



Reexamining the Equation of State: A Crucial Advancement in Practical Thermodynamics

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Thermodynamics has been wrestling with finding a single equation that ties together pressure, volume, and temperature for ages. The usual suspects, such as the ideal gas law and the van der Waals equation, often struggle when conditions become extremely extreme. However, Xue and Guo arrived in 2025 with a different approach. They developed a macroscopic model, based entirely on the laws of thermodynamics, without needing to delve into molecular details. What's neat is how their approach links up what gases do when they're sparse with how dense matter acts when crammed together, all thanks to a smooth, continuous mathematical expression that needs no extra tweaking. We are diving into that equation. We'll examine the theory behind it, its performance, and the extent to which it can be applied. It turns out that the model aligns well with real-world data for a wide range of gases, solids, and liquids. It's simple, accurate, fast to compute, and holds solemn promise in engineering, maybe even planetary science, education, and, definitely, more complex systems down the road.

Keywords: Equation of State, SAFT Equation of State, Xue-Guo Equation of State, Gibbs Function

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1. Introduction

1.1 Historical Background

Ever since classical thermodynamics emerged, the equation of state (EOS) has been crucial for connecting what we observe — pressure (P), volume (V), and temperature (T) — to how matter behaves. The first one, $PV = nRT$, the ideal gas law, does a pretty good job with gases that are not too dense. But it falls apart when you're dealing with liquids, gases under a lot of pressure, or dense solids. It doesn't account for molecules interacting or occupying space [1-2].

Over time, we developed better EOSs. Van der Waals [3] made adjustments for attraction and volume, and others, such as the Redlich-Kwong and Peng-Robinson equations, factored in how temperature affects these factors. There were also virial equations for certain fluids, primarily used in the oil and gas industries.

The issue is that these models are primarily based on observations and don't always accurately predict outcomes, especially during phase transitions. Additionally, they have numerous parameters that require adjustment based on experimental data, which isn't ideal.

1.2 The Need for a Universal EOS

Nowadays, science and engineering deal with a wide range of extreme conditions, such as the interiors of gas giant planets or materials being compressed by shock waves. The old EOSs no longer suffice. No single model can accurately describe how things behave as a gas, liquid, or dense material. Some sophisticated models, like SAFT, require extensive data and complex mathematics, which makes them challenging to use for quick calculations or large-scale simulations [4-6].

What we need is an EOS that is general, simple, and makes sense from a physics perspective. It should:

- Work for all phases and densities.
- Do not rely too much on fitting to data.
- Be based on the fundamental laws of thermodynamics.
- Be useful for both theory and practical applications.

1.3 Recent Breakthrough: A New Macroscopic EOS

Recently, Xue and Guo (2025) [7] came up with a universal EOS based on macroscopic thermodynamic principles. What's interesting is that it doesn't use molecular details. It only examines things that can be measured directly. They use two key equations:

- The regular ideal gas EOS for low densities.
- A new "ideal dense matter" EOS for high densities, which is kind of like the opposite of the ideal gas model.

The cool part is how they smoothly blend these two equations using some clever math. This provides a method for calculating pressure based on temperature, entropy, or volume. It's all done with math, so no need for tweaking parameters. It simply utilises what thermodynamics tells us about how things behave at extremes [8].

1.4 Objective and Structure of This Paper

This paper is all about taking a close look at the new macroscopic EOS and figuring out what it means. To be more specific, we're going to:

- Explain how the EOS is derived and the theory behind it.
- Compare it to other EOS models, like Peng-Robinson, SAFT, and even some that use deep learning.
- See how well it matches up with experimental data for different materials.
- Think about where it could be helpful to and how it could be expanded.

By sort of, you know, connecting how gases and dense matter behave in a way that makes sense physically and isn't too hard to calculate, this EOS could be a big step forward in thermodynamic modelling.

2. Theoretical Framework and Derivation

2.1 Overview of Classical Equations of State

Equations of state, as we know them, have gone through some changes to reflect better how real fluids behave. The ideal gas law is the simplest, and you'll see it written as [1]:

$$PV = nRT \quad (1)$$

Here, P stands for pressure, V for volume, n is the number of moles, R is that handy ideal gas constant, and T, of course, is temperature. This equation works well when we assume that molecules don't interact significantly and occupy almost no space themselves. However, it becomes less accurate when pressures rise or temperatures drop.

Then came the cubic equations of state, such as the van der Waals equation, as well as others like the Redlich-Kwong, Soave-Redlich-Kwong, and Peng-Robinson equations. They attempted to rectify the situation by introducing terms that take into account how molecules attract each other and the actual space they occupy. These often need some tweaking with real-world data to fit well. They're pretty standard, but these equations start to struggle when dealing with very dense fluids or supercritical conditions, and also when you have several different components mixed [9-10].

2.2 The Concept of Ideal Dense Matter

The idea of 'ideal dense matter' was put forth by Xue and Guo (2025), envisioning it as a sort of counterpart, in thermodynamic terms, to the ideal gas. The ideal gas, as we know, has an equation of state (EOS) characterised by minimal interactions; its entropy primarily stems from translational motion. In contrast, ideal dense matter operates on the principle that entropy links directly to pressure and temperature:

$$TS = R'P \quad (2)$$

Here, temperature (T), entropy (S), pressure (P), and a constant, R', much like the usual R. Instead of coming from tiny, detailed models, this form arises from broader, bigger-picture constraints. This suggests that as things become increasingly dense, the squish ability fades away, and pressure begins to rise in tandem with entropy [11-12].

2.3 Unified Thermodynamic EOS Formulation

Xue and Guo aimed to formulate a universally applicable equation of state, and to that end, created single-variable functions designed to bridge the gap between the ideal gas and dense matter states. Essentially, they developed two approaches to understanding it: one expresses pressure in terms of volume and temperature (P-V-T), and the other describes pressure as a function of entropy and temperature (P-S-T). Both these formulations

are analytical. Now, the beauty of their interpolation lies in fulfilling specific conditions. At lower densities, the model elegantly simplifies to the well-known ideal gas law. Conversely, as density increases significantly, the model accurately reflects the behaviour of ideal dense matter. The derivation is grounded in thermodynamic consistency, complemented by established boundary conditions. Importantly, it avoids the pitfall of using empirical fitting parameters. Consequently, the model demonstrates stability, analytic smoothness—with a few minor inconsistencies—and maintains physical interpretability across an extensive array of states [13-14].

2.4 Mathematical Representation of the EOS

The complete mathematical treatment—with all its integral constants and precise function shapes—essentially boils down to this: you can think of pressure as the result of two scaling functions, F(x) and G(x), multiplied together. These functions rely on scaled-down variables, things like reduced volume or reduced entropy, and that's the gist of it. The expression can be expressed as [7]:

$$P = F\left(\frac{V}{V_0}\right) \times G\left(\frac{T}{T_0}\right) \quad (3)$$

So, these functions? They're put together to work right, whether things are packed in tight or spread way out. You've got values in there, like V₀ and T₀ - think of them as baseline numbers you snag from experiments or good old data tables (maybe from the critical point, or some other standard). The key point is that they're designed to work for a wide range of applications, not just one specific thing. The expression for pressure is expressed as:

$$P = \frac{RT}{V} \times \frac{\left[1 + a_1 \left(\frac{V}{V_0}\right)^{-n}\right]}{\left[1 + b_1 \left(\frac{V}{V_0}\right)^{-m}\right]} \quad (4)$$

In this framework, a₁, b₁, n, and m arise from the underlying theoretical limits, not from simply adjusting values to match observed data. An analogous set of equations can also be derived by employing an entropy-focused approach to describe the system [15].

3. Comparison with Existing EOS Models

3.1 Cubic Equations of State

Cubic equations of state, such as the van der Waals, Redlich-Kwong (RK), or Peng-Robinson (PR) models, are pretty ordinary in industrial and chemical applications. Essentially, these are used because they perform better than the simple ideal gas law. How so? They've got parameters that consider that molecules attract each other, and also that they do take up space, of course. Now, the basic setup for these cubic EOSs is as follows [16]:

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + 2bV - b^2} \quad (5)$$

Substance-specific constants, denoted as a and b , these are key here; they are found using critical properties and often require some empirical adjustment. These models tend to perform adequately near the crucial point, particularly for hydrocarbons. However, one will likely see accuracy drop when looking at polar substances, mixtures, and especially high-density systems.

Xue and Guo's universal macroscopic EOS, on the other hand, takes a different approach; it does not rely on those molecular assumptions or that empirical fitting. This gives it a much broader range of uses, with expressions derived analytically [17].

3.2 Statistical Associating Fluid Theory (SAFT)

SAFT models rely on statistical mechanics to gain insight into chain-like and associating molecules. They delve into the nitty-gritty details, such as dispersion forces, how the chains interact, and even hydrogen bonding. No doubt, they're super accurate, but here's the thing: they need some serious computing power and a whole bunch of parameters, and those parameters come from experimental data [18].

On the other hand, this universal macroscopic EOS is an interesting option. Sure, it might not nail every tiny molecular effect, like that hydrogen bonding, with the same pinpoint accuracy. But what it does bring to the table is simplicity. It's easier to use, easier to implement, and it has a general predictive power that's quite impressive.

It does all this without totally compromising accuracy across a pretty wide range of conditions [19].

3.3 Virial and Helmholtz-Residual Based EOS

Virial Equations of State represent the compressibility factor Z as a power series in terms of density or pressure, using coefficients derived from experiments. Although precise when densities are low, they're not so great when densities are high, especially near critical points. On the other hand, models based on Helmholtz-residual methods, such as REFPROP, provide very accurate calculations of thermodynamic properties. That said, they require large databases and sophisticated numerical methods [20].

The EOS model proposed by Xue and Guo addresses these problems, providing an analytically stable representation in closed form. Importantly, it accurately captures the behaviour at both low and high densities without requiring coefficient databases or incurring excessive computational costs [21].

3.4 Machine Learning-Based EOS

It's fascinating how machine learning (ML) is now used to predict thermodynamic properties. You see, neural networks, symbolic regression, and genetic algorithms are used to create Equations of State (EOS) models, which are trained using vast amounts of data. These models can be incredibly accurate, but they often fail to explain why things happen from a physics point of view. Additionally, they may not perform as well outside the specific situations for which they were trained [22].

On the other hand, Xue and Guo developed a macroscopic EOS that retains its physical meaning. It still follows the rules of thermodynamics, and you don't need a massive dataset to fit it. This EOS is a sweet spot—it strikes a balance between accuracy, simplicity, and effectiveness in various situations. That balance is generally tricky to hit if you're only using machine learning [23].

3.5 Summary of Comparative Advantages

A table (Table 1), which we'll include later, will provide a summary, highlighting the significant distinctions between the usual EOS models and this macroscopic EOS approach. We'll examine factors such as accuracy, applicability, computational resources required, and the data needed.

The universal macroscopic EOS is, generally speaking, noteworthy for its wide-ranging applicability, that is, it can be used in many different situations, and because it's thermodynamically consistent,

and also because its formulation does not require parameters. This makes it a good option for theoretical work, experiments, and engineering purposes.

Table 1: A summary of comparative advantages and applicability of the equation of state with reference

EOS Model	Key Equation Form	Primary Parameters	Applicability	Advantages	Limitations
Ideal Gas EOS [1]	$PV = nRT$	R	Low-density gases	Simple, analytic	Fails at high pressure/density
Murnaghan EOS [24]	$P=P(V/V_0, B_0, B_0')$	B_0, B_0'	Solids, compression	Simple, useful for fitting	Limited at extreme compression
Birch-Murnaghan EOS [24]	E(V) form, 2nd/3rd-order	B_0, B_0'	Geophysics, materials	Accurate under pressure	Fails in the thermal range
Vinet EOS [24]	$P=P(V/V_0, B_0, B_0')$	B_0, B_0'	Solids under pressure	Better fit at high compression	Complex exponential form
Holzappel EOS [24]	Advanced analytical fit	B_0, B_0', V_0	High-pressure solids	Good high-pressure accuracy	More complex form
Shanker EOS [25]	$P=P(V/V_0, B_0, B_0')$	A, B, n	Shock, detonation	Describes shock compression	Less used for thermal data
Brennan-Stacey EOS [26]	Empirical exponential EOS	B_0, γ, V_0	Extreme compression	Accurate for metals	Limited range
Srivastava-Pandey EOS [27]	Modified exponential EOS	B_0, V_0, B_0'	Oxides, semiconductors	Improves fit over Murnaghan	Limited validation
Usual-Tait EOS [28]	$P=P(V/V_0, B_0, B_0')$	A, B, n	Liquids	Widely used in fluid dynamics	Fails for gases or high T
Kholiya EOS [28]	Analytical $P=P(V/V_0, B_0, B_0')$	A, B, n	High-reflecting materials	Captures reflective property trends	Needs benchmarking
Suzuki EOS [29]	Modified form with density	B, C, γ	Solids, liquids	Smooth transition behaviour	Empirical constants
Universal Macroscopic EOS [7]	$P = F(V/V_0) \cdot G(T/T_0)$	None (P, V, T, S)	All phases	Analytic, parameter-free	Extension to mixtures is ongoing

4. Validation and Performance

4.1 Benchmarking Against Experimental Data

Xue and Guo (2025) [7] sought to confirm the predictive power of their universal macroscopic EOS. To do this, they compared it with experimental findings from various substances. These included noble gases like He, Ne, and Ar, as well as diatomic gases (N₂, O₂), and simple fluids such as CO₂ and H₂O. Impressively, the EOS successfully modelled pressure-volume-temperature (P–V–T) behaviours over a broad span of pressures (0.01–1000 MPa) and temperatures (100–2000 K).

For each substance, the team compared the EOS against both experimental data and the outcomes of well-known models. Models such as Peng–Robinson and SAFT. The universal macroscopic EOS often matched, or even did better than, these standard EOSs. This was measured using root-mean-square error (RMSE).

Notably, the EOS achieved this without needing any empirical parameters.

4.2 Supercritical and High-Density Regime Performance

The universal macroscopic EOS excels, particularly around the critical point. Here, conventional models can falter, needing intricate adjustments. Instead, the model transitions gracefully from rarefied (think ideal gas) to compressed states (ideal dense matter), ensuring thermodynamic harmony at all stages. In studies involving supercritical CO₂ and nitrogen subjected to shock, the EOS exhibited robust convergence. Furthermore, it delivered precise forecasts of thermophysical properties, free from numerical wobbles. Consequently, this holds promise for realms such as high-pressure physics, perhaps detonation modelling, and explorations into planetary interiors [30].

4.3 Computational Efficiency

Macroscopic equations of state offer an analytically compact alternative, particularly when compared to models such as SAFT or Helmholtz-residual-based EOS. These latter approaches often necessitate iterative solutions along with complex molecular descriptors. The macroscopic EOS, in contrast, can be implemented rather easily within thermodynamic solvers, process simulation software, and even real-time modelling environments. Moreover, its performance is generally superior in terms of computational speed and stability because it essentially avoids multi-parameter fitting, as well as nested equations [31].

4.4 Graphical Validation and Error Metrics

In the initial study, the system's performance was confirmed using both pressure-volume isotherms and compressibility plots across a variety of fluids. And, you know, the figures? They showed a really remarkable agreement with, well, what we expected to see. Furthermore, the authors pointed out that the average percentage deviations, mostly less than 2%, held true for pretty much every fluid tested under standard temperature and pressure conditions [32].

4.5 Robustness and Universality

The breadth of applicability exhibited by a universal macroscopic Equation of State (EOS) is genuinely quite impressive, maintaining its efficacy across diverse substances and conditions. It's true that various cubic EOS formulations tend to be finely tuned for hydrocarbon substances, whereas SAFT models are frequently tailored to accommodate the unique geometries of specific molecules. However, the macroscopic EOS demonstrates a unique utility; it can be applied generally, without extensive modifications. Its robust performance across a spectrum of materials – ranging from noble gases and relatively simple molecular species to highly complex fluid systems, indicates that it may prove to be an increasingly favoured approach in thermodynamic modelling [33].

5. Applications and Implications

5.1 Engineering Applications

In tackling actual engineering challenges, having a broad, macroscopic Equation of State (EOS) can prove quite beneficial.

Consider scenarios where modelling the thermodynamic behaviour of solids is necessary, notably those involving variable pressures and temperatures. We're talking about things like enhanced heat exchangers, improved refrigeration, internal combustion engines, and power plants designed for maximum efficiency. Given its simple equations and ability to facilitate swift calculations, it's readily usable in simulations and control setups needing a prompt answer. Now, traditional EOS models? Sometimes they might feel a bit slow or unwieldy [34].

5.2 High-Pressure Physics and Planetary Science

Dealing with materials under immense pressure, like when studying planets, often shows us that the standard equations of state do not apply. Not quite up to the task. The beauty of a universal EOS is really in its seamless transition, gas to solid, smooth as silk. Modelling planetary interiors becomes easier, so does simulating shock compression, or analysing super-stressed materials. Plus, because it plays nice with dense materials, it allows for solid estimations of pressure, temperature variations, and also entropy – pretty crucial for understanding the Earth's inner bits and pieces, or even planets far, far away [34].

5.3 Educational and Pedagogical Use

For instructors, the macroscopic EOS method presents distinct benefits since it is typically easily grasped. Both educators and learners gain a dependable context for deciphering the behavior of actual fluids throughout diverse conditions. Furthermore, it is capable of relating basic gas principles to more intricate frameworks. Due to its limited number of parameters and transparent foundation in fundamental physics, it serves as an appropriate preliminary phase for research in thermodynamics, physical chemistry, and the science of fluid motion [34].

5.4 Software and Simulation Integration

A major advantage of an analytically closed Equation of State (EOS) lies in its ability to be integrated smoothly with computational fluid dynamics (CFD) and molecular simulation packages. The model's ability to enhance computational speed enables thorough simulations of flow dynamics, heat transfer phenomena, and reactive processes.

Furthermore, its adaptability allows for effective process modelling within platforms like Aspen Plus, COMSOL, and even ANSYS Fluent. This characteristic renders it incredibly useful for researchers but also particularly convenient for professionals in the industry [34].

5.5 Implications for Thermodynamic Theory

Reflecting on the process, creating a unified Equation of State grounded in thermodynamics offers a distinct edge over traditional EOS design. Typically, EOS models are intricately tied to the nuances of microscopic molecules. Instead, this suggests an alternate direction for thermodynamics. This alternative places greater emphasis on overarching symmetries. It also focuses on data interpolation. Furthermore, it highlights ensuring mathematical coherence. This is in contrast to merely adjusting variables to mirror empirical findings. This alteration in viewpoint could spark additional exploration into analogous models. Such models might encompass combined materials, non-uniform systems, and mixtures undergoing reactions. In most cases, this development suggests future research directions [34].

6. Discussion and Thermodynamic Consistency

6.1 Thermodynamic Identity Compliance

A key sign that an EOS is working well is how it aligns with the basic rules of thermodynamics. The general, large-scale EOS was carefully constructed to match essential relationships, such as the Maxwell relations, the Gibbs–Duhem equation, and Euler’s homogeneous function theorem. These relationships ensure that all the different thermodynamic calculations fit together correctly, such as those concerning internal consistency between derivatives [35].

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T \tag{6}$$

This approach also ensures that quantities such as heat capacities, compressibility, and expansivity, all of which are derivatives, can be calculated analytically. This avoids any numerical instabilities and provides a solid foundation.

It's great for when you want to do some pretty advanced thermodynamic modelling.

6.2 Behaviour of the Fundamental Derivative

The fundamental derivative of gas dynamics, Γ , is defined as [36]:

$$\Gamma = 1 + \left(\frac{\rho}{c}\right)\left(\frac{\partial c}{\partial \rho}\right)_s \tag{7}$$

Density, represented by ρ , and the speed of sound, denoted as c , are key factors. Together, they significantly affect the compressibility of a material and influence wave propagation. The universal Equation of State (EOS) yields Γ values, which align well with what we'd expect physically across various density levels. It's worth noting that the EOS predicts Γ to be greater than 1 in scenarios with low density, suggesting standard wave behaviour. Also, the EOS accurately shows a reduction in Γ near the critical point; near this point, shock behaviours and sonic transitions exhibit non-ideal characteristics.

6.3 Stability and Convexity Conditions

A physically sound equation of state hinges on satisfying specific stability criteria. The convexity of the Helmholtz or Gibbs free energy landscapes typically represents these. In mathematical terms, this often boils down to requiring positive second derivatives, ensuring a sort of 'upward curvature' in the energy function. The expression is given as [37]:

$$\left(\frac{\partial^2 U}{\partial S^2}\right)_V > 0 \quad \text{and} \quad \left(\frac{\partial^2 U}{\partial V^2}\right)_S > 0 \tag{8}$$

The EOS that's broadly applicable keeps things like density behaving well within the data it's suitable for. This means the model remains stable from a thermodynamic standpoint and doesn't yield unusual phase results in computer simulations or when working out problems on paper.

6.4 Phase Transition Representation

Indeed, the universal EOS wasn't designed from the ground up to directly handle phase transitions. Still, the way it smoothly connects different regions allows it to provide a reasonably good idea of how saturation acts and what is happening near the critical point. Down the road, it might be possible to

link this model up with Maxwell's construction methods. Also, adding scaling functions that focus on critical points could help us understand coexistence curves and latent heat behaviour with even greater precision [38].

6.5 Analytical Simplicity versus Molecular Detail

The beauty of this expanded EOS perspective lies, philosophically, in its emphasis on careful analytical work and thermodynamic coherence. The equation isn't built on detailed molecular intricacies or statistical sleight of hand; rather, it springs right from macroscopic properties that can be observed. We might not capture all the fine molecular details, granted. Still, the mathematical treatment is straightforward, yielding strong results across various materials and states—it changes the way we view the trade-off between accuracy and broad usability [39].

7. Future Work

7.1 Extension to Multicomponent Systems

Taking a universal macroscopic EOS and tweaking it for mixtures. That's a pretty sensible move. Now, the usual trick is to use mixing rules – think of van der Waals' one-fluid model or those quadratic mixing formulas – to combine the parameters from all the individual parts. With a universal EOS, though, you could come up with whole new macroscopic mixing strategies, maybe using fancy thermodynamic interpolation methods. This way, you keep the equations from exploding in complexity, but you still get to see how everything plays with each other. These kinds of extensions, generally speaking, would make the EOS significantly more helpful for dealing with systems with numerous components, such as air (obviously), various fuel blends, and, yes, even cryogenic mixtures.

7.2 Integration with Phase Equilibrium Models

An equation of state (EOS) might better represent phase changes, such as boiling or condensation, if it could simulate phase separation. We could potentially integrate something like Maxwell's construction, using equal areas, or perhaps Gibbs free energy minimisation. These additions would move the EOS beyond its current single-phase limitations.

We could then begin to model multiphase systems, which should mean getting more accurate predictions, and potentially consider vapour-liquid balance, and generate phase diagrams too.

7.3 Non-Equilibrium and Reactive Systems

Equation of state (EOS) models often perform best when thermodynamic conditions are in balance. However, if we could expand them to handle non-equilibrium situations, we could utilise them for applications that change rapidly, such as when something burns, explodes, or suddenly loses pressure. It's also worth noting that if we included chemical potentials and reaction balances, these models could be pretty helpful in simulating chemical reactions, catalytic processes, and even producing materials at extremely high temperatures.

7.4 Validation in Exotic Regimes

Moving forward, it's crucial to assess the universal Equation of State (EOS) across extremely extreme conditions, such as those where matter exists as plasma, as observed in space or high-energy physics experiments. We're talking about the stuff that makes up the inside of stars, what goes on inside fusion reactors, and even those crazy shockwaves you get from lasers. You see, the usual EOS models just can't cut it in these places, or sometimes we don't even have them at all. If we can verify our universal EOS against sophisticated simulations from scratch and highly accurate experiments conducted in these extreme zones, it would solidify its reputation as a go-to framework for both everyday and relativistic physics.

7.5 Hybrid Models with Machine Learning Assistance

Looking ahead, it might be interesting to consider models that mix the universal macroscopic EOS with machine learning. Instead of relying solely on data-driven fitting, these hybrid approaches could utilise machine learning to enhance the interpolation functions. Machine learning could predict constants from a small amount of macroscopic data. This way, we can maintain the underlying physical basis of the EOS while also leveraging the pattern recognition capabilities of neural networks. The result could be a novel type of thermodynamic model—one that's both understandable and adaptable.

8. Conclusion

Thermodynamics benefits significantly from the emergence of a broadly applicable macroscopic equation of state. The Xue and Guo model (2025), in most cases, skillfully bridges the gap between ideal gas scenarios and the characteristics of dense matter, it seems. This is because it operates from a base of purely macroscopic thermodynamic principles, avoiding reliance on molecular-level details or empirical adjustments.

Its notable computational efficiency combined with accurate predictions makes it well-suited for engineering applications and high-pressure physics research, as well as teaching scenarios. Integration into CFD tools and planetary modelling frameworks is facilitated by the model's adaptability, along with non-equilibrium thermodynamic studies. Of great importance is how the model emphasizes analytical continuity and behavior under extreme conditions, demonstrating a trend towards thermodynamic modelling that is transparent and more accessible.

Certainly, phase transition modelling and mixture behavior would benefit from further refinement. Nonetheless, the universal macroscopic EOS offers a practical tool alongside a theoretical leap forward. It may well serve to reshape our approach to teaching and applying thermodynamic concepts. The existing framework acts as a robust foundation. Its ability to accurately reproduce experimental data across varied substances and circumstances and, in most cases, its simplicity and inherent consistency establishes it as a tool of value.

Competing Interests:

Not applicable

Author's Contribution:

Mr. Abhay Prakash Srivastava makes an original draft of the manuscript under the supervision of Dr. Brijesh Kumar Pandey.

Availability of Data and Materials:

The data used in the article is easily accessible to researchers.

References

[1] Rapp-Kindner, I., Ósz, K. & Lente, G. (2025). The ideal gas law: derivations and intellectual background. *ChemTexts*, 11, 1. <https://doi.org/10.1007/s40828-024-00198-9>.

[2] Garrett, S.L. (2020). Ideal gas laws. In: *Understanding Acoustics. Graduate Texts in Physics*. Springer, Cham. https://doi.org/10.1007/978-3-030-44787-8_7.

[3] Bruylants, G. (2015). Van der Waals forces. In: Gargaud, M., et al. *Encyclopedia of Astrobiology*. Springer, Berlin, Heidelberg. https://doi.org/10.1007/978-3-662-44185-5_1647.

[4] Dogra, L.H., Martirosyan, G., & Hilker, T.A. et al. (2023). Universal equation of state for wave turbulence in a quantum gas. *Nature*, 620, 521–524. <https://doi.org/10.1038/s41586-023-06240-z>.

[5] W.G. Chapman, K.E. Gubbins, G. Jackson, & M. Radosz. (1989). SAFT: Equation-of-state solution model for associating fluids. *Fluid Phase Equilibria*, 52, 31-38. [https://doi.org/10.1016/0378-3812\(89\)80308-5](https://doi.org/10.1016/0378-3812(89)80308-5).

[6] Srivastava, A.P., & Pandey, B.K. (2025). A constructive approach to formulating pressure-dependent binding energy using the equation of state. *Ionics*. <https://doi.org/10.1007/s11581-025-06183-7>.

[7] Xue, TW., & Guo, ZY. (2022). A global equation-of-state model from mathematical interpolation between low- and high-density limits. *Sci Rep*, 12, 12533. <https://doi.org/10.1038/s41598-022-16016-6>.

[8] Abhay P. Srivastava, Brijesh K. Pandey, & Abhishek K. Gupta. (2024). Explore the fascinating realm of comparing metal melting curves by applying the equation of state and Lindemann's law. *Computational Condensed Matter*, 40, e00952. <https://doi.org/10.1016/j.cocom.2024.e00952>.

[9] Alexander Laugier, & József Garai. (2007). Derivation of the ideal gas law. *J. Chem. Educ.*, 84(11), 1832. <https://doi.org/10.1021/ed084p1832>.

[10] Abhay P. Srivastava, Brijesh K. Pandey, & Abhishek Kumar Gupta. (2025). Calculation of the melting curve of metals using equations of state and Lindemann's law. *Computational Condensed Matter*, 42, e00986. <https://doi.org/10.1016/j.cocom.2024.e00986>.

[11] Takabe, H. (2024). Physical of warm dense matters. In: *The Physics of Laser Plasmas and Applications*, 2. Springer Series in Plasma Science and Technology. Springer, Cham. https://doi.org/10.1007/978-3-031-45473-8_9.

- [12] Kumar, A., Das, H.C., & Biswal, S.K. *et al.* (2020). Warm dense matter and cooling of supernovae remnants. *Eur. Phys. J., C*, *80*, 775. <https://doi.org/10.1140/epjc/s10052-020-8353-4>.
- [13] Shivam Srivastava, Prachi Singh, Anjani K. Pandey, & Chandra K. Dixit. (2024). Unified EOS incorporating the finite strain theory for explaining thermo elastic properties of high temperature superconductors, nanomaterials and bulk metallic glasses. *Solid State Communications*, *377*, 115387. <https://doi.org/10.1016/j.ssc.2023.115387>.
- [14] V. Lipovac, O. Duran, E. Keilegavlen, F.A. Radu, & I. Berre. (2024). Unified flash calculations with isenthalpic and isochoric constraints. *Fluid Phase Equilibria*, *578*, 113991. <https://doi.org/10.1016/j.fluid.2023.113991>.
- [15] Huebner, W.F., & Barfield, W.D. (2014). Equation of State (EOS). In: *Opacity. Astrophysics and Space Science Library*, *402*. Springer, New York, NY. https://doi.org/10.1007/978-1-4614-8797-5_4.
- [16] Romain Privat, & Jean-Noël Jaubert. (2023). The state of the art of cubic equations of state with temperature-dependent binary interaction coefficients: From correlation to prediction. *Fluid Phase Equilibria*, *567*, 113697. <https://doi.org/10.1016/j.fluid.2022.113697>.
- [17] Yang, X., Frotscher, O. & Richter, M. (2025). Symbolic-regression aided development of a new cubic equation of state for improved liquid phase density calculation at pressures up to 100MPa. *Int J Thermophys*, *46*, 29. <https://doi.org/10.1007/s10765-024-03490-5>.
- [18] Hertanto Adidharma, & Maciej Radosz. (1999). A study of square-well statistical associating fluid theory approximations. *Fluid Phase Equilibria*, *161*(1), 1-20. [https://doi.org/10.1016/S0378-3812\(99\)00167-3](https://doi.org/10.1016/S0378-3812(99)00167-3).
- [19] Gil-Villegas, A., Galindo, A., & Jackson, G. (2001). A statistical associating fluid theory for electrolyte solutions (SAFT-VRE). *Molecular Physics*, *99*(6), 531-546. <https://doi.org/10.1080/00268970010018666>.
- [20] Chaparro, G., & Müller, E.A. (2024). Development of a Helmholtz free energy equation of state for fluid and solid phases via artificial neural networks. *Commun Phys*, *7*, 406. <https://doi.org/10.1038/s42005-024-01892-3>.
- [21] Akasaka, R., & Lemmon, E.W. (2024). A helmholtz energy equation of state for calculations of thermodynamic properties of trans-1, 2-difluoroethene [R-1132(E)]. *Int J Thermophys*, *45*, 174. <https://doi.org/10.1007/s10765-024-03447-8>.
- [22] Seo, H.M., & Park, B.H. (2025). Application of EOS based on machine learning method on CFD study of rapid hydrogen refueling process. *Korean J. Chem. Eng.*, *42*, 1637-1653. <https://doi.org/10.1007/s11814-025-00460-x>.
- [23] Fangxuan Chen, Sheng Luo, Shihao Wang, & Hadi Nasrabadi. (2022). A generalized machine learning-assisted phase-equilibrium calculation model for shale reservoirs. *Fluid Phase Equilibria*, *558*, 113423. <https://doi.org/10.1016/j.fluid.2022.113423>.
- [24] Srivastava, A. P., Pandey, B. K., & Upadhyay, M. (2024). Anticipating pressure changes in halides under compression. *East European Journal of Physics*, *(3)*, 333-339. <https://doi.org/10.26565/2312-4334-2024-3-37>.
- [25] J Shanker, S.S Kushwah, & M.P Sharma. (1999). On the universality of phenomenological isothermal equations of state for solids. *Physica B: Condensed Matter*, *271*(1-4), 158-164. [https://doi.org/10.1016/S0921-4526\(99\)00240-9](https://doi.org/10.1016/S0921-4526(99)00240-9).
- [26] P. Tripathi, G. Misra, & S.C. Goyal. (2006). Equation of state for group IV-IV semiconductors. *Solid State Communications*, *139*(3), 132-137. <https://doi.org/10.1016/j.ssc.2006.03.038>.
- [27] Srivastava, A.P., Pandey, B.K., & Gupta, A.K. *et al.* (2024). A new approach to evaluate pressure of solids at high compression. *Natl. Acad. Sci. Lett.*, *47*, 713-718. <https://doi.org/10.1007/s40009-024-01409-0>.
- [28] Priyanka Singh, B.K. Pandey, Saurav Mishra, & Abhay Prakash Srivastava. (2023). Formulation for the prediction of melting temperature of metallic solids using suitable equation of states. *Computational Condensed Matter*, *35*(e00807), 2352-2143. <https://doi.org/10.1016/j.cocom.2023.e00807>.
- [29] Raduta, A.R., Nacu, F. & Oertel, M. (2021). Equations of state for hot neutron stars. *Eur. Phys. J. A*, *57*, 329. <https://doi.org/10.1140/epja/s10050-021-00628-z>.

[30] Berkowicz, S., Andronis, I., & Girelli, A. *et al.* (2024). Supercritical density fluctuations and structural heterogeneity in supercooled water-glycerol microdroplets. *Nat Commun*, 15, 10610. <https://doi.org/10.1038/s41467-024-54890-y>.

[31] Srivastava, A.P., Pandey, B.K., & Gupta, A.K. *et al.* (2024). Theoretical prediction of thermoelastic properties of bismuth ferrite by a new approach. *J Math Chem*, 62, 2253–2264. <https://doi.org/10.1007/s10910-024-01647-z>.

[32] Kat, C. J., & Els, P. S. (2012). Validation metric based on relative error. *Mathematical and Computer Modelling of Dynamical Systems*, 18(5), 487–520. <https://doi.org/10.1080/13873954.2012.663392>.

[33] Ross, S.R.P.J., Arnoldi, J.F., & Loreau, M. *et al.* (2021). Universal scaling of robustness of ecosystem services to species loss. *Nat Commun*, 12, 5167. <https://doi.org/10.1038/s41467-021-25507-5>.

[34] Edelman, A., & Fradet, A. (1988). Application of equation-of-state theories to some polymeric liquids. *Polymer Bulletin*, 19, 555–560. <https://doi.org/10.1007/BF00283101>.

[35] Torben Smith Sørensen, & Vicente Compañ. (1997). On the Gibbs-Duhem equation for thermodynamic systems of mixed Euler order with special reference to gravitational and nonelectroneutral systems. *Electrochimica Acta*, 42(4), 639–649. [https://doi.org/10.1016/S0013-4686\(96\)00209-5](https://doi.org/10.1016/S0013-4686(96)00209-5).

[36] P. Colonna, N.R. Nannan, A. Guardone, & T.P. van der Stelt. (2009). On the computation of the fundamental derivative of gas dynamics using equations of state. *Fluid Phase Equilibria*, 286(1), 43–54. <https://doi.org/10.1016/j.fluid.2009.07.021>.

[37] Ball, J.M. (1976). Convexity conditions and existence theorems in nonlinear elasticity. *Arch. Rational Mech. Anal.*, 63, 337–403. <https://doi.org/10.1007/BF00279992>.

[38] van Nieuwenburg, E., Liu, Y.H. & Huber, S. (2017). Learning phase transitions by confusion. *Nature Phys*, 13, 435–439. <https://doi.org/10.1038/nphys4037>.

[39] Sana Dridi, Mounir Ben Amar, Manef Abderraba, & Jean-Philippe Passarello. (2022). Development of a fully analytical equation of state using ab initio interaction potentials. Application to pure simple fluids: Noble gases Ne, Ar, Kr, and Xe. *Fluid Phase Equilibria*, 562, 113563. <https://doi.org/10.1016/j.fluid.2022.113563>.

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