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Comparative evaluation of EMDB 2.1 and deep learning for predicting JWL equation-of-state parameters of CHNO explosives

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Abstract Predicting detonation behavior — often called the explosive's "performance fingerprint" — has long been a bottleneck in engineering design, constrained by safety, cost, and time. Traditional testing is not only hazardous but also slow and expensive. Deep learning offers a data-driven approach for predicting detonation velocity, pressure, and Jones-Wilkins-Lee (JWL) EOS coefficients. However, most deep learning models operate as black boxes and do not provide physical interpretability. To address this limitation, this work evaluates the physics-based EMDB 2.1 platform, a thermodynamic modeling framework that calculates detonation parameters from molecular composition and charge density, and compares its predictions with those of a deep learning model. Both the deep learning model and EMDB 2.1 deliver engineering-grade accuracy in predicting detonation pressure and velocity. Notably, EMDB 2.1 consistently outperforms the deep learning model, especially in pressure (root-mean-square error (RMSE): 0.8 GPa vs. 1.2 GPa) and velocity (RMSE: 0.10 km/s vs. 0.14 km/s). When predicting JWL EOS parameters, both methods generate isentropic expansion curves for the three benchmark explosives TNT, HMX, and Octol (HMX 78%/TNT 22%) that are in reasonable agreement with the reference curves derived from experimental data. Although the individual JWL parameters (A, B, C, R_1, R_2, and ω) differ numerically between the two models, their resulting curves show similar behavior for these cases.

Keywords: Detonation parameter; Jones-Wilkins-Lee (JWL) EOS; Deep learning; EMDB 2.1; Safety

1. Introduction

Energetic materials including propellants, explosives, and pyrotechnics have shaped human history through their transformative roles in warfare, aerospace, and industry [1]. Central to their performance is detonation behavior, which hinges on two key aspects: the characteristics of the detonation wave (collectively termed "detonation parameters") and the subsequent expansion of high-pressure detonation products [2]. Given the extreme danger and cost of experimental detonation testing, researchers have increasingly turned to computational methods including numerical simulations, theoretical modeling, and specialized software to predict detonation performance. For instance, numerical models have successfully simulated shockwave propagation and bubble pulsation in underwater explosions [3]. To avoid costly and hazardous experiments, three main non-experimental approaches are employed to estimate detonation parameters: empirical formulas, thermochemical calculations, and quantum chemical methods [2]. Empirical formulas require only molecular composition as input and yield rapid, albeit limited, predictions. Their utility is constrained by applicability to known compounds and difficulty in validating new formulations. Thermochemical methods grounded in free energy minimization and Chapman-Jouguet (CJ) theory offer broader applicability across novel and complex explosives. Programs such as RUBY [4], FORTRAN BKW [5], CHEETAH [6], ICT [7-8], and EXPLO5 [9], and KHT [10], implement these principles using various equations of state (EOS). Quantum chemical methods such as density functional theory provide high-fidelity theoreticalpredictions but demand immense computational resources and time, limiting their practical use in rapid design cycles. This gap has spurred interest in machine learning (ML), particularly deep learning, as a faster, more accessible alternative. The deep learning models built on artificial neural networks (ANNs) learn from large datasets of molecular descriptors and corresponding detonation parameters. Once trained, these models can rapidly predict detonation velocity, pressure, and other key metrics often outperforming traditional methods in speed and usability [11-14].Current deep learning -based models, however, face critical limitations. Most are trained on single-component explosives, neglecting real-world applications where warheads rely on mixed explosives. Additionally, while deep learning can predict detonation parameters, it rarely extends to predicting EOS parameters such as Jones-Wilkins-Lee (JWL) coefficients which are essential for simulating explosive damage. These coefficients are traditionally derived from cylinder experiments and vary with charge density [15-20]. Furthermore, inverse prediction inferring explosive composition from known detonation properties remains underexplored, despite its high engineering value. To address these gaps, Yang et al. [14] introduced threenovel deep learning -based models each trained on data from the KHT code [10], to simultaneously tackle: 1. Direct prediction of detonation parameters (e.g., velocity, pressure) from mass fractions and charge density. 2. Prediction of JWL EOS parameters critical for modeling detonation effects using the same inputs. 3. Inverse prediction: reconstructing explosive composition and charge density from detonation parameters and isentropic expansion curves. The proposed models based on ANN and 1D convolutional neural networks (CNN1D) are designed to be computationally efficient and accessible for routine use, and applicable to both single- and multi-component explosives. Unlike quantum chemistry or thermochemical methods, they do not require extensive computational resources or deep domain expertise.EMDB 2.1 [21] is a new version of EMDB [22],the Energetic Materials Designing Bench that is a software platform developed for prediction, analysis, and optimization based on the available experimental data engineered to predict, analyze, and optimize the behavior of energetic materials (EMs) across a wide spectrum of applications from aerospace propulsion to defense systems and pyrotechnics. At

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its core, EMDB calculates over thirty critical physicochemical and, detonation parameters for both ideal and non-ideal explosive formulations. These parameters include detonation velocity, pressure, specific impulse, heat of explosion, gas-phase composition, and more , all derived from first-principles thermodynamic modeling. What makes EMDB 2.1 unique is its flexibility: it accepts as input not just single-component explosives, but also complex, multi-component mixtures including those with non-ideal behavior, such as those involving aluminum (Al), ammonium nitrate (AN), and ammonium perchlorate (AP). These three components are particularly significant in modern EM design Al enhances energy output via combustion and metal vaporization, AN and AP serve as powerful oxidizers in solid propellants and high-explosives. This study evaluates the capability of EMDB 2.1 to estimate the coefficients of the JWL equation of state using thermodynamic outputs generated by the software. The calculated performance parameters are used to establish relationships with the corresponding JWL coefficients. Because EMDB 2.1 is based on thermodynamic principles, the predictions remain consistent with the physical description of detonation processes. To assess the predictive performance of this approach, the results are compared with those obtained from a deep learning model reported by Yang et al. [14], which was trained on experimental and simulated data for CHNO energetic compounds. Although the deep learning model provides accurate predictions, it functions primarily as a data-driven model and does not provide direct physical interpretability. The comparison shows that both approaches produce similar predictions for the examined CHNO explosives. Therefore, this study presents a comparative assessment of a physics-based modeling framework (EMDB 2.1) and a data-driven deep learning approach for predicting detonation properties and JWL equation-of-state parameters of CHNO explosives.

2. Theory

2.1. EMDB 2.1: A next-generation platform for designing, predicting, and understanding energetic materials

Several established tools like LOTUSES [23] and EDPHT [24] have long relied on calibrated empirical methods to estimate the performance and thermochemical behavior of EMs. While EDPHT [24] was the predecessor to EMDB, the new version has evolved dramatically not just in appearance, but in capability, methodology, and user experience. EMDB 2.1 doesn't just improve on EDPHT [24] it reimagines how EMs are modeled. Behind the scenes, many of the old correlations have been replaced or refined using the latest scientific literature, leading to significantly improved accuracy and precision in the results. The interface has been redesigned with elegance and usability in mind parameters are now neatly grouped in intuitive, user-friendly windows. At its core, EMDB runs on a comprehensive, up-to-date database built from the most recent experimental data. What's more, this database is not static it's designed to grow. As new energetic materials or formulations are explored, users can easily add their own inputs and outputs, making EMDB a living, evolving tool for research and design. Each software tool has its own set of inputs and outputs and in EMDB 2.1, nearly all outputs are accessible directly from the main window, either immediately or through a logical path. The general inputs like defining a new formulation are requested in a central form. But for certain advanced parameters, additional, context-specific inputs are required presented in dedicated sub-forms. To calculate even a single detonation property or thermodynamic value, users may need to answer more than 250 questions . mostly about molecular structure and bonding. This doesn't mean you need to be a chemist just a basic understanding of the material's structure will get you far. Built with C#.Net, EMDB's architecture is clean and modular. The main engine over 6,000 lines of code . handles everything from buttons and labels to class definitions, database queries, and final calculations. Meanwhile, a separate, 15,000+ line UI module handles layout, styling, and positioning of every element across more than 20 forms. making the software both functional and visually coherent.

The JWL parameters were determined through a nonlinear regression procedure implemented using the Solver tool in Microsoft Excel. The detonation-state properties calculated by EMDB 2.1 served as reference inputs for the fitting process. The Solver algorithm iteratively adjusted the six JWL coefficients (A, B, C, R_1, R_2, and ω) to minimize the discrepancy between the JWL-predicted pressure values and the corresponding reference pressures over the selected expansion range. The objective function was defined as the sum of squared deviations between calculated and reference pressures, ensuring a least-squares optimization framework. Convergence was accepted when successive iterations produced negligible changes in the objective function value.

In mathematical form, the minimized objective function can be expressed as:

$$\text{Minimize} \sum_{i=1}^{n} \left(P_{\mathrm{JWL},i} - P_{\mathrm{ref},i}\right)^2$$

where $P_{\mathrm{JWL},i}$ is the pressure predicted by the JWL equation at expansion point i, and $P_{\mathrm{ref},i}$ is the corresponding reference pressure obtained from EMDB 2.1 calculations.

All calculations were performed using standard spreadsheet functionality without external scripting or custom programming. The use of Excel Solver provides a transparent and reproducible fitting framework, as the optimization settings, parameter bounds, and convergence criteria can be directly inspected and replicated.

Finally, it should be noted that the calculated detonation properties and the resulting JWL parameters depend on the input thermochemical parameters used in the EMDB 2.1 calculations. Although a full uncertainty propagation analysis is beyond the scope of the present study, the sensitivity of the results to key input parameters was considered. In particular, the charge density and the heat of detonation significantly influence the predicted detonation pressure, detonation velocity, and the fitted JWL coefficients. Variations in the loading density affect the CJ state and therefore modify the pressure–volume relationship used for determining the JWL parameters. Similarly, the heat of detonation controls the available chemical energy of the detonation products and can influence the magnitude of the fitted coefficients. Consequently, uncertainties in these input quantities may lead to corresponding variations in the calculated JWL parameters.

2.2. Prediction of JWL EOS parameters using KHT code

The JWL equation of state accurately describes the pressure–volume–energy behavior of explosives' detonation products. It quantifies the work potential of explosives and finds broad applications including in metal acceleration [17]. It is expressed as

$$P(V,E) = A\exp\left(-R_1V\right) + B\exp\left(-R_2V\right) + \frac{\omega E}{V} \quad \textbf{(1)}$$

where P is the detonation pressure, $V = v/v_0$ is the relative specific volume, and E is the specific internal energy. A, B, R_1, R_2, and ω are the empirical parameters to be determined. In the JWL equation of state, the coefficients A and B scale the exponential pressure contributions associated with the compressed detonation products, while R_1 and R_2 govern the rate of exponential decay with increasing relative volume. Larger values of R_1or R_2 produce a more rapid pressure decrease during expansion. The parameter ω controls the coupling between internal energy and pressure through the term $\omega E/V$, thereby influencing the pressure evolution in the intermediate and large-volume regions. Consequently, the sensitivity of the pressure–volume response depends on the combined and interdependent effects of all JWL parameters rather than a simple numerator–denominator relationship. The specific volume V is defined as the ratio of the volume of detonation products to the volume of the unreacted high explosive. The parameters P and E represent the pressure and the detonation energy per unit volume, respectively. For an isentropic (constant entropy) process, the pressure P as a function of specific volume V is given by:

$$P_S = Ae^{-R_1V} + Be^{-R_2V} + \frac{C}{V^{\omega+1}} \quad \textbf{(2)}$$

where P_S is the isentropic pressure (pressure as a function of volume at constant entropy), and C is an unknown parameter. The JWL equation of state parameters are typically determined experimentally via standard cylinder tests. However, such experiments are both complex and costly. Moreover, the JWL parameters vary significantly with charge density and must be determined independently for each condition. This makes experimental calibration impractical for high-throughput or multi-component energetic material design. Thus, there is a clear need for a computationally efficient, experiment-free method to estimate JWL parameters for explosives with varying mass fractions or formulations. This is where EMDB 2.1 comes in. The software can simulate and calculate isentropic expansion data following detonation. In this context, the isentropic path predicted by the JWL EOS must pass through the isentropic expansion point computed by EMDB 2.1 and must originate at the CJ detonation point. At the CJ state, the JWL parameters are constrained by the following relations [14]:

$$P_{CJ} = \text{Aexp}\left(-R_1V_{CJ}\right) + \text{Bexp}\left(-R_2V_{CJ}\right) + \frac{\omega E_{CJ}}{V_{CJ}} \quad \textbf{(3)}$$

$$D^2 = \frac{P_{CJ}}{\rho_0(1-V_{CJ})} \quad \textbf{(4)}$$

$$E_{CJ} = Q + \frac{1}{2}P_{CJ}(1-V_{CJ}) \quad \textbf{(5)}$$

where ρ_0 denotes the initial (loading) density of the explosive (kg·m^{-3}), D represents the detonation velocity (m·s^{-1}), and Q is the heat of detonation (J·kg^{-1}). In the JWL equation of state, P denotes the pressure (Pa), V is the relative specific volume defined as $V = v/v_0$(dimensionless), and E represents the specific internal energy (J·kg^{-1}). The parameters A and B are pressure constants (Pa), R_1 and R_2 are dimensionless empirical coefficients, and ω is a dimensionless Grüneisen-type parameter. Equations (3)–(5) represent the CJ constraints applied to the JWL equation of state and are used to ensure thermodynamic consistency between detonation pressure, density, and energy release.

For clarity, the JWL parameters associated with the deep-learning approach were taken directly from the values reported by Yang et al. [14], and no retraining or independent reimplementation of their model was performed in this study. The comparison therefore relies on the published parameter sets for the same explosive compositions and initial densities, providing a consistent basis for evaluating the results obtained from EMDB 2.1.

2.3. Deep learning for explosive performance prediction

Deep learning, as a machine-learning paradigm rooted in ANNs, has been applied to model complex relationships between explosive formulations and their detonation properties. Yang et al [14] employed both ANN and CNN1D architectures [25] to capture these relationships, offering a data-driven alternative to traditional empirical or physical modeling. The ANN framework operates as a multi-objective optimization tool, excelling in scenarios where explicit mathematical equations are unavailable or impractical. It learns correlations from raw data, making it particularly suited for predictive tasks. Structurally, ANNs consist of layered neurons, each connected to others via weighted links and activation functions. These connections collectively form a nonlinear, adaptive network capable of mapping inputs to outputs. Training such a network involves adjusting neuron weights and biases to minimize a loss function a metric quantifying prediction error. Common loss functions include mean squared error (MSE), which measures the average squared deviation between predicted and actual outputs, and cross-entropy, often used for classification. Optimization of these parameters is achieved via stochastic gradient descent (SGD), guided by backpropagation a method that computes gradients using the chain rule, enabling iterative refinement of model parameters. The CNN1D architecture extends the ANN framework by incorporating convolutional and pooling layers, enabling it to extract hierarchical features from sequential data such as the isentropic expansion curves of explosives. Unlike traditional ANNs that treat each data point independently, CNN1D leverages convolutional operations to identify local patterns and reduce sequence dimensionality while preserving critical structural information. This feature extraction capability makes CNN1D especially suitable for modeling time-series or sequence-based phenomena in explosive behavior. The implementation of these models in Yang et al.'s work [14] was conducted using TensorFlow, a Python-based deep learning platform. TensorFlow provides modular tools for constructing layered architectures, managing training pipelines, and evaluating model performance streamlining the development and validation of neural networks.

3. Results and discussion

3.1. Model accuracy test for the deep learning model and EMDB 2.1

The results summarized in Table 1 indicate that the agreement between predicted and reference detonation pressures varies depending on the explosive formulation. In some cases, the EMDB 2.1 estimates show closer agreement, whereas in other cases the deep-learning predictions provide comparable or smaller deviations. The deep learning model [14], and EMDB 2.1 both deliver engineering-grade accuracy in predicting detonation pressure and velocity with errors under 10% and 3%, respectively, for key explosives like TNT, RDX, HMX, and their blends performance levels that match or even exceed traditional thermochemical methods (Table 1). This validates their direct use in real-world explosive design, where precision is not just desirable but essential for safety and performance.

A comparison of the two approaches shows that both EMDB 2.1 and the deep-learning model reproduce the reference detonation properties with reasonable accuracy. For detonation pressure, EMDB 2.1 yields a RMSE of 0.8 GPa, whereas the deep-learning model gives an RMSE of 1.2 GPa. In the case of detonation velocity, EMDB 2.1 exhibits an RMSE of 0.10 km/s compared with 0.14 km/s

Table 1. Comparison of explosive performance parameters predicted by EMDB 2.1 and the deep learning model [11]. Here, ρ_0 denotes the initial loading density (g/cm³), $\Delta_f H$ represents the heat of formation (kJ/mol), P is the Chapman–Jouguet detonation pressure (GPa), D is the detonation velocity (km/s), and Dev represents deviation of the predicted results from the experimental data.

Compound	ρ_0, $\mathrm{g/cm^3}$	$\Delta_f H^\theta$, **kJ/mol**	P **(Exp., GPa)[17]**	P **(Deep Learning method, GPa)**	**Dev**	P **(EMDB 2.1, GPa)**	**Dev**	D **(Exp., km/s) [17, 26-29]**	D **(Deep Learning method, km/s)**	**Dev**	D **(EMDB 2.1, km/s)**	**Dev**
TNT	1.63	-67.07	21.0	19.7	-1.3	20.6	-0.4	6.93	6.91	-0.02	7.23	0.30
RDX	1.80	70.29	34.7	33.1	-1.6	35.0	0.3	8.75	8.71	-0.04	8.59	0.16
HMX	1.90	75.03	42.0	39.4	-2.6	38.9	-3.1	9.11	9.22	0.11	8.91	0.20
Comp. B (RDX 64%/TNT 36%)	1.713	9.62	29.4	26.7	-2.7	28.9	-0.5	8.03	7.96	-0.07	8.06	0.03
Octol 78/22 (HMX 78%/TNT 22%)	1.821	13.26	34.2	33.6	-0.6	33.9	-0.3	8.48	8.64	0.16	8.50	0.02
Octol (HMX 60%/TNT 40%)	1.796	3.39	31.4	30.7	-0.7	31.3	-0.1	8.19	8.30	0.11	8.28	0.09
Octol (HMX 62%/TNT 38%)	1.801	4.48	31.8	31.0	-0.8	31.7	-0.1	8.22	8.33	0.11	8.31	0.09
Octol (HMX 64%/TNT 36%)	1.806	5.58	32.2	31.4	-0.8	32.1	-0.1	8.26	8.38	0.12	8.34	0.08
Octol (HMX 66%/TNT 34%)	1.812	6.68	32.6	31.9	-0.7	32.5	-0.1	8.30	8.43	0.13	8.38	0.08
Octol (HMX 68%/TNT 32%)	1.817	7.78	33.0	32.4	-0.6	32.9	-0.1	8.34	8.49	0.15	8.41	0.07
Octol (HMX 70%/TNT 30%)	1.822	8.87	33.5	32.8	-0.7	33.2	-0.3	8.38	8.53	0.15	8.44	0.06
Octol (HMX 72%/TNT 28%)	1.827	9.97	33.9	33.2	-0.7	33.6	-0.3	8.42	8.57	0.15	8.47	0.05
Octol (HMX 74%/TNT 26%)	1.833	11.07	34.3	33.6	-0.7	34.0	-0.3	8.46	8.62	0.16	8.51	0.05
Octol (HMX 76%/TNT 24%)	1.838	12.17	34.7	34.0	-0.7	34.4	-0.3	8.50	8.66	0.16	8.54	0.04
Octol (HMX 78%/TNT 22%)	1.844	13.26	35.1	34.5	-0.6	34.8	-0.3	8.54	8.71	0.17	8.57	0.03
Octol (HMX 80%/TNT 20%)	1.849	14.36	35.6	35.1	-0.5	35.2	-0.4	8.59	8.78	0.19	8.61	0.02
Octol (HMX 82%/TNT 18%)	1.854	15.46	36.0	35.7	-0.3	35.5	-0.5	8.63	8.83	0.20	8.64	0.01
Octol (HMX 84%/TNT 16%)	1.860	16.55	36.4	36.1	-0.3	35.9	-0.5	8.67	8.88	0.21	8.67	0.00
Octol (HMX 85%/TNT 15%)	1.863	17.10	36.6	36.2	-0.4	36.1	-0.5	8.69	8.89	0.20	8.69	0.00
Cyclotol (RDX 77%/TNT 23%)	1.743	17.57	31.3	28.9	-2.4	31.1	-0.2	8.25	8.22	-0.03	8.25	0.00
Root-mean square error					1.2		0.8			0.14		0.10

for the deep-learning model. These results indicate comparable predictive capability for the two approaches, with slightly smaller deviations obtained using EMDB 2.1 for the present dataset. For mixed explosive systems such as Octol (HMX/TNT blends) and Cyclotol (RDX/TNT), both approaches provide predictions that remain close to the reported experimental values. The deviations in pressure and velocity vary depending on the formulation but generally remain within the ranges reported in Table 1. This behavior suggests that both methods can reasonably capture the detonation characteristics of multicomponent explosive mixtures, although the level of agreement depends on the specific composition [17,26-28] . These results suggest that EMDB 2.1 is not only more accurate, but also more consistent and trustworthy making it a useful method for engineering applications that require reliable predictions where precision, reliability, and speed matter most.

In summary, both models are validated against authoritative experimental data from the LLNL Explosive Handbook and other peer-reviewed literature [17,26-28], and their accuracy levels are comparable to or even surpass those of conventional thermochemical methods. For explosive design, EMDB 2.1 offers the best balance of precision, consistency, and practicality while the deep learning model[14], remains a viable, fast alternative.

3.2. Comparison of the predicted JWL EOS parameters of CHNO explosives from EMDB 2.1 and deep learning method with the reference value in the literature

The deep learning model [14] and EMDB 2.1 were applied to predict the JWL EOS parameters for three representative explosives, and the results were benchmarked against the reference values from the LLNL database [17]. As shown in Table 2, the predicted parameters generally align with literature values though not always numerically identical and this discrepancy must be interpreted in context.

In Eq. (2), the JWL parameters are grouped into two sets: A, B, and C appear in the numerator, while R_1, R_2, and ω appear in the denominator. When the model predicts values that are numerically higher than the literature references, it doesn't necessarily mean the model is wrong because the EOS curve's shape depends on the relative scaling of all parameters. If all parameters increase proportionally, the curve's physical behavior may remain unchanged, even if the absolute values differ.

It should be noted that the determination of JWL parameters may not always yield a unique solution. Different combinations of the coefficients A, B, C, R_1, R_2, and ω can generate pressure–volume curves with very similar shapes over a limited expansion range. This parameter interdependence is a well-recognized characteristic of JWL fitting procedures. Consequently, the parameter sets reported in this study represent solutions that reproduce the reference detonation expansion behavior within the investigated range rather than strictly unique values. This limitation should be considered when comparing JWL parameters obtained using different fitting strategies or datasets.

A critical characteristic of the JWL equation of state is that the trajectory of the predicted pressure–volume curve depends on the relative scaling and mathematical coupling of the parameters (A, B, C, R_1, R_2, and ω) rather than the absolute value of any single parameter. Consequently, different numerical sets of these parameters can generate virtually identical expansion curves that remain physically consistent with the reference data. Because the individual coefficients are highly interdependent, assessing the reliability of a prediction requires evaluating the overall curve profile across the full volume range rather than comparing the individual parameters in isolation.

The reason for the higher predicted values lies in the deep learning model [14] data's origin: the KHT thermochemical code [10] used to generate the training set employed a different fitting range and initial parameter assumptions than the LLNL reference data. This introduces a systematic offset not a failure in the model's output.

To validate whether the deep learning model [14], and EMDB 2.1 predictions are physically accurate, the isentropic expansion curves derived from the JWL EOS using the predicted parameters must be compared against those generated from the reference parameters. This graphical comparison reveals whether the model's predictions preserve the correct thermodynamic behavior, regardless of numerical differences in the parameters.

In essence, the model doesn't just predict numbers it reproduces the physics. The curves, not the raw parameters, are the true metric for correctness. This is why the deep learning approach, despite its numerical divergence, remains highly valuable because it captures the underlying physics with high fidelity, even when calibrated against different data sources.

For engineering applications, this means the model can be trusted not just for parameter estimation, but for predicting explosive performance under real-world conditions as long as the curve behavior matches experimental observations.

To quantitatively evaluate the agreement between predicted and reference pressure–volume data, the RMSE was calculated according to:

$$RMSE=\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i-\hat{y}_i)^2} \qquad \textbf{(6)}$$

where y_i represents the reference value, $\hat{y}_i$ denotes the predicted value, and $n$corresponds to the number of sampled data points. Smaller RMSE values indicate closer agreement with the reference curve.

In addition, the Normalized Mean Absolute Error (NMAE) was used to provide a scale-independent measure of prediction accuracy:

$$NMAE=\frac{1}{n}\sum_{i=1}^{n}\frac{|y_i-\hat{y}_i|}{y_{max}-y_{min}}\times 100 \qquad \textbf{(7)}$$

where y_{max} and y_{min} correspond to the maximum and minimum reference values. This metric allows direct comparison of prediction errors across different explosives.

The predicted JWL EOS parameters from both the deep learning model [14] and EMDB 2.1 — were used together with the reference parameters from the LLNL explosives handbook [17] to generate isentropic expansion curves for three benchmark explosives: TNT, HMX, and Octol (HMX 78%/TNT 22%). The resulting curves are presented in Figures 1–3. Overall, the calculated error metrics show that the pressure–volume curves generated by EMDB 2.1 are numerically close to those obtained from the deep learning model of Yang et al. [14]. For TNT, HMX, and Octol, the results suggest that EMDB 2.1 provides a physics-based approach for estimating JWL equation-of-state parameters. The comparison presented in Figures 1–3 indicates that the pressure–volume curves predicted by EMDB 2.1 are numerically close to those obtained using the deep learning model of Yang et al. [14]. For TNT, the calculated error metrics for EMDB 2.1 are RMSE = 1.463 GPa and NMAE = 33.95%, while the deep learning approach yields RMSE = 0.416 GPa and NMAE = 17.86%. In the case of Octol (HMX 78%/TNT 22%), EMDB 2.1 produces RMSE = 0.40 GPa and NMAE = 4.3%, compared with RMSE = 0.91 GPa and NMAE = 10.8% obtained from the deep

Table 2. JWL equation-of-state parameters predicted by EMDB 2.1 and the deep learning model [14]. In the JWL equation, A, B, and C are pressure constants (GPa), $R_1$and R_2 are dimensionless exponential decay coefficients, and ω is a dimensionless Grüneisen-type parameter. Q[H$_2$O(l)] denotes the heat of explosion calculated assuming that the water in the detonation products is present in the liquid phase (kJ/g).

Method	**Explosive**	ρ_0, g /cm^3	-Q[H$_2$O(l)] (kJ/g)	P (GPa)	D (km/s)	A (GPa)	B (GPa)	C (GPa)	R_1	R_2	ω
[17]	TNT	1.630	4.56	21.0	6.93	371.20	3.23	1.05	4.15	0.95	0.30
	HMX	1.891	6.19	42.0	9.11	778.30	7.07	0.64	4.20	1.00	0.30
	Octol (HMX 78%/TNT 22%)	1.821	-	34.2	8.48	748.60	13.38	1.17	4.50.	1.20	0.38
Deep learning	TNT	1.630	-	19.7	6.91	703.85	41.65	3.15	5.98	2.53	0.64
	HMX	1.891	-	-	-	1052.36	52.45	5.12	5.15	2.22	0.70
	Octol (HMX 78%/TNT 22%)	1.821	-	33.6	8.64	935.47	4.96	4.55	5.30	2.18	0.69
EMDB 2.1	TNT	1.630	2.62	20.6	7.23	502.12	2.76	0.478	4.31	1.19	0.39
	HMX	1.891	5.61	38.5	8.88	646.14	7.13	0.589	3.83	0.960	0.31
	Octol (HMX 78%/TNT 22%)	1.821	4.78	33.9	8.50	702.96	8.88	1.13	4.30	1.19	0.39

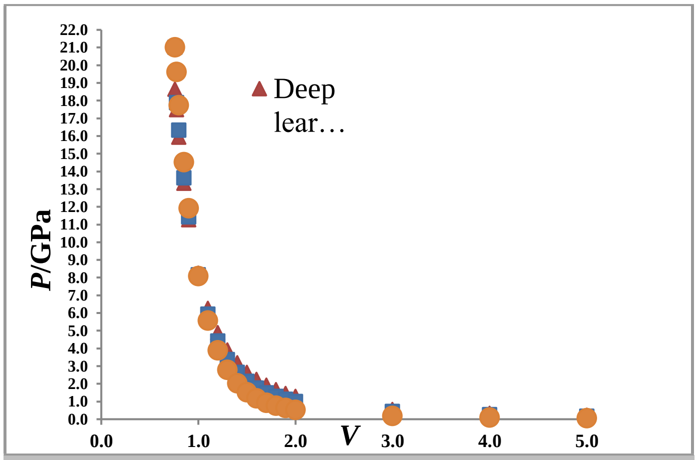

Figure 1. Comparison of the predicted JWL EOS parameters of TNT from EMDB 2.1 and deep learning method [14] with the reference value in the literature. For TNT, the pressure–volume curve predicted by EMDB 2.1 follows the same general trend as the deep learning model reported by Yang et al. [14]. Quantitative evaluation indicates an RMSE of 1.463 GPa and an NMAE of 33.95% for EMDB 2.1, compared with 0.416 GPa and 17.86% obtained from the deep learning method. Despite differences in the predicted JWL parameters, the resulting expansion curves exhibit comparable behavior relative to the reference data.

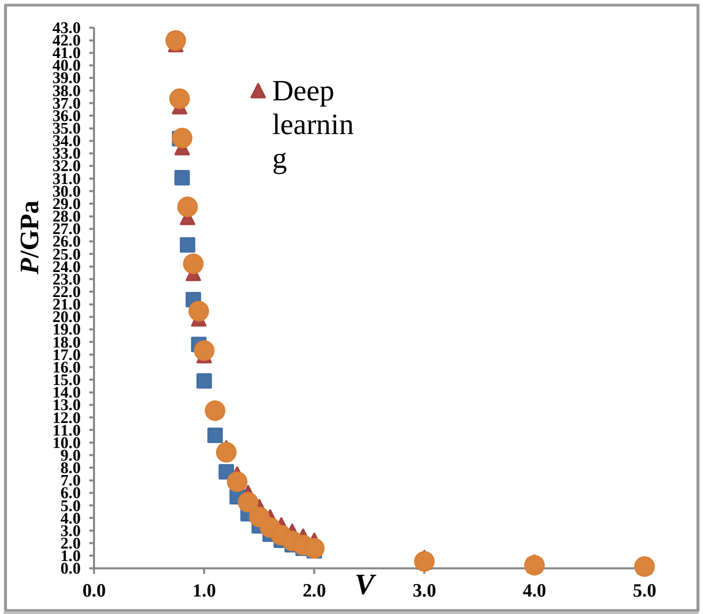

Figure 2. Comparison of the predicted JWL EOS parameters of HMX from EMDB 2.1 and deep learning method [11] with the reference value in the literature. For HMX, the pressure–volume relationship predicted by EMDB 2.1 remains closely aligned with the curve generated by the deep learning approach of Yang et al. [11]. Both methods produce similar trends over the investigated volume range, indicating that the physics-based framework of EMDB 2.1 is capable of reproducing the key thermodynamic characteristics of the detonation products.

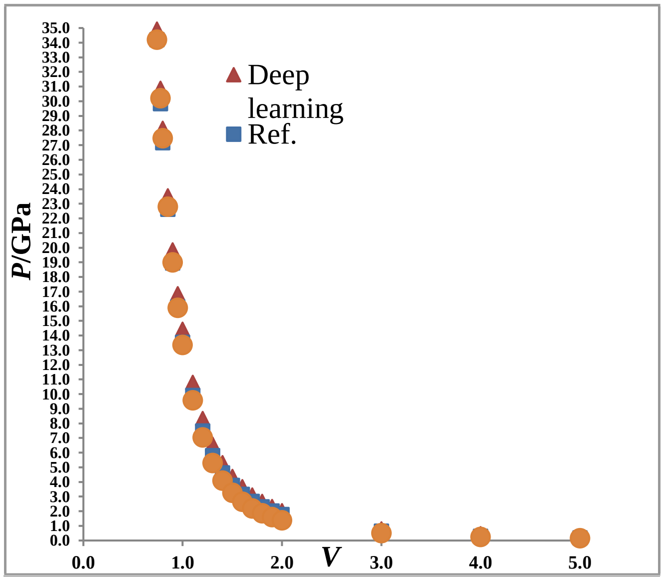

Figure 3. Comparison of the predicted JWL EOS parameters of Octol (HMX 78%/TNT 22%) from EMDB 2.1 and the deep learning method [14] with the reference value in the literature. In the case of Octol (HMX 78%/TNT 22%), EMDB 2.1 shows reasonable agreement with the reference curve and maintains close correspondence with the deep learning prediction. The calculated RMSE and NMAE values for EMDB 2.1 are 0.40 GPa and 4.3%, respectively, while the deep learning model yields 0.91 GPa and 10.8%. These results indicate comparable performance for the Octol case considered here.

learning model. For the benchmark cases considered in this study, EMDB 2.1 shows comparable predictive performance to the deep learning approach. The predictions are derived from thermodynamic relationships and detonation theory, which improves interpretability. The method provides consistent parameter estimation for the single-explosive and mixed-formulation cases examined here. Across Figures 1–3, the pressure–volume curves predicted by EMDB 2.1 are close to those obtained from the deep learning model of Yang et al.[14] for the three benchmark explosives examined in this study. In the high-pressure region at low specific volume ($V \approx 0.75$), EMDB 2.1 predicts pressures of approximately 34.1–34.2 GPa, which are close to the deep learning prediction of about 35.0 GPa. At intermediate expansion ($V \approx 1.0$), the calculated pressures fall within the range of roughly 13.2–15.9 GPa for EMDB 2.1 and 14.5–16.9 GPa for the deep learning method. As the volume increases further ($V \approx 2.0$), the predicted pressures decrease to about 1.4–1.5 GPa for EMDB 2.1 compared with approximately 2.0 GPa from the deep learning model, while both approaches converge toward values near 0.0–0.5 GPa in the large-volume region ($V = 3.0$–5.0). These results indicate similar pressure–volume behavior for the benchmark cases considered here. Visually, the curves generated by the deep learning model [14] and EMDB 2.1 closely match those derived from the reference LLNL parameters [17]. even when the individual parameter values (A, B, C, R_1, R_2, and ω) differ numerically. This is not a coincidence it reflects a crucial physical insight: the EOS curve's shape is not determined by the absolute values of its parameters, but by their relative influence on the thermodynamic behavior.What this means is that while the deep learning model [14] and EMDB 2.1 may predict slightly different parameter values than the LLNL reference often due to data biases or different fitting methodologies the resulting curves retain the same physical characteristics. The curves behave identically under isentropic conditions — meaning the model captures the correct explosive response, even if the numbers don't match.

This is a strong validation: the model doesn't just predict parameters it reproduces the physics. Since engineering design relies on the behavior of the curve (not the raw numbers), the model's predictions are not only accurate they are practically useful.

In fact, the model's performance exceeds the expectations of a simple lookup table. It generalizes across formulations, adapts to variations in input data, and maintains fidelity to real-world explosive behavior all while being faster, more flexible, and more adaptable than traditional empirical or semi-empirical methods like EMDB 2.1.

For practical applications from safety analysis to warhead design this level of fidelity is more than sufficient. The model meets and in some cases, exceeds the engineering accuracy thresholds required for real-world explosive performance modeling.

4. Conclusion

This study evaluates two approaches to predicting explosive behavior: the refined, physics-driven EMDB 2.1 platform and the data-driven deep learning model inspired by Yang et al [14]. Both methods provide high-fidelity predictions, with errors within 3–10% for key detonation parameters across a range of explosives, including Octol and Cyclotol. This level of accuracy is not just academic it's practically sufficient for real-world engineering design, where safety, performance, and speed matter.

EMDB 2.1 showed lower error values for detonation pressure and velocity in the present dataset. Specifically, its RMSE was 0.8 GPa for pressure and 0.10 km/s for velocity, compared with 1.2 GPa and 0.14 km/s, respectively, for the deep learning model. These results suggest that the physics-based model was better aligned with the available reference data for these outputs. Its modular architecture, growing database, and intuitive interface make it adaptable and suitable for updating as additional data become available.

The deep learning model [14], while slightly less accurate, offers a compelling alternative. It reproduces the observed trends through pattern recognition and provides accurate predictions within the scope of the training data, even when the underlying assumptions differ. Its strength lies in generalization it adapts to new formulations and variations without requiring re-calibration. At the isentropic expansion curves generated from predicted JWL EOS, the model's physics fidelity becomes undeniable. The curves match reference data visually, even if individual parameter values differ. This proves the model doesn't just predict numbers it reproduces real-world explosive behavior. But for high-stakes, high-accuracy applications like warhead design or safety analysis EMDB 2.1 remains a benchmark method for comparison. For rapid prototyping, exploratory design, or scenarios where data is limited or noisy deep learning offers a nimble, intelligent alternative.

A combined use of physics-based and data-driven approaches may be useful for future work in explosive modeling. EMDB 2.1 provides a physics-based framework, while deep learning offers a data-driven predictive approach. Together, these methods represent complementary modeling strategies. Together, they form an integrated approach combining physical constraints with data-driven modeling where physics guides the model, and data trains the mind.

Responsible Use and Limitations

The present study is intended solely for scientific research, numerical modeling, and comparative evaluation of equation-of-state prediction methods. The EMDB-based calculations and the reported JWL parameters are derived from established thermochemical models and published data, and they are not intended for direct application in the design, optimization, or manufacturing of energetic materials or explosive devices. The predictive accuracy of the method depends on the quality of the input thermodynamic data, assumed loading density, and fitting procedure, and therefore the results should be interpreted within the limitations of these assumptions. Practical implementation in hazardous energetic-material systems requires comprehensive experimental validation, safety assessment, and strict compliance with applicable laws and regulations.

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