently the states of the conservation equations, may impose significant limitations on the accuracy and numerical performance of dynamic simulations of vapor-compression cycles. The benefits of using P and q as thermodynamic coordinates for refrigerant mixtures are evident, but require a reformulation of the conservation equations to take full advantage of their benefits.

3. CYCLE MODELS

In the previous section, we discussed the implications of using pressure P and specific enthalpy h as thermodynamic coordinates of a dynamic model of a vapor-compression cycle that uses a refrigerant mixture as a working fluid, and suggested the use of P and vapor quality q as a more numerically efficient set of coordinates for these complex fluids. This change in coordinates requires the reformulation of the conservation equations using this alternate set of states for the purposes of model implementation. We will first describe the balance equations using the conventional (P, h) coordinates, and then illustrate the changes need to change to (P, q) coordinates.

For one-dimensional compressible flow with constant cross-sectional area, neglecting gravitational effects and axial heat conduction, the governing equations of mass, momentum, and energy can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial G}{\partial z} = 0 \tag{14}$$

$$\frac{\partial G}{\partial t} + \frac{\partial}{\partial z}\left(\frac{G^2}{\rho} + P\right) = -\frac{4\tau_w}{D_H} \tag{15}$$

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial (Gh)}{\partial z} = \frac{4Q''}{D_H} \tag{16}$$

where ρ, G, P, e, h, τ_w, D_H, and Q'' denote density, mass flux, pressure, specific internal energy, specific enthalpy, wall shear stress, hydraulic diameter, and wall heat flux, respectively. These equations form the basis of many dynamic vapor-compression cycle models.

In conventional dynamic HVAC cycle models, pressure P and specific enthalpy h are commonly selected as the thermodynamic state variables. This choice is largely dictated by the thermodynamic property formulation: when refrigerant properties are parameterized directly in terms of (P, h), other quantities such as density and temperature can be evaluated without requiring an additional thermodynamic inversion. As a result, the governing equations can be discretized in a form that is both numerically convenient and computationally efficient. A representative formulation of this type was presented by Qiao et al. (2015), where the one-dimensional conservation equations were discretized using P and h as the primary state variables.

In the present work, however, the refrigerant property routines are reformulated using pressure P and vapor quality q as the independent variables. As the property model is now naturally expressed in these coordinates, it is also natural to adopt (P, q) as the thermodynamic state variables in the governing equations. This choice eliminates the need to repeatedly recover q from (P, h), which would otherwise require the solution of a local nonlinear equation in the two-phase region for zeotropic mixtures. The change in state variables is therefore not only mathematically straightforward, but also aligned with the structure of the property model itself.

The finite-volume method is used to discretize the governing equations because it preserves the conservation form and has been widely used for thermal-fluid systems. As in many previous dynamic cycle models, a staggered-grid arrangement is adopted to decouple the mass and energy balances from the momentum balance. In this arrangement, the mass and energy equations are evaluated in the volume cells, while the momentum equation is evaluated in the flow cells between adjacent control volumes, as illustrated in Figure 4.

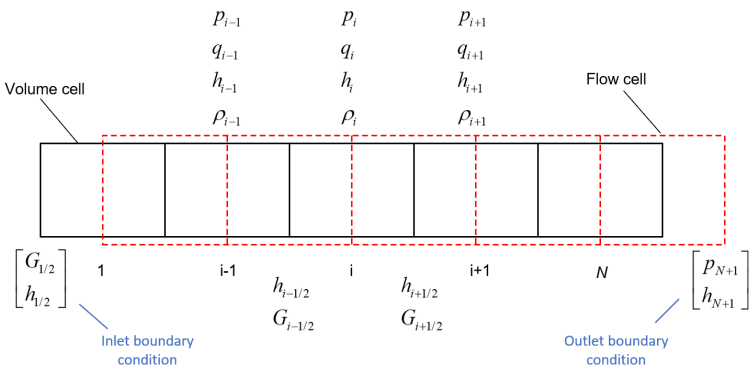

Figure 4: Finite volume model with staggered grid scheme.

To simplify the analysis, the homogeneous equilibrium model (HEM) is adopted for two-phase flow. Under this assumption, the liquid and vapor phases are in thermodynamic equilibrium and share the same phasic velocity. For an inhomogeneous flow formulation, the reader is referred to Qiao et al. (2015). The two-phase refrigerant can therefore be treated as a single pseudo-fluid, and the conservation equations can be expressed directly in terms of the chosen thermodynamic coordinates. Using (P, q) as the state variables, the semi-discretized mass and energy equations for control volume *i* become

$$\frac{\partial \rho_i}{\partial P_i}\frac{dP_i}{dt} + \frac{\partial \rho_i}{\partial q_i}\frac{dq_i}{dt} = \frac{G_{i-1/2} - G_{i+1/2}}{\Delta z_i} \tag{17}$$

$$\left(\rho_i \frac{\partial h_i}{\partial P_i} - 1\right)\frac{dP_i}{dt} + \rho_i \frac{\partial h_i}{\partial q_i}\frac{dq_i}{dt} = \frac{G_{i-1/2}(h_{i-1/2} - h_i) - G_{i+1/2}(h_{i+1/2} - h_i)}{\Delta z_i} + \frac{4Q_i''}{D_H} \tag{18}$$

The variables defined at the flow-cell faces, such as $h_{i\pm1/2}$, are evaluated using a first-order upwind scheme according to the direction of the mass flux. For example,

$$h_{i+1/2} = \begin{cases} h_i, & G_{i+1/2} \geq 0, \\ h_{i+1}, & G_{i+1/2} < 0, \end{cases}$$

and similarly for other convected quantities.

The corresponding momentum balance on the staggered flow cell is obtained from Eq. (15). In its most general form, this equation includes both the dynamic momentum and acceleration terms. However, for the class of applications considered here, these terms are neglected to reduce computational cost, following the analysis in Qiao et al. (2023), which showed that the dominant system dynamics are typically governed by mass and energy storage and transport rather than by momentum transients. Under this approximation, the momentum equation reduces to

$$\frac{P_{i+1} - P_i}{\Delta z_i} = -\frac{4\tau_{w,i+1/2}}{D_H} \tag{19}$$

The resulting equation is used to compute the mass flux through each flow cell, since the pressure drop is generally modeled as a function of mass flux.

It is worth noting that the transformed governing equations retain essentially the same structure as the conventional (P, h)-based formulation. The primary difference is that the thermodynamic derivatives now appear with respect to P and q, rather than P and h. Once the refrigerant properties are parameterized in terms of (P, q), these derivatives can be obtained directly from the property routines, so no additional thermodynamic inversion is required during simulation. This makes the reformulated model especially attractive for zeotropic mixtures, for which the two-phase state is more naturally described by pressure and quality than by pressure and enthalpy alone.

In this work, the vapor quality q is defined as an extended thermodynamic quality variable. Within the two-phase region, $0 \leq q \leq 1$, and q has its usual interpretation as vapor quality. Outside the two-phase region, the definition is extended

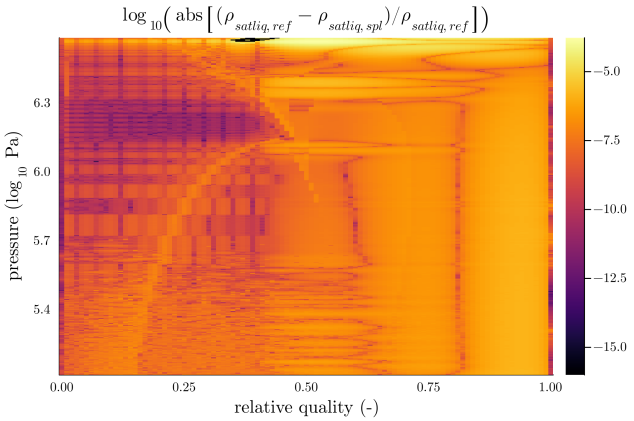

Figure 5: Heatmap showing the relative error of the saturated liquid density function over the entire interpolation domain.

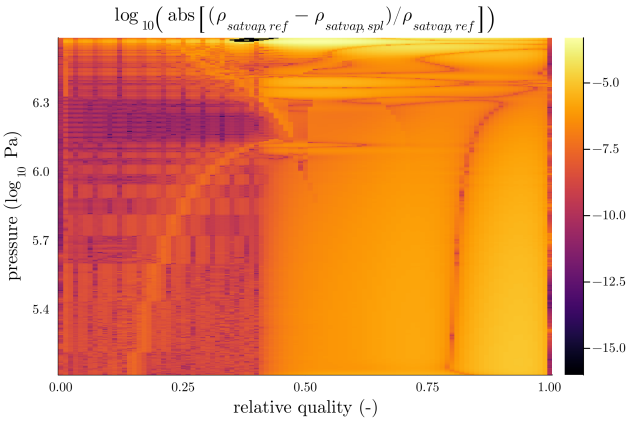

Figure 6: Heatmap showing the relative error of the saturated vapor density function over the entire interpolation domain.

so that q may take values less than zero or greater than one. In this sense, $q < 0$ corresponds to a subcooled liquid state, while $q > 1$ corresponds to a superheated vapor state. This extended definition permits a unified thermodynamic coordinate to be used across single-phase and two-phase regions, which simplifies implementation and reduces the need for repeated switching between state representations during simulation.

Overall, adopting (P, q) as the state variables yields a formulation that is fully analogous to the conventional (P, h) model, while being better matched to the mixture property routines developed in this work. The resulting model preserves the conservation-law structure of the original formulation, but provides a more natural and computationally efficient description of zeotropic refrigerant behavior, particularly in the two-phase region.

4. RESULTS

These methods were initially tested by implementing this refrigerant property model in the Julia numerical computing language (Bezanson et al., 2017) as a refinement of the methods described in earlier work (Laughman & Qiao, 2021). REFPROP version 10 was used to obtain samples of the reference data for the thermodynamic properties of R454C, and we used 5$^{\text{th}}$-order B-splines to build the interpolating functions describing the individual properties, such as the saturated liquid and vapor densities, saturated liquid and vapor specific enthalpies, and so forth. These properties were sampled over a wide range of pressures (130 kPa to 3.8 MPa) and qualities ($q \in [0, 1]$).

Figures 5 and 6 illustrate a heatmap that visualizes the log absolute relative error for both the saturated liquid density and saturated vapor density over the entirety of the two-phase region. This particular error metric was used to effectively visualize the range of relative errors that span many orders of magnitude. It is clear that the maximum relative error for both functions is on the order of 10^{-4}, and that the average relative error is closer to 10^{-6}, which is acceptable for many applications in model-based design of vapor-compression equipment. These methods use 25 coefficients in the quality direction, and about 250 coefficients in the pressure direction, resulting in the storage of approximately 6500 coefficients for the function over the entire domain. While a full timing analysis of the computational requirements for these methods is beyond the scope of this paper, timing tests for the saturated liquid and vapor density functions indicate that these functions require approximately 320 ns of compute time.

In order to demonstrate the efficacy of the refrigerant property models formulated with pressure P and vapor quality q as independent variables, a vapor-compression heat pump cycle model is constructed in Modelica using R454C as the working fluid. A library of refrigerant properties for R454C needed to implement the cycle was generated in Julia and interfaced to the Modelica language (Modelica Association, 2017). The model is operated in heating mode and is first allowed to reach steady state at a compressor speed of 50 Hz. At t = 10,000 s, the compressor speed is increased by a step change from 50 Hz to 80 Hz. The resulting transient responses of the cycle pressures and the apparent temperature glide in the two heat exchangers are shown in Figs. 7 and 8, respectively. This model is quite fast, with approximately

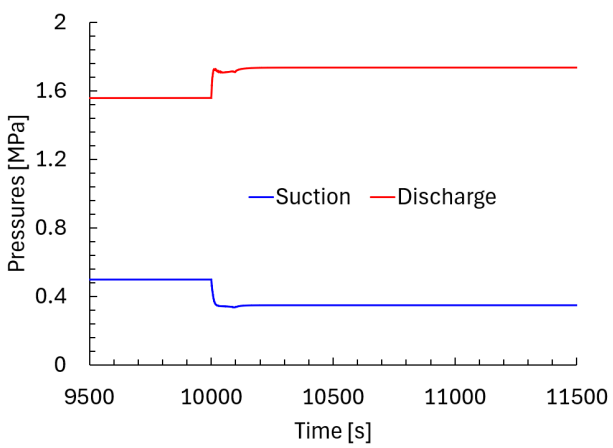

Figure 7: Dynamic response of the suction and discharge pressures after a compressor speed step change from 50 Hz to 80 Hz at t = 10,000 s.

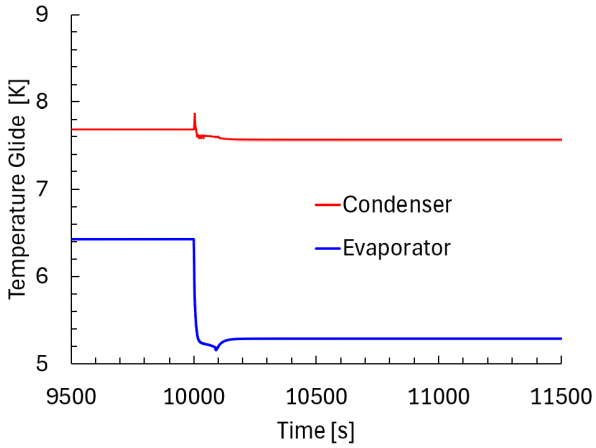

Figure 8: Dynamic response of the apparent temperature glide in the condenser and evaporator after the compressor speed step change.

8000 equations being solved over the 20,000 second time horizon in 13 seconds of CPU time.

Figure 7 shows the suction and discharge pressure dynamics for this cycle as well. After the compressor speed is increased, the discharge pressure rises while the suction pressure decreases, which is consistent with the increased refrigerant circulation rate and larger compressor pressure lift. Both pressures then settle to new steady-state values after a short transient.

In comparison, Figure 8 shows the apparent temperature glide in the condenser and evaporator. Since R454C is a zeotropic mixture, phase change occurs over a finite temperature range rather than at a single saturation temperature. In this study, the apparent temperature glide is evaluated from the refrigerant states at the boundaries of the two-phase region while accounting for local pressure variation along each heat exchanger. For the condenser, the apparent temperature glide is defined as

$$\Delta T^{\mathrm{app}}_{\mathrm{glide,cond}} = T_{\mathrm{dew}}\left(P_{\mathrm{cond,2ph,in}}\right) - T_{\mathrm{bub}}\left(P_{\mathrm{cond,2ph,out}}\right), \tag{20}$$

where $P_{\mathrm{cond,2ph,in}}$ is the pressure at the beginning of condensation and $P_{\mathrm{cond,2ph,out}}$ is the pressure at the end of condensation. For the evaporator, the apparent temperature glide is defined as

$$\Delta T^{\mathrm{app}}_{\mathrm{glide,evap}} = T_{\mathrm{dew}}\left(P_{\mathrm{evap,2ph,out}}\right) - T_{\mathrm{bub}}\left(P_{\mathrm{evap,2ph,in}}\right), \tag{21}$$

where $P_{\mathrm{evap,2ph,in}}$ is the pressure at the beginning of evaporation and $P_{\mathrm{evap,2ph,out}}$ is the pressure at the end of evaporation.

After the compressor speed step, the apparent temperature glide responses remain smooth, indicating that the (P,q)-based refrigerant property models can robustly evaluate zeotropic two-phase states during dynamic operation. The condenser glide changes only slightly, while the evaporator glide decreases more noticeably due to the reduced low-side pressure and redistribution of the two-phase region. These results provide a dynamic verification case for the proposed refrigerant property formulation under realistic heat pump operating transients.

5. DISCUSSION

Model-based design practices for vapor-compression cycles that use zeotropic refrigerant mixtures as the working fluid are becoming increasingly common due to the need to reduce the environmental impact of this equipment and address regulatory concerns. While the conventional choice of (P,h) for state variables is effective for pure fluids and azeotropic mixtures, this choice presents some limitations when applied to zeotropic mixtures. The use of (P,q) as coordinates, along with the creation of interpolating functions for the saturated liquid and vapor properties in the two-phase region, enables the computationally effective and accurate description of the thermophysical properties for these refrigerants. Modification of the models to re-express the conservation equations in these new coordinates allows

the models to take full advantage of the computational efficiency of this refrigerant property model formulation, and implementation of the properties in the Julia language and of a complete vapor-compression cycle using R454C in the Modelica language demonstrates the efficacy of these methods for practical system design.

NOMENCLATURE

D_H	hydraulic diameter (m)	S	entropy ($J\,K^{-1}$)
e	specific internal energy ($J\,kg^{-1}$)	T	temperature (K)
G	mass flux ($kg\,m^{-2}\,s^{-1}$)	U	internal energy (J)
G	Gibbs free energy (J)	V	volume (m^3)
h	specific enthalpy ($J\,kg^{-1}$)	x_i	liquid-phase mole fraction of component i (–)
K_i	phase-equilibrium ratio of component i (–)	y_i	vapor-phase mole fraction of component i (–)
N	number of moles (mol)	z	axial coordinate (m)
N_c	number of mixture components (–)	z_i	overall mole fraction of component i (–)
P	pressure (Pa)	μ_i	chemical potential of component i ($J\,mol^{-1}$)
Q''	heat flux ($W\,m^{-2}$)	ρ	density ($kg\,m^{-3}$)
q	vapor quality (–)	τ_w	wall shear stress (Pa)

Subscripts

bub	bubble point	i	component or control-volume index
cond	condenser	l	saturated liquid phase
dew	dew point	v	saturated vapor phase
evap	evaporator	2ph	two-phase region

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