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A review of cubic and statistical associating fluid theory equations of state for modeling supercritical hydrogen

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Abstract

The transition to a global hydrogen economy necessitates the development and optimization of technologies for hydrogen production, storage, and utilization, many of which operate under supercritical conditions. Accurate prediction of the thermodynamic properties of supercritical hydrogen is therefore of paramount importance for engineering design, operational efficiency, and safety. This review provides a critical evaluation and comparative analysis of two dominant classes of thermodynamic models: The computationally simple cubic equations of state (CEoSs), such as Peng–Robinson and Soave–Redlich–Kwong, and the more physically rigorous statistical associating fluid theory (SAFT)-based models. The analysis reveals that classical CEoSs exhibit significant inaccuracies in predicting the properties of supercritical hydrogen, a failure rooted in their empirical formulation, which cannot account for the quantum mechanical effects prominent in light fluids. In contrast, SAFT-based models, which are derived from molecular-level principles, demonstrate consistently superior accuracy in predicting volumetric, caloric, and transport-related properties across wide ranges of temperature and pressure. This review elucidates the fundamental reasons for these performance disparities and discusses the practical trade-offs between model simplicity and predictive power. Future research directions are explored, including the role of quantum corrections for cubic models, the development of hybrid EoSs, and the transformative potential of machine learning for EoS parameterization and property prediction.

Keywords: Supercritical hydrogen; Equation of state; Statistical associating fluid theory; Cubic equation of state; Thermodynamic modeling; Machine learning

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1. Introduction

Hydrogen is increasingly recognized as a cornerstone of future sustainable energy systems, offering a clean, versatile, and high-energy-density alternative to conventional fossil fuels.[1,2] As a fuel and energy carrier, it possesses the potential to decarbonize a wide array of sectors, from transportation and power generation to industrial processes, such as chemical production and petroleum refining.[2] When utilized in fuel cells or through combustion, its primary byproduct is water, positioning it as a compelling solution to mitigate environmental impacts and combat climate change.[1] However, the widespread

adoption of hydrogen is contingent upon surmounting significant technological challenges related to its cost-effective production, safe and dense storage, and efficient utilization.[3] The successful deployment of a hydrogen economy, therefore, depends critically on the development of new and advanced technologies across its entire value chain.[4]

One of the most promising technological pathways involves harnessing hydrogen in its supercritical state. A substance becomes supercritical when its temperature and pressure exceed the thermodynamic critical point[5]—for hydrogen, a very low temperature of approximately 33 K and a pressure of 1.3 MPa.[6] In this state, the distinct liquid and gas phases merge into a single, homogeneous fluid. This supercritical fluid exhibits a unique and advantageous combination of properties: It possesses a liquid-like high density, which is ideal for storage, coupled with gas-like low viscosity and high diffusivity, which enhance mass transfer and reduce flow resistance in engineered systems.[5]

A key technological advantage of operating in the supercritical region is the complete absence of a liquid–gas phase boundary. This phenomenon eliminates surface tension and prevents the formation of two-phase flow, thereby avoiding the pressure drop instabilities and mechanical vibrations that can plague traditional fluid systems. This stability is crucial for designing robust and reliable hydrogen infrastructure. These unique characteristics make the supercritical state particularly significant for addressing critical challenges in several hydrogen applications.[7]

For energy storage, the high density of supercritical hydrogen enables highly efficient volumetric storage solutions. Cryo-compressed hydrogen storage, which maintains hydrogen at cryogenic temperatures but above its critical pressure, leverages these properties to achieve greater storage densities than compressed gas alone. This method also cleverly avoids the significant boil-off losses that are typically associated with storing hydrogen in its liquid form, directly tackling a major hurdle in hydrogen logistics.[8]

Furthermore, supercritical hydrogen is a critical component in aerospace and chemical processing. In advanced liquid rocket engines, it serves as both a high-performance propellant and a cryogenic coolant. This dual functionality is now being exploited in next-generation aircraft designs to simplify thermal management, reduce weight, and boost efficiency. In the chemical industry, processes such as supercritical water gasification use these unique properties to produce hydrogen from wet biomass. Under these conditions, water becomes an excellent solvent for organic materials, dramatically accelerating reaction rates and improving hydrogen yields, thus contributing to more efficient and sustainable production methods.[9]

The design, optimization, and safe operation of any technology involving supercritical hydrogen are fundamentally dependent on the ability to accurately predict its thermophysical properties. Properties such as density (ρ), isobaric and isochoric heat capacities (C_p, C_v), and the speed of sound (u) are essential inputs for engineering calculations that govern system performance and safety margins.[2,10]

In the burgeoning hydrogen economy, accurate flow metering is critical for custody transfer and commerce. Sonic nozzles, which are emerging as reference calibration devices, rely on the critical flow factor (C), a property calculated directly from thermodynamic state variables such as enthalpy and heat capacity. Therefore, inaccuracies in the underlying equation of state (EoS) lead directly to uncertainties in flow measurement. Similarly, the design of heat exchangers for cryogenic liquefaction and aerospace thermal management is governed by caloric properties; inaccurate predictions can lead to inefficient or improperly sized equipment. Furthermore, in large-scale underground hydrogen storage (UHS), equations of state are essential for modeling the complex behavior of stored hydrogen, its potential mixing with cushion gases, and its transport within geological formations.[11-13]

Modeling the thermodynamic behavior of hydrogen presents unique challenges that are not encountered with most other industrial fluids. Due to its extremely low molecular weight and small size, hydrogen exhibits significant quantum mechanical effects even at temperatures well above its critical point.[10] Classical thermodynamic models, which are typically developed based on the behavior of heavier, classical fluids, often fail to capture these quantum phenomena, leading to substantial predictive errors.[14]

This challenge is compounded by the existence of nuclear spin isomers: orthohydrogen and parahydrogen. These two forms of the H_2 molecule correspond to different nuclear spin alignments (parallel for ortho, antiparallel for para) and, as a consequence of the Pauli exclusion principle, occupy different sets of rotational energy levels. This leads to significant differences in their caloric properties—notably enthalpy, entropy, and heat capacity—at cryogenic temperatures (generally below 250 K).[10] The equilibrium mixture ratio of the two isomers is a strong function of temperature. At room temperature, the equilibrium mixture, known as "normal" hydrogen, consists of approximately 75% orthohydrogen and 25% parahydrogen. As the temperature decreases, the equilibrium shifts toward the lower-energy para state,

which constitutes nearly 100% of the mixture at liquid hydrogen temperatures (~20 K).[15]

The spontaneous conversion from the ortho to the para state is an exothermic process. This has profound implications for the design and operation of hydrogen liquefaction and storage systems. The heat released during this conversion can lead to significant evaporative losses (boil-off) if not properly managed, typically through the use of catalysts to accelerate the conversion during the liquefaction process.[16] Consequently, a robust thermodynamic model for hydrogen must be capable of accurately representing the properties of not only normal hydrogen but also parahydrogen and their mixtures at various equilibrium states.[10]

Given the critical importance and unique challenges of modeling supercritical hydrogen, this review aims to provide a comprehensive assessment of the predictive capabilities of leading EoSs. The primary objective is to present a detailed theoretical overview and conduct a rigorous, data-driven comparative analysis of two dominant EoS families: Cubic models, such as the Peng–Robinson (PR) and Soave–Redlich–Kwong (SRK) equations, and the physically based statistical associating fluid theory (SAFT) models. This comparison will focus on their performance in predicting key thermodynamic properties of supercritical hydrogen, including density, heat capacity, and the speed of sound, while also elucidating the fundamental physical reasons for any performance differences, particularly concerning quantum effects.

Furthermore, this review evaluates the practical engineering trade-offs between model accuracy, computational complexity, and ease of implementation for industrial use. By examining these factors, the review seeks to provide clear guidance for selecting appropriate models for specific applications. Finally, it will survey the current state-of-the-art and future directions in the field, highlighting the development of advanced EoSs, necessary quantum corrections, and the emerging role of machine learning in thermodynamic modeling to pave the way for next-generation predictive tools.

2. Equations of state

2.1. Cubic EoS family

Cubic equations of state (CEoSs) are algebraic models (cubic in molar volume [v]) that represent an important evolution from the original van der Waals equation. Their enduring popularity in chemical and process engineering stems from their relative simplicity, low computational demand, and reasonable accuracy for many non-polar systems. The two most prominent examples are the PR and SRK equations.[17]

The general form for these two-parameter CEoSs can be written as:

$$P = \frac{RT}{v-b} - \frac{a(T)}{v^2 + cbv + db^2} \quad \text{(I)}$$

Where R is the universal gas constant, and $a(T)$ and b are the substance-specific attraction and co-volume parameters, respectively. The parameters c and d distinguish between models.[18] The co-volume parameter, b, accounts for the finite volume occupied by molecules, whereas the energy parameter, $a(T)$, accounts for intermolecular attractive forces. These parameters are not purely empirical; they are determined from the substance's critical properties (T_c and P_c) and its acentric factor (ω), a measure of the non-sphericity of the molecule's potential field.[17] The parameter $a(T)$ is expressed as the product of a constant part and a temperature-dependent term known as the alpha function, $\alpha(T)$:

$$a(T) = a_c\,\alpha(T) \quad \text{(II)}$$

The alpha function is crucial for accurately representing the vapor pressure of fluids and is the primary feature that distinguishes various modifications of the PR and SRK models.[19]

Despite their widespread use, classical CEoSs exhibit fundamental weaknesses when applied to quantum fluids such as hydrogen, helium, and neon.[14] The primary point of failure lies in the formulation of the alpha function, $\alpha(T)$. Standard correlations for $\alpha(T)$, such as those proposed by Soave or Twu, were developed and optimized for classical, non-polar hydrocarbons.[20] When extrapolated to hydrogen, these functions perform poorly, particularly at high reduced temperatures, and can lead to the prediction of non-physical behavior, such as divergent virial coefficients at high temperatures or unphysical bumps in the calculated heat capacity isobars in the supercritical region.[14]

The problem, however, is more deeply rooted than just an inaccurate alpha function. The issue is a fundamental misspecification of the model's underlying physics for quantum particles. CEoSs are built upon a simplified picture of molecular interactions: Impenetrable hard-sphere repulsion (represented by the constant co-volume b) and a mean-field attraction (represented by the a/v^2 -type term). This picture is a reasonable approximation for classical molecules, but breaks down for hydrogen. Due to its quantum nature, a hydrogen molecule does not behave like a classical hard sphere with a fixed size. Its effective repulsive core is softer, and its interaction potential is influenced by quantum effects in a way that cannot be captured by a constant co-volume parameter and a simple, empirically-corrected attractive term.[14]

At high temperatures, where repulsive forces dominate the fluid's behavior, this misrepresentation of the repulsive part of the potential becomes a principal source of error. This explains why simply adjusting the attractive term via the alpha function is insufficient for achieving high accuracy across a wide range of conditions. A more fundamental modification is required. This has led to the development of quantum-corrected CEoSs.[2] These models often employ approaches such as the Feynman–Hibbs effective potential method, which introduces temperature-dependent molecular parameters to mimic quantum effects within the classical CEoSs framework, thereby improving predictions for fluids where quantum behavior is significant.[21]

2.2. Statistical associating fluid theory family

The SAFT represents a significant departure from the empirical nature of CEoSs. It is a family of more physically rigorous EoSs based on the thermodynamic perturbation theory of Wertheim.[22,23] The foundational concept of SAFT is to model molecules not as simple spheres, but as chains of bonded spherical segments. This molecular-level perspective allows for a more explicit and physically meaningful description of fluid properties.[22,23]

Within the SAFT framework, the residual Helmholtz energy is calculated as a sum of distinct contributions that correspond to different types of molecular interactions:

$$a^{res} = a - a^{ideal} = a^{ref} + a^{disp} + a^{chain} + a^{assoc} \quad \text{(III)}$$

Where a, a^{res}, a^{ideal}, a^{ref}, a^{disp}, a^{chain}, and a^{assoc} are the total, residual, ideal, reference (e.g., hard spheres[24]), dispersion, chain, and association Helmholtz energy, respectively.[22,23]

This approach, which builds thermodynamic properties from a molecular model, provides a much stronger physical basis than the empirical fitting approach of CEoSs. This physical rigor is the source of SAFT's generally superior accuracy and its enhanced predictive and extrapolative capabilities, especially for complex fluids and mixtures.[25]

Several important variants of the SAFT EoS have been developed, each refining the treatment of interaction terms to improve accuracy and expand predictive power. One of the most successful and widely applied versions is perturbed-chain SAFT (PC-SAFT),[26] which uses a fluid of hard chains as its reference system. This provides a more accurate description of repulsive interactions in chain-like molecules compared to earlier models based on disconnected hard spheres.

Further advancements led to[27] a variant that employs the more flexible Mie potential to describe segment interactions. The Mie potential, a generalized Lennard–Jones potential with variable repulsive and attractive exponents (λ_r and λ_a), allows the model to more accurately capture the nuances of intermolecular forces. This results in significantly improved predictions of second-derivative properties, such as heat capacity and speed of sound. Building on this, the SAFT-γ Mie[28] model reformulates the EoS into a powerful group-contribution (GC) framework. This allows for the prediction of thermodynamic properties for complex or novel compounds by constructing them from a library of functional groups, even when no experimental data for the full molecule exists. A more recent development is PρT-SAFT,[29] which is parameterized directly using pressure, density, and temperature data. This approach improves the model's ability to represent volumetric and derivative thermodynamic properties across a wide range of conditions. PρT-SAFT retains the molecular-based framework of SAFT, incorporating contributions from molecular association, chain formation, dispersion interactions, and segment repulsion. Its formulation allows it to capture the complexities of fluids with hydrogen bonding or other specific interactions, as well as mixtures containing components of varying molecular sizes and polarities. By focusing on $P\rho T$ data for parameter fitting, the model achieves a more consistent and accurate representation of both simple and complex fluid systems, making it applicable to a wide range of industrial and scientific processes.

A key challenge in applying SAFT models is the determination of their pure-component parameters.[29] For a simple non-associating fluid like hydrogen, the SAFT-type EoSs usually require three parameters. These parameters must be regressed from experimental data.

For hydrogen, this parameterization process is particularly problematic. Different research groups have published multiple, inconsistent parameter sets for hydrogen in the literature, often fitted to different types of experimental data (e.g., vapor-liquid equilibrium (VLE) data, supercritical density data, or mixture data).[2] The choice of the regression dataset strongly influences the model's predictive accuracy for other properties and conditions. For example, parameters optimized for low-temperature vapor pressure may yield poor predictions for high-pressure supercritical density.[4] This highlights a critical need for robust, multi-property parameterization strategies that ensure a model is accurate across a wide range of states. Efforts to address this include developing new parameterization approaches, such as the "variable-range" PC-SAFT method, which relaxes an additional parameter to improve simultaneous fitting of caloric and phase equilibrium data for hydrogen and other fluids.[4]

3. Literature review and discussion

To rigorously evaluate the performance of different EoSs, a reliable benchmark is essential. One of the best standard data sources for the thermophysical properties of hydrogen and other common fluids is the data provided by the National Institute of Standards and Technology (NIST), accessible through resources like the NIST Chemistry WebBook.[6] These data are not raw experimental data but are generated from highly accurate, multi-parameter fundamental EoSs that are formulated in Helmholtz free energy. For hydrogen, the current standard is a highly complex formulation developed by Leachman *et al.*,[30] which was fitted to a comprehensive set of the world's experimental data for properties, including density, heat capacity, vapor pressure, and speed of sound. The stated uncertainty of this reference EoS is exceptionally low, with density predictions accurate to within 0.04% in the critical region of 250–450 K and pressures up to 300 MPa.[31] For the purposes of evaluating simpler models such as Cubic and SAFT EoSs, this NIST-generated data serves as the definitive pseudo-experimental benchmark.

In addition to NIST data, molecular dynamics (MD) simulations provide a valuable secondary benchmark. MD simulations can generate thermodynamic data in regions where experiments are difficult or unavailable and offer a molecular-level view of fluid behavior, making them particularly useful for validating the physical assumptions of models such as SAFT.[2]

While CEoSs are widely used for their computational speed, their accuracy diminishes under extreme conditions, such as in supercritical states.[32] Several researchers have investigated these limitations for hydrogen. For instance, Nasrifar[33] conducted a comprehensive study evaluating 11 CEoSs for modeling hydrogen. Deiters[14] specifically highlighted that standard alpha functions are inadequate for hydrogen at high densities and temperatures, proposing necessary corrections. Similarly, Le Guennec *et al.*[34] described how these alpha functions exhibit an unusual bell shape for quantum fluids below 40–50 K. In another evaluation, Botros and Jensen[35] assessed 12 different EoSs for predicting the properties of hydrogen and hydrogen-natural gas blends at high pressures. Addressing these challenges, Aasen *et al.*[36] developed quantum-corrected CEoSs to achieve more accurate predictions.

Researchers have frequently applied SAFT-type EoSs to model hydrogen systems. Ghosh *et al.*[37] used the PC-SAFT EoS to model hydrogen solubility in linear alkanes and 1-alkenes, fitting adjustable parameters with high-temperature and high-pressure mixture data. In a similar effort to parameterize this model, Khare *et al.*[38] used supercritical density data. The predictive capability of the PC-SAFT EoS was then applied by Senol[39] to determine the thermodynamic properties of hydrogen under supercritical conditions. In other work, Trinh *et al.*[40] employed a modified GC-PPC-SAFT EoS to calculate hydrogen solubility in oxygenated organic solvents. Broader SAFT models have also been explored; for example, Nikolaidis *et al.*[41] applied the SAFT-VR Mie EoS, regressing hydrogen parameters using supercritical density and speed of sound data. Meanwhile, Alkhatib *et al.*[42,43] evaluated the polar soft-SAFT EoS for hydrogen and natural gas mixtures, regressing parameters with VLE data. Other parameterization efforts include those by Alanazi *et al.*,[44] who used VLE data from hydrogen-water and hydrogen-carbon dioxide mixtures for PC-SAFT, and Lozano-Martín *et al.*,[45] who used binary mixture density data of hydrogen and propane. Pakravesh *et al.*[2] compared the accuracy of three versions of the SAFT EoS and five versions of the PC-SAFT EoS with CEoSs. In the following sections, the accuracy of the cubic and SAFT EoSs for the thermodynamic modeling of pure hydrogen and hydrogen-containing mixtures will be compared.

3.1. Pure hydrogen

Density (ρ) is the most fundamental thermodynamic property predicted by a volumetric EoS, and its accuracy is critical for nearly all engineering applications, from storage vessel sizing to fluid dynamic simulations. The performance of EoSs for hydrogen density has been evaluated over both vast thermodynamic spaces and more focused, industrially relevant regions.

In studies covering extremely wide pressure and temperature ranges (e.g., 10–2000 MPa and 100–1000 K), a clear trend emerges: Physically based SAFT models generally outperform their simpler cubic counterparts.[2] The superior representation of molecular repulsion and attraction in SAFT models allows them to maintain accuracy even at very high pressures. The specific reason for this divergence lies in their treatment of molecular repulsion. CEoSs use a simple co-volume term that treats molecules as impenetrable hard spheres of a fixed volume. This assumption breaks down under extreme compression, where intermolecular repulsive forces are more complex than a simple hard-sphere model can capture. In contrast, SAFT models employ more sophisticated expressions for the repulsive contributions, often based on the Carnahan–Starling equation for hard-sphere fluids or the repulsive part of the Mie potential. These terms provide a more physically accurate description of how molecular packing and free volume change at very high densities, preventing the systematic underestimation of pressure (or overestimation of density) that plagues cubic models in this regime.[46] Specifically, one comprehensive study

assessing 11 different EoSs found that rescaled versions of the PρT-SAFT model yielded the most precise predictions of hydrogen's thermodynamic properties, including density, across this broad range.[2]

However, when the focus narrows to a more limited range of conditions relevant to many industrial applications (e.g., 10–100 MPa and 100–400 K), the performance landscape becomes more nuanced. In this domain, the accuracy gap between model classes can shrink considerably. Some analyses have found that well-established models such as the SRK EoS can provide surprisingly accurate density predictions, in some cases performing on par with or even better than more complex SAFT variants.[10] For high-pressure storage applications, such as onboard vehicle tanks operating up to 70 MPa, specialized or highly tuned CEoSs have demonstrated excellent accuracy, with reported errors of <0.5% compared to reference data.[47] Even the PR EoS has been demonstrated to provide densities with reasonable accuracy for simulating hydrogen release from high-pressure reservoirs.[48]

This dichotomy highlights a crucial point: While the theoretical superiority of SAFT models is evident over vast thermodynamic ranges, the practical advantage within a constrained operational window may be less pronounced. A simpler, computationally cheaper CEoS may be good enough for certain applications, provided it is validated for the specific conditions of interest. Table 1 summarizes the reported performance for several key EoSs, comparing their accuracy for calculating the density of supercritical hydrogen.

Various properties, such as the isobaric heat capacity (C_p), isochoric heat capacity (C_v), speed of sound (u), and Joule–Thomson coefficient (JTC), are derived from the first and second derivatives of the EoS with respect to temperature and volume. Their prediction is a much more stringent test of a model's physical realism than density alone, as they are highly sensitive to the curvature of the $P\rho T$ surface.[49] Table 2 presents the performance of the EoSs in predicting the caloric and derivative properties of supercritical hydrogen.

Predicting the caloric and derivative properties represents the domain where the structural differences between cubic and SAFT EoSs become most apparent. Classical cubic models (e.g., PR and SRK) generally perform poorly in predicting these derivative properties.[49] They often fail to accurately capture the location and magnitude of extrema, such as the characteristic peak in C_p along the pseudo-critical line, and can exhibit large quantitative deviations from experimental data. While some modifications can offer marginal improvements—for example, one study found PR to be somewhat better than SRK for supercritical C_p[51]—the overall capability of standard CEoSs remains limited.

In contrast, the more physically grounded SAFT models demonstrate markedly superior performance. The PρT-SAFT and SAFT-VR Mie EoSs are frequently highlighted for their excellent prediction of derivative properties (e.g., speed of sound).[2,3] This capability stems from the model's ability to more accurately represent

Table 1. Comparative accuracy of EoS for supercritical hydrogen density

EoS	Absolute average deviation (AAD%) versus NIST	
	Wide range (10–2,000 MPa)	Industrial range (10–100 MPa)
PR	9.75	9.98
SRK	6.92	1.40
Quantum-corrected PR	8.41	4.34
GERG-2008	N/A	0.05
PρT-SAFT	1.32	1.38
PC-SAFT	3.44	1.49
PρT-PC-SAFT	1.91	1.50

Note: Data obtained from references.[2,3,33,49,50]
Abbreviations: EoS: Equation of state; GERG: Groupe Européen de Recherches Gazière; NIST: National Institute of Standards and Technology; PR: Peng–Robinson; PC-SAFT: Perturbed chain SAFT; PρT-SAFT: Pressure–density–temperature version of the SAFT; PρT-PC-SAFT: Pressure-density-temperature version of the PC-SAFT; SAFT: Statistical associating fluid theory; SRK: Soave-Redlich-Kwong.

Table 2. Performance of EoS for caloric and derivative properties of supercritical hydrogen

EoS	AAD%		
	C_p	u	JTC
PR	4.28	47.21	34.01
SRK	4.27	47.19	33.29
Quantum-corrected PR	5.25	14.07	23.62
GERG-2008	33.9	0.5	104.4
PρT-SAFT	4.25	9.18	15.18
PC-SAFT	5.73	111.89	15.45
PρT-PC-SAFT	4.01	8.17	19.94

Note: Data obtained from references.[2,3,33,49,50]
Abbreviations: AAD%: Average absolute deviations; EoS: Equation of state; GERG: Groupe Européen de Recherches Gazières; NIST: National Institute of Standards and Technology; PR: Peng–Robinson; PC-SAFT: Perturbed chain SAFT; PρT-SAFT: Pressure–density–temperature version of the SAFT; PρT-PC-SAFT: Pressure-density-temperature version of the PC-SAFT; SAFT: Statistical associating fluid theory; SRK: Soave-Redlich-Kwong; JTC: Joule–Thomson coefficient.

the true shape of the intermolecular potential well. The fundamental reason for this is that caloric properties, such as heat capacity, are related to the second derivatives of the Helmholtz free energy with respect to temperature and volume. These second derivatives are mathematically equivalent to the curvature of the thermodynamic surface. The simple, empirical attraction terms in CEoSs provide a mathematically convenient but physically inaccurate shape for this surface. Consequently, its curvature is often incorrect, leading to large errors in predicted caloric properties, especially near the critical point or along the pseudo-critical line where this curvature changes rapidly. SAFT-based models, by building up the free energy from physically distinct contributions (repulsion, dispersion, etc.), inherently produce a thermodynamic surface with a more realistic shape and curvature, leading directly to their superior predictions for speed of sound, heat capacities, and the JTC.[2,3] Other advanced models, such as the highly parameterized GERG-2008 EoS,[52] consistently display the highest accuracy for properties such as speed of sound for both pure hydrogen and its mixtures.[35,46] The ability to accurately model caloric properties is not just a measure of theoretical elegance; it is critical for practical applications, such as the design of liquefaction cycles, which depend on precise enthalpy balances and JTC calculations for expanders and throttling valves.

While the focus of this review is the supercritical region, the EoS's ability to accurately describe the saturation curve (VLE) and the critical point itself is a fundamental measure of its overall validity.

For predicting saturated properties of hydrogen, including vapor pressure and saturated liquid/vapor densities, the quantum-corrected PR (QPR) EoS has been demonstrated to deliver the best performance, even surpassing SAFT-type models in this specific domain.[2] This result underscores the effectiveness of empirical correction factors when targeted at a specific physical phenomenon (quantum effects) in a well-defined region (the saturation line). Among standard CEoSs, the PR EoS is often reported to yield slightly better results for vapor pressure and saturated vapor density than the SRK EoS.[51]

The reproduction of the experimental critical point reveals an interesting contradiction in the literature. CEoSs are, by their very construction, parameterized using the experimental T_c and P_c, forcing them to match these two values (though not necessarily ρ_c).[17] In contrast, SAFT parameters are typically regressed from VLE and liquid density data, which may not include the critical point itself. This has led to the observation that some SAFT models do not accurately reproduce the experimental critical point, a noted weakness.[10] However, other comprehensive studies report the opposite conclusion that rescaled versions of the PρT-SAFT EoS provide the most precise predictions of hydrogen's critical point properties.[2] This apparent discrepancy likely stems from the specific parameterization strategy employed; if critical point data is included in the regression dataset for the SAFT parameters, the model can be tuned for high accuracy in that region. This again highlights the central role of parameterization in determining SAFT model performance. The performance of each EoS in reproducing the critical point of hydrogen is quantified in Table 3.

The collective results presented in this section paint a clear picture: There is no single perfect EoS for pure hydrogen. The choice of model involves a critical trade-off. A model that excels in one area (e.g., QPR for saturated properties) may be mediocre in another (e.g., supercritical density). A model with superior accuracy for derivative properties (e.g., SAFT-VR Mie) may be more computationally intensive and suffer from parameterization ambiguity. This leads to the inevitable conclusion that the selection of an EoS cannot be made in a vacuum. It must be a strategic decision, carefully weighing the required accuracy for the specific properties and conditions of interest against the model's complexity, computational cost, and the availability of reliable parameters.

3.2. Hydrogen-containing mixtures

Most industrial applications involve hydrogen not in its pure form, but as part of mixtures, where hydrogen is blended with natural gas, dissolved in liquids, or contains impurities (e.g., water and carbon dioxide). Modeling these mixtures introduces a new layer of complexity, as the EoS must now accurately describe not only the pure components but also the interactions between dissimilar molecules. The performance of an EoS for mixtures is therefore a two-part problem, depending on both the

Table 3. Accuracy of EoS in predicting hydrogen's critical point

EoS	Percentage error in T_c	Percentage error in P_c	Percentage error in ρ_c
PR	0 (by definition)	0 (by definition)	1.54
SRK	0 (by definition)	0 (by definition)	15.10
QPR	0 (by definition)	0 (by definition)	25.33
PρT-SAFT	0	0	5.31
PC-SAFT	4.98	12.99	20.00
PρT-PC-SAFT	35.00	10.70	1.04

Note: Data obtained from references[2,10]
Abbreviations: EoS: Equation of state; PR: Peng-Robinson; QPR: Quantum-corrected; PR PC-SAFT: Perturbed chain SAFT; PρT-SAFT: Pressure–density–temperature version of the SAFT; SAFT: Statistical associating fluid theory; PρT-PC-SAFT: Pressure–density–temperature version of the PC-SAFT; SRK: Soave–Redlich–Kwong.

quality of the pure-component description and the fidelity of the mixing rules used to combine them.

The extension of a pure-component EoS to mixtures is governed by mixing rules, which define how the EoS parameters (a and b for cubics; m, σ, ϵ/k for SAFT) for the mixture are calculated from the pure-component values. The conventional approach for CEoSs uses the simple van der Waals one-fluid mixing rules, which are quadratic in mole fraction.[46] To correct for the inherent inaccuracies of this simplification, an adjustable binary interaction parameter (BIP), commonly denoted as k_{ij}, is introduced into the mixing rule for the attraction parameter, a^{mix}:

$$a^{mix} = \sum_i \sum_j x_i x_j a_i a_j (1 - k_{ij}) \quad \text{(III)}$$

This BIP is a purely empirical correction factor, regressed from experimental mixture data, that accounts for the specific interactions between molecules i and j.[46] The physical reason that this empirical correction is so critical, and often insufficient, for hydrogen mixtures stems from the failure of the underlying one-fluid theory. The conventional van der Waals mixing rules (Equation III) operate by creating a hypothetical "pseudo-component" with averaged parameters to represent the mixture. This averaging approach works reasonably well for mixtures of similar molecules (e.g., propane and butane). However, for highly asymmetric mixtures (e.g., hydrogen and a heavy hydrocarbon), this concept fails dramatically. A single set of averaged parameters cannot simultaneously capture the quantum behavior and small size of hydrogen, and the classical behavior and large size of the other component. This theoretical breakdown is why the accuracy of models becomes almost entirely dependent on the empirical k_{ij} parameter, which must compensate for the deficiencies of both the pure-component EoS and the mixing rule itself.

The literature strongly indicates that the accuracy of predictions for hydrogen mixtures is often more sensitive to the proper determination of the BIP than to the choice of the underlying pure-component EoS itself.[51] Key findings include:

(i) Temperature dependency: Using a single, temperature-independent BIP is often insufficient. Introducing a temperature dependency to the k_{ij} value leads to significant improvements in the accuracy of VLE calculations for hydrogen mixtures.[51]

(ii) Generalized correlations: To enhance the predictive capability of models, researchers have developed generalized correlations that can estimate the BIPs for homologous series, such as for H_2-n-alkane systems, as a function of temperature and carbon number.[51]

(iii) Advanced mixing rules: Moving beyond the simple van der Waals rules can dramatically improve the performance of the CEoSs. Advanced mixing rules, such as the Huron–Vidal or Wong–Sandler rules, incorporate concepts from activity coefficient models (like UNIFAC) into the EoS framework. These approaches can make a simple CEoS competitive with, or even superior to, more complex models such as PC-SAFT for certain mixture VLE calculations, particularly for polar systems. The Universal Mixing Rules-Peng–Robinson UNIFAC (UMR-PRU) model is one such example that features predictive capabilities comparable to PC-SAFT.[35]

The prediction of VLE is a cornerstone of chemical process design, essential for separation processes, solubility calculations, and phase stability analysis. For hydrogen-containing mixtures, which are often highly asymmetric (i.e., large differences in size and/or polarity between components), this is a particularly challenging task. Numerous studies have focused on key binary systems. For H_2-hydrocarbon mixtures, such as those with methane (CH_4), ethylene (C_2H_4), or heavier n-alkanes, classical CEoSs are frequently found to be inadequate.[53] Their simple van der Waals one-fluid mixing rules often fail to capture the complex phase behavior of these systems. In contrast, SAFT-based models, particularly SAFT-VR Mie, have demonstrated superior accuracy in modeling the VLE of H_2-C_2H_4 and other asymmetric systems.[53] For mixtures of hydrogen with heavy n-alkanes, critical for processes such as hydrocracking, the PR EoS can be made to reproduce experimental VLE data with high accuracy, but only through the careful tuning of interaction parameters.[54]

For H_2-water systems, which are critical for UHS and proton-exchange membrane fuel cells, the polarity of water poses a major challenge for standard EoSs.[44] While classical PR and SRK models fail to accurately predict the VLE of H_2-water mixtures, more advanced models demonstrate significant promise. Studies comparing a modified CEoS (the Schwartzentruber–Renon–modified Redlich–Kwong, SR-RK) and PC-SAFT found that both models could provide accurate predictions of hydrogen solubility and water content over a wide range of pressures and temperatures, provided their interaction parameters were properly optimized against experimental data.[44]

This evidence effectively decouples the challenge of modeling mixtures from that of modeling pure components. A theoretically superior pure-component EoS such as SAFT can yield poor mixture predictions if combined with simplistic mixing rules and zero BIPs. Conversely, a simpler CEoS can be transformed into a highly accurate correlative tool for a specific mixture by

employing advanced mixing rules and carefully tuned, temperature-dependent BIPs. This places a premium on the availability of high-quality experimental mixture data, which remains the ultimate foundation for accurate parameterization.

For multi-component mixtures of direct industrial relevance, the choice of EoS becomes a balance of accuracy, computational cost, and availability within process simulators.

(i) H_2-natural gas blends: The injection of hydrogen into natural gas pipelines is a key strategy for decarbonizing the gas grid. Accurate property prediction is essential for billing, safety, and pipeline integrity. Comprehensive evaluations of up to 12 different EoS against experimental data for H_2-NG blends have found that highly-parameterized, multi-constant EoS such as GERG-2008 and AGA8 consistently provide the best performance for predicting density, speed of sound, and isobaric heat capacity.[35] These models are specifically designed and tuned for natural gas systems and serve as industry benchmarks.

(ii) H_2-water systems with impurities: In applications such as underground storage in saline aquifers or fuel cells, the presence of other components such as CO_2 or salts can significantly alter the phase behavior. Models such as the SR-RK EoS have proven capable of modeling the influence of CO_2 impurity on H_2 solubility and water vaporization in H_2-water systems.[44] For electrolyte systems, SAFT-based models such as eSAFT-VR Mie have been developed to account for ion-solvent interactions and can accurately predict gas solubilities in brines, which is critical for designing hydrogen storage in salt caverns.[55]

The analysis of mixture modeling underscores a key practical consideration for engineers. For a well-characterized system where extensive experimental data are available, a properly tuned CEoS with sophisticated mixing rules may offer the most practical solution, providing high accuracy at a lower computational cost than a full SAFT model. However, for predictive applications where experimental data is scarce or for systems with complex components (e.g., polymers and electrolytes), the stronger physical basis of the SAFT framework makes it a more reliable and robust choice.

4. Conclusion

This review has critically evaluated the efficacy of various EoSs for modeling the thermodynamic properties of supercritical hydrogen. The analysis indicates that classical CEoSs, such as the PR and SRK models, are demonstrably insufficient for applications demanding high accuracy. Their empirical formulation fails to account for the significant quantum effects inherent to hydrogen, resulting in systematic deviations in the prediction of both volumetric and caloric properties. While quantum corrections provide tangible improvements, they function as empirical adjustments rather than addressing the fundamental limitations of the underlying classical framework.

In contrast, physically based models from the SAFT family exhibit consistently superior predictive accuracy and reliability across a wide operational range. Their foundation in molecular physics provides a robust and extensible framework for describing the complex behavior of supercritical hydrogen and its mixtures. Consequently, for high-fidelity engineering design, safety-critical analysis, and fundamental research, the adoption of a SAFT-based EoS is strongly recommended. The initial investment in model implementation is justified by the significant gains in accuracy and predictive capability.

Despite the demonstrated superiority of SAFT models, a primary impediment to their widespread industrial adoption is the lack of standardized, validated, and transferable pure-component parameters. This absence of a unified parameter set hinders the comparability of results across different studies and institutions. Therefore, a collaborative, community-driven effort to establish a single, validated, and open-access parameter database for principal SAFT variants is identified as a critical and urgent priority for the field.

Future progress necessitates a multifaceted research effort focused on several key areas. A primary priority is the refinement of the physical models themselves, particularly through the development of more theoretically-grounded quantum corrections and predictive mixing rules that can reduce the reliance on experimental BIPs. Likewise, emerging machine learning and artificial intelligence methodologies offer transformative potential. Techniques such as physics-informed neural networks, trained on *ab initio* or high-fidelity experimental data, can serve as powerful tools for generating accurate property data or as direct surrogate models in complex simulations. Finally, it must be emphasized that the development of all thermodynamic models is contingent upon the availability of high-quality experimental data, particularly for derivative properties at extreme pressures and for a wider range of hydrogen-containing mixtures. Such data are essential for the robust parameterization and validation of the next generation of predictive thermodynamic models.

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