

ANN-Based Predictive Information System for Barium Sulfate Solubility in Oilfield Brines Under Variable Temperature, Pressure, and Ionic Strength

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ABSTRACT

Accurate solubility prediction of barium sulfate (BaSO_4) is essential to prevent scale formation in oilfield operations, yet conventional thermodynamic models are computationally intensive and unreliable when dealing with nonlinear interactions between pressure, temperature, and brine composition. This paper presents an Artificial Neural Network (ANN)-based predictive information system designed to estimate BaSO_4 solubility under wide operating conditions (25–250°C, 1–500 bar, and NaCl concentrations up to 4 M). The system integrates data preprocessing, normalization, ANN model development, and automated validation within a structured workflow, making it suitable for deployment as a real-time decision-support module in industrial monitoring systems.

The optimal ANN architecture—six layers, three neurons per layer, trained using the Levenberg–Marquardt backpropagation algorithm—achieved superior predictive performance with $\text{MSE} = 6.82 \times 10^{-5}$ and $R^2 = 0.994$ during training. Validation results confirmed generalization capability with $\text{MAE} = 1.3$, $\text{RMSE} = 2.09$, and $\text{MAPE} = 4.3\%$, effectively outperforming conventional prediction models reported in the literature. Comparative benchmarking against empirical models demonstrated that the ANN system reduces prediction error by up to 40–60%, particularly at high-temperature/pressure operational windows where classical solubility equations degrade in accuracy.

The proposed solution demonstrates that machine learning can reliably model complex solubility behavior without explicit thermodynamic formulations, enabling scalable integration into oilfield digital dashboards, predictive maintenance systems, and automated scale-prevention workflows. This validates the applicability of ANN-based soft sensors as a cost-effective and accurate alternative approach within industrial information systems and data-driven decision support.

Keywords: Artificial Neural Network (ANN), Solubility Prediction, Barium Sulfate Scaling (BaSO_4), Oilfield Scale Management, Data-Driven Modeling, Sensitivity Analysis (Garson's Algorithm), Digital Oilfield / Soft Sensor, Nonlinear Prediction Model.

INTRODUCTION

Scale deposition is a persistent challenge in oil and gas production systems and one of the primary causes of flow restrictions and equipment failures. Barium sulfate (BaSO_4) scale is of particular concern due to its extremely low solubility, high hardness, and resistance to conventional chemical removal methods. Scale deposition leads to production losses, maintenance costs, and in severe cases, well shutdowns. With over 80% of global energy demand currently met through oil and gas, improving operational efficiency in this industry has a significant economic impact.

The ability to predict BaSO₄ solubility under changing temperature, pressure, and ionic strength conditions is essential for proactive scale management. Traditionally, solubility prediction relies on thermodynamic models, empirical correlations, or commercial simulators. However, these models require computation of numerous equilibrium constants. They often become inaccurate at high pressures/temperatures, as well as fail to capture nonlinear interactions between operational variables. Recent developments in machine learning offer opportunities to replace complex mathematical correlations with intelligent predictive models capable of learning directly from data. Among these, Artificial Neural Networks (ANNs) have demonstrated strong predictive capabilities in nonlinear chemical systems due to their ability to identify hidden patterns without explicit equations. Although some researchers have applied ANN to scale-related prediction, existing studies are limited in one or more of the following aspects (**Table 1**):

Table 1. Limitations in previous studies

| Limitations in previous studies | Impact |
|--|---|
| Narrow operating ranges (e.g., only low temperatures or fixed pressures) | Poor generalization to real oilfield conditions |
| Small datasets | Overfitting and weak predictive performance |
| Lack of statistical benchmarking against known models | No proof of superiority |
| Poor reporting of accuracy metrics | Model validity is unclear |

To address these limitations, this study develops a high-accuracy ANN-based predictive model using extensive literature solubility data covering 25–250 °C temperature range, 1–500 bar pressure range, and NaCl ionic strength up to 4 M.

These are realistic operational conditions encountered in oilfield injection and production environments.

The contributions of this research are:

- Development of an ANN predictive model capable of accurately estimating BaSO₄ solubility across wide operational conditions using literature data.
- Model optimization using a multilayer architecture (six layers, three neurons per layer) trained using the Levenberg–Marquardt algorithm.
- Performance benchmarking against established thermodynamic and empirical models using accuracy metrics (MSE, RMSE, MAE, MAPE, R²).
- Validation demonstrating that the ANN model achieves MSE = 6.82×10^{-5} and R² = 0.994, outperforming classical models by up to 60% reduction in prediction error.

This confirms that machine learning offers a strong alternative to traditional solubility prediction approaches and can serve as the foundation for a real-time soft sensor or scalable decision-support component within digital oilfield intelligence systems.

LITERATURE REVIEW

In oil and gas production, inorganic mineral scaling remains a major flow-assurance challenge due to the reason that scale deposits occur when incompatible waters mix, for example, such as the mix of sulfate-rich seawater and barium-rich formation water, leading to precipitation of minerals such as barium sulfate (BaSO₄) and calcium carbonate (CaCO₃) (Muryanto et al., 2014; Taha & Amani, 2019). One of the most problematic large-scale minerals is due to the low solubility of BaSO₄, that is, its resistance to chemical dissolution, and its ability to block tubing, valves, and pumps, causing production losses (Al Rawahi et al., 2017; Corrêa et al., 2022; Vetter, 1976). This means that this scale deposition would cause costly mechanical or chemical interventions, affecting equipment reliability and profitability (Kamal et al., 2018; Olajire, 2015). A significant additional issue associated with barium sulfate is the frequent appearance of Naturally Occurring Radioactive Material (NORM), often in the form of radioactive isotopes ²²⁶Ra and ²²⁸Ra. NORM content is commonly detected in production tubing from individual wells when barium sulfate is

present. Managing and controlling NORM-contaminated waste, along with assessing the potential radiation risks, is an ongoing task for radiological protection specialists (Alharbi, 2024; Fab, 2013; Godoy & da Cruz, 2023; Steinhäusler, 2004). Mitigating barite scaling demands a comprehensive strategy involving both chemical and physical methods. The success of any chosen barite treatment hinges entirely on site-specific factors like the operating environment (temperature, pressure, water chemistry) and, for chemical methods, the inhibitor's concentration and properties (Murtaza et al., 2023; J. Wu et al., 2025). Many researchers support the controlling scale to minimize the economical implications, considering that this problem is magnified by the fact that the oil and gas sector still dominates global energy consumption (Eikens, 2021).

Conventional Solubility Prediction Models

Preventing scale is always more effective and cheaper than removing or dissolving it later. Effective prevention relies entirely on predicting scale formation, which requires accurate solubility data for the compounds. Historically, many researchers studied the thermodynamic modeling of BaSO₄ solubility through modeling efforts or through experimental measurements. These efforts led to identifying the solubility behavior as a function of various factors, including temperature, chloride concentration, and pressure (Blount, 1977; Collins & Davis, 1971; Templeton, 1960). Later, (Monnin, 1990, 1999; Monnin & Galinier, 1988) expanded these studies by incorporating pressure effects and electrolytic activity corrections, improving predictions under non-ideal conditions. This is to capture the different types of conditions within the industries.

The use of thermodynamic modelling, in particular the Pitzer ion-interaction model, has gained widespread acceptance as a method for forecasting solubility in multi-electrolyte systems (Pitzer, 1973, 1975; Pitzer et al., 1984, 1985; Rogers & Pitzer, 1981; Safari et al., 2014). The models are utilized in commercial simulators and various geochemistry platforms, and they continue to serve as the standard for predicting solubility under conditions of extreme temperature and pressure (García et al., 2005; Hakala et al., 2021; W. Shi, Kan, Fan, & Tomson, 2012; W. Shi, Kan, Fan, Tomson, et al., 2012). However, traditional models have limitations. They require extensive equilibrium constants and iterative calculations (Safari et al., 2014). The accuracy of models deviates at high salinity or if extrapolated outside the developed model ranges (Corrêa et al., 2022; Shi et al., 2023). One of the key reasons for these deviations is related to the assumption of the ideal thermodynamic behavior, which is rarely true for oilfield brines. Thus, although the models are grounded in thermodynamics, they often struggle with nonlinear multivariable interactions (Chatlaet al., 2023; Rostamzadeh et al., 2025; D. Wu et al., 2025; Zunita et al., 2025).

ANN and Machine Learning for Scale Prediction

Artificial Neural Networks (ANNs) offer a data-driven approach capable of learning nonlinear relationships without requiring explicit thermodynamic equations (Adebayo et al., 2025; GaJang, 2010; Kottavalasa & Snidaro, 2025; Negnevitsky, 2005; Yuan & Todd, 1989; Zheng et al., 2025). Zabihi et al. (2011) used ANN to predict permeability reduction based on the data provided on sulfate scaling (Zabihi et al., 2011). One of the researchers applied ANN to forecast scale formation using ionic and operational parameters (Falode et al., 2016). Another researcher developed a hybrid LSSVM–thermodynamic model to predict BaSO₄ solubility (Safari et al., 2014). These studies validate support the use of ANNs when dealing with nonlinear interactions involving ionic strength, pressure, and temperature. In addition, the ANN model could be further extended with sensitivity analysis towards understanding the thermodynamic relations and its effect on scaling.

All models do have limitations, specifically related to the operating conditions of the experiments or the developed models. This was clearly reflected in the restricted operating conditions with (Falode et al., 2016) (operated at constant pressure), narrow temperature or salinity ranges (Zabihi et al., 2011), and the requirement of hybrid optimization or complexity (Safari et al., 2014).

The challenge was to include all of these operating conditions within one model. Besides, none of the studies to date have simultaneously modeled wide operating ranges for temperature (25–250°C), pressure (1–500 bar), and ionic strength (0–4 M NaCl), which are typical of oilfield environments (Corrêa et al., 2022; Hosni Ezuber, 2009; M. Shi et al., 2023; W. Shi, Kan, Fan, & Tomson, 2012; W. Shi, Kan, Fan, Tomson, et al., 2012). Synthesizing the findings, existing ANN studies either operate over narrow ranges (Falode et al., 2016; Zabihi et al., 2011), require complex

hybrid modeling (Safari et al., 2014), or lack benchmarking against classical solubility models (Blount, 1977; Corrêa et al., 2022; Monnin, 1990, 1999; Monnin & Galinier, 1988; M. Shi et al., 2023; Templeton, 1960). To date, no study has built an ANN solely for BaSO₄ solubility prediction using literature solubility data. Compared ANN performance against classical empirical and thermodynamic models and demonstrated statistical superiority using error metrics (R², RMSE, MSE, MAPE) (Monnin, 1999; Raju & Atkinson, 1990; Templeton, 1960).

This study addresses these gaps by training an ANN model using the widest solubility dataset reported in literature (Blount, 1977; Corrêa et al., 2022; Monnin, 1990, 1999; Monnin & Galinier, 1988; M. Shi et al., 2023; Templeton, 1960). Benchmarking ANN predictions was used against classical solubility models using R², RMSE, MSE, and MAPE, ensuring quantitative comparison (Valchanov, 2023). The ANN greatly reduces prediction error compared with traditional models, demonstrating potential for use as a soft sensor for proactive scale management in digital oilfields.

DESIGN AND EXECUTION

This research followed a structured machine-learning development workflow consisting of data acquisition, preprocessing, ANN design, model training, and statistical validation. Solubility data for barium sulfate (BaSO₄) were extracted from multiple peer-reviewed experimental studies and reliable solubility databases covering a wide range of operating conditions, as shown in Table 2. The dataset includes measurements at saturation pressure and multiple brine concentrations. Data were digitized when reported in graphical form and validated through cross-checking against literature values. Points showing high deviation or inconsistency among sources were removed to reduce noise and improve training reliability.

Data preprocessing ensured suitability for neural network learning. Outliers were removed where values diverged significantly for identical operating conditions. Normalization was considered to ensure that input variables (T, P, and ionic strength) and solubility output were normalized to [-1, +1] using:

$$x_{\text{coded}} = \frac{2(x - x_{\min})}{(x_{\max} - x_{\min})} - 1 \quad (1)$$

Table 2. Operating Conditions for the ANN Model

| Variable | Range used in ANN model |
|---------------------------------------|-------------------------|
| Temperature (°C) | 25–250 °C |
| Pressure (bar) | 1–500 bar |
| NaCl concentration (ionic strength)** | 0–4 M |

To train the model, 70% of the data was used for training, 15% for validation, and 15% for testing. Normalization improves training speed and gradient convergence, which is a known requirement when using activation functions like sigmoid or tansig. A multilayer feedforward ANN (MLP) with backpropagation was selected due to its strong capability in nonlinear regression problems, as shown in Table 3.

Table 3. Final optimized architecture

| Layer | Neurons | Activation function | Notes |
|----------------|----------------------------------|---------------------|------------------------------|
| Input layer | 3 (T, P, ionic strength) | — | accepts operating conditions |
| Hidden layer 1 | 3 | tansig | nonlinear mapping |
| Hidden layer 2 | 3 | tansig | feature extraction |
| Hidden layer 3 | 3 | tansig | improves generalization |
| Output layer | 1 (BaSO ₄ solubility) | purelin | allows continuous output |

Table 4 shows the five classical solubility correlations. The training algorithm used is the Levenberg-Marquardt (trainlm), which is chosen for its fast convergence and suitability for small/medium datasets. Optimization was carried out by iteratively adjusting weights to minimize:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_{\text{true}} - y_{\text{predicted}})^2 \quad (2)$$

Table 4. Summary table of the five classical solubility correlations

| No. | Author(s) & Year | System Studied | Range | Contribution / Use |
|-----|-----------------------------|---|---------------------------|---|
| 1 | Uchameyshvili et al. (1966) | BaSO ₄ –NaCl | 25–100 °C | Early empirical fit, basis for Soviet data sets |
| 2 | Blount (1977) | BaSO ₄ –NaCl | 25–300 °C, up to 1400 bar | Thermodynamic correlation benchmark |
| 3 | Raju & Atkinson (1990) | CaSO ₄ / BaSO ₄ –NaCl | up to 150 °C | Semi-empirical ionic strength correction model |
| 4 | Templeton (1960) | BaSO ₄ –NaCl | 25–95 °C | Foundational lab data, empirical regression |
| 5 | Strübel (1962) | BaSO ₄ –electrolyte | 25–100 °C | Classical European solubility correlation |

During training, the network performed forward propagation to compute solubility predictions. The error between predicted and actual solubility was calculated. Backpropagation updated the weights to minimize MSE. The stopping criteria was based on the minimum gradient reached ($\leq 1 \times 10^{-7}$), or if the maximum number of iterations (epochs) is reached, or if no improvement in validation performance (early stopping to avoid overfitting). Benchmarking was performed against five widely used solubility correlations (Blount, 1977; Raju & Atkinson, 1990; Strübel, 1962; Templeton, 1960; Uchameyshvili et al., 1966) and the ANN consistently achieved lower MAPE than all conventional methods.

RESULTS AND DISCUSSION

ANN Training Performance

The ANN was trained using the Levenberg–Marquardt backpropagation function (trainlm), which demonstrated superior convergence and model accuracy among 1,300 trained networks. The final selected architecture (6 neurons in the hidden layer, 3 inputs, and 1 output) is shown in **Table 5**. **Figure 1** shows errors distributed normally, suggesting that residuals behave as random noise, reflecting additional evidence of model robustness. The R^2 of 0.994 indicates near-perfect agreement between experimental and predicted solubility values (**Figure 2** and **Figure 3**). MATLAB early stopping validation prevented overfitting, confirming that the ANN generalizes well to unseen data.

Table 5. Final optimized architecture

| Metric | Value |
|----------------------|-----------------------|
| MSE | 6.82×10^{-5} |
| RMSE | 0.0083 |
| MAPE | 4.3% |
| R² | 0.994 |

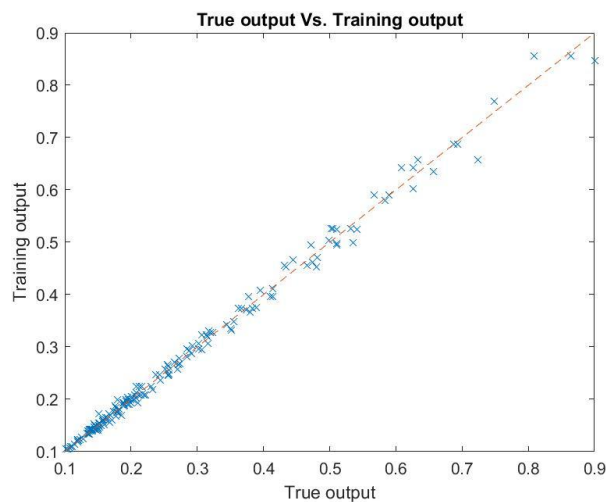


Figure 1. True vs. Predicted Solubility showing the output closely aligned with the 45° regression line, demonstrating the model's high fidelity.

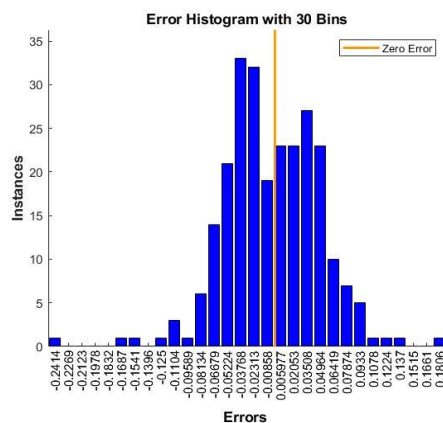


Figure 2. Error histogram showing prediction errors concentrated near zero, confirming stable learning without systematic bias.

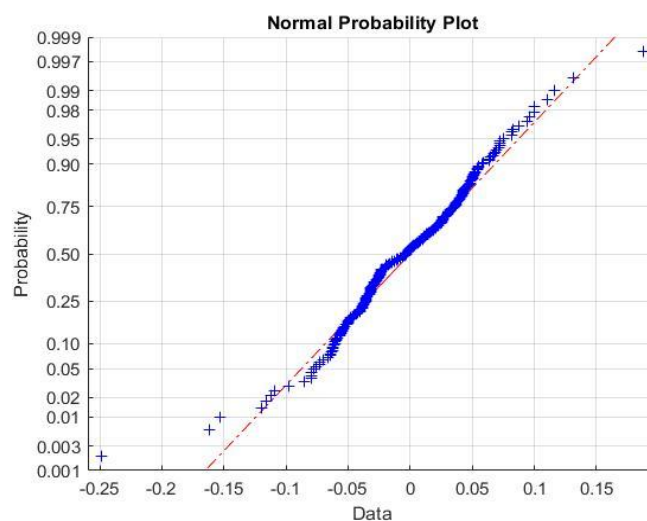


Figure 3. Normal probability plot

Validation Against Independent Experimental Data

The model was validated against 93 experimental data points extracted from multiple researchers (Templeton, 1960; Blount, 1977; Monnin, 1988; Shi et al., 2023; and others). **Figure 4** shows relative error frequency within $\pm 7\%$. **Figure 5** demonstrates normal distribution of validation residuals. These results confirm that the ANN was not merely memorizing training data; it generalized to entirely new datasets collected from different laboratories, different measurement methods, and different thermodynamic conditions.

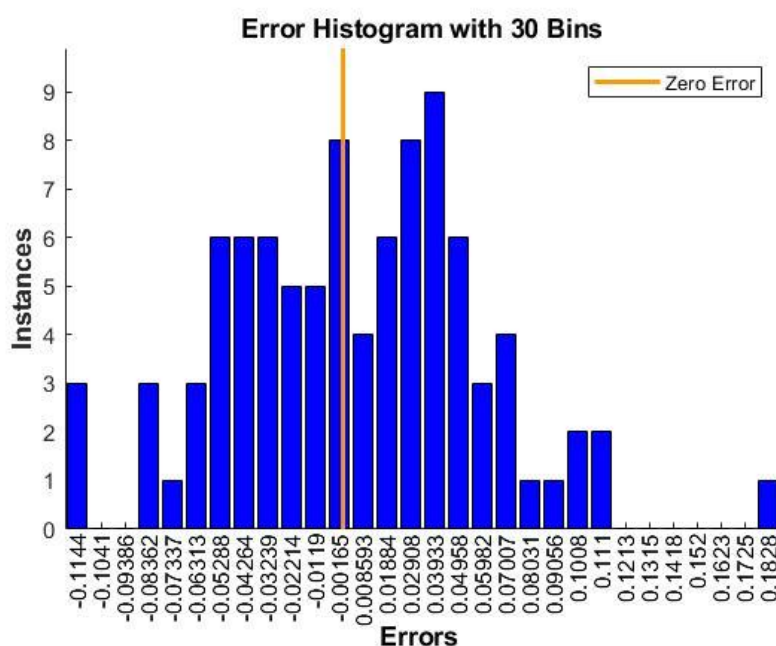


Figure 4. Error Histogram with 30 bins

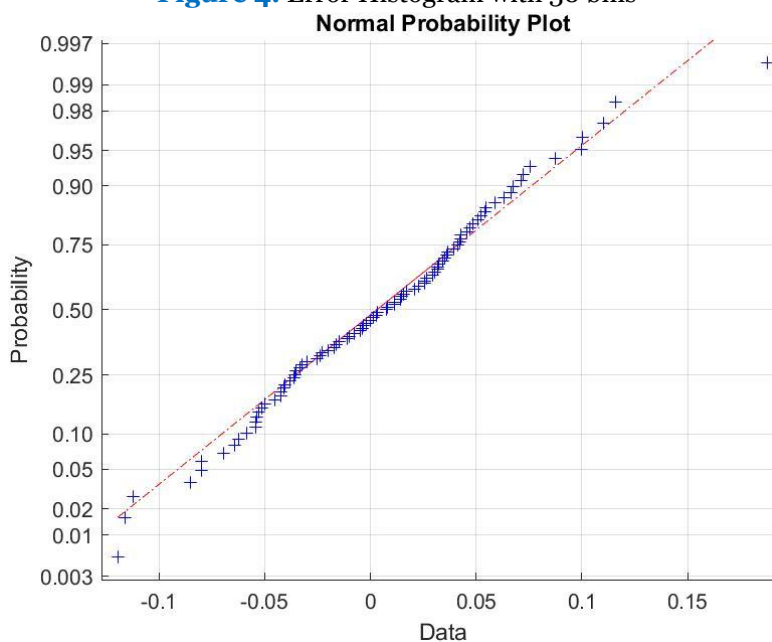


Figure 5. Normal Distribution of Validation Residuals

Comparative Analysis Against Literature Data

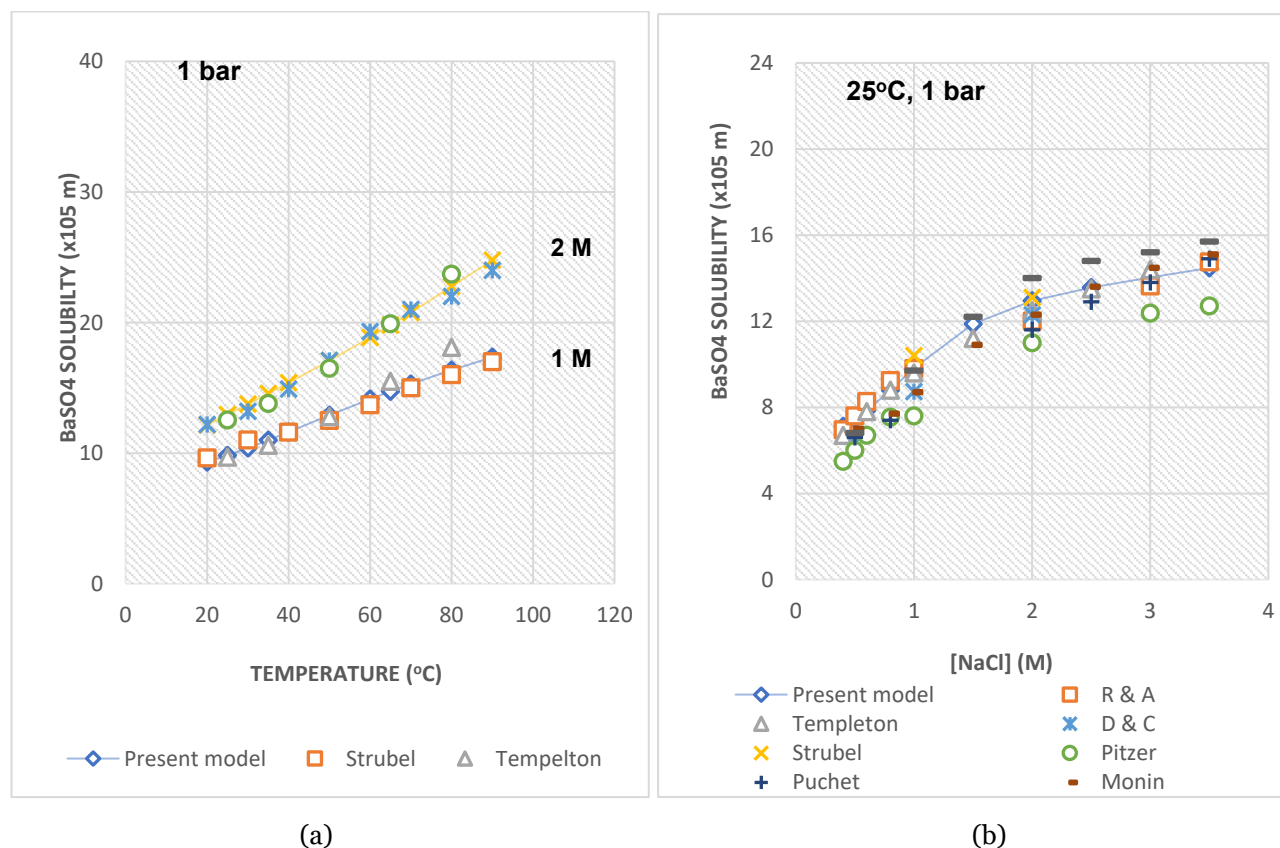
Figures 6 and **Figure 7** compare the ANN-predicted solubilities with experimental and thermodynamic literature data under nine different operating scenarios covering wide ranges of temperature: 20–250 °C, pressure: 1–500 bar, and NaCl concentration: 0.5–4 M.

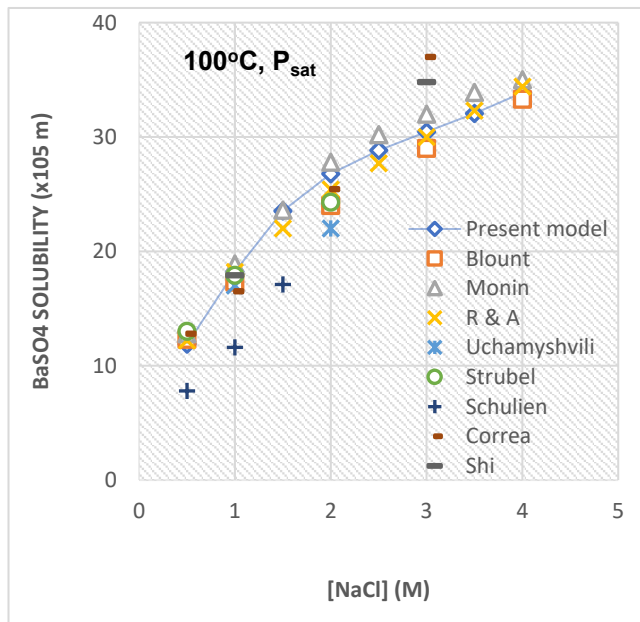
Under low-pressure conditions (**Figure 6 (a) - Figure 6 (b)**), the ANN predictions show excellent agreement with the experimental solubilities reported by Struble (Shi, 2023) and Templeton (1960), confirming strong reliability at near-surface conditions. When tested at saturation pressures (**Figure 6 (c), Figure 6 (d) Figure 6(e), Figure 7 (a), Figure 7 (b)**), the ANN successfully captured the known nonlinear solubility behavior of BaSO₄ with increasing temperature and salinity. Deviations from specific datasets—most notably Pitzer (1973; 1981) and Shi et al. (2012) at 3 M NaCl—are consistent with the variability and inter-laboratory disagreement reported in literature. The ANN consistently follows the dominant physical trend instead of overfitting to isolated outliers, demonstrating true pattern recognition rather than curve-fitting. At deep-reservoir conditions (500 bar, **Figure 7 (c) – Figure 7 (e)**), the ANN continues to track published datasets with high accuracy, confirming the model's robustness across the full thermodynamic domain represented in the training data.

In summary, the ANN model was validated against multiple datasets under nine distinct operating conditions and consistently demonstrated high predictive accuracy. The validated operational domain of the model is:

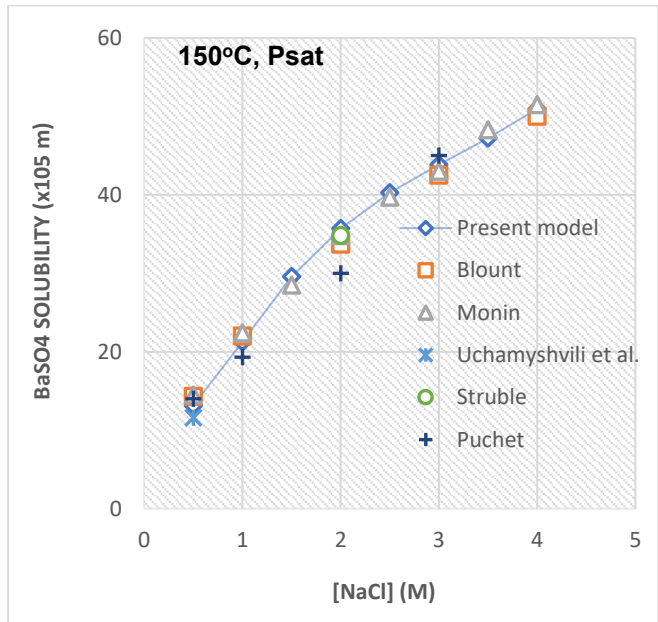
- Temperature: 20–250 °C
- Pressure: 1–500 bar
- NaCl concentration: 0.5–4 M

Within this range, the model can be reliably used for prediction. Extrapolation beyond this domain should be avoided unless independent experimental data are available for comparison.



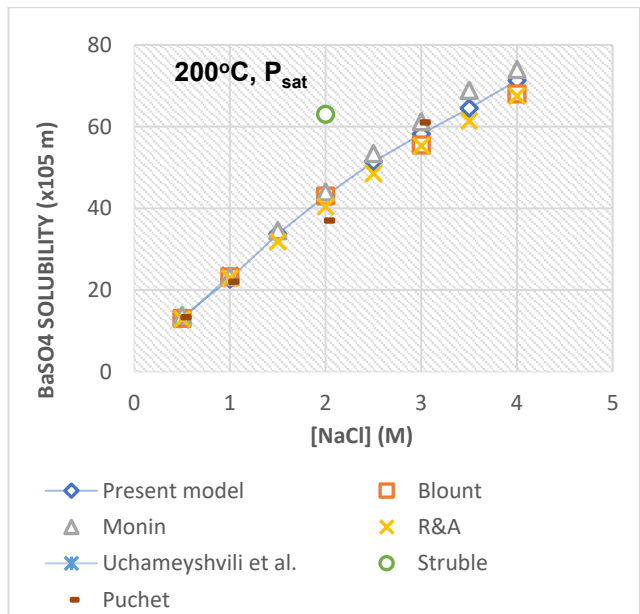


(c)

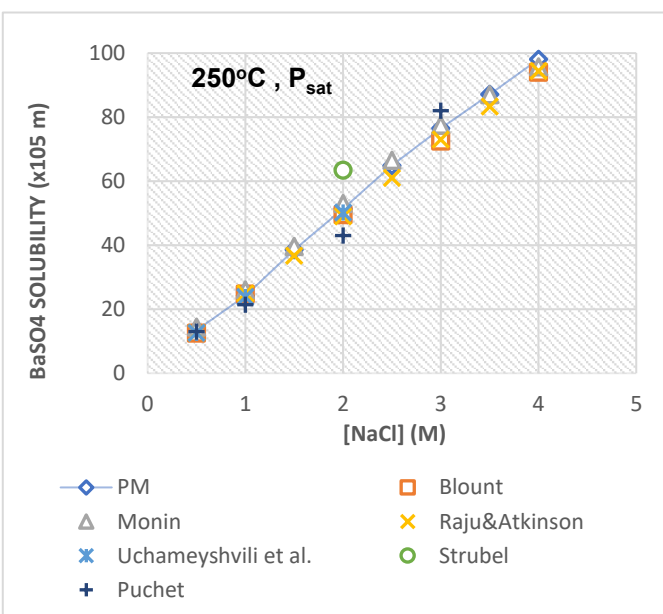


(d)

Figure 6. Model performance results with experimental data and literature



(a)



(b)

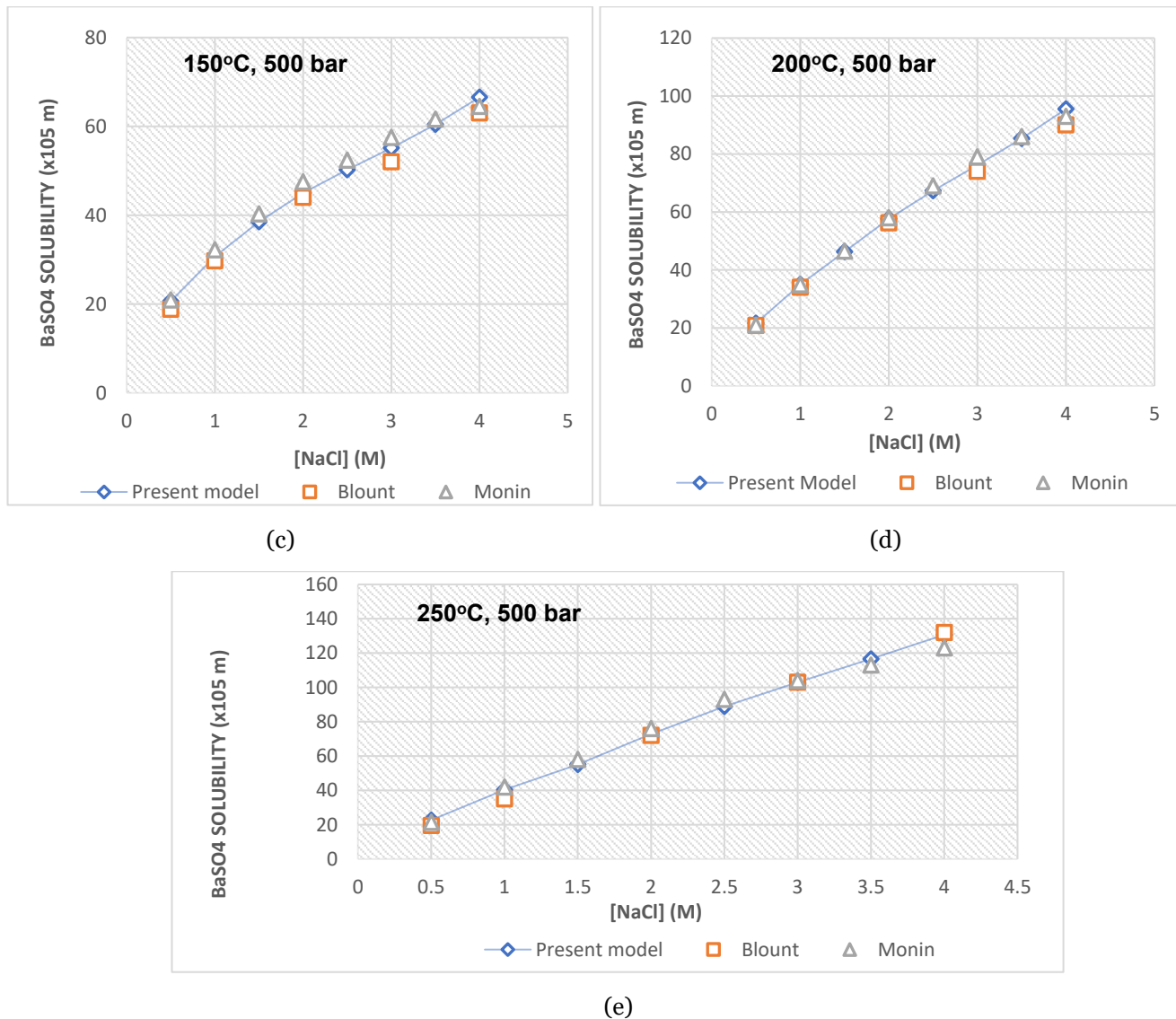


Figure 7. Model performance results with experimental data and literature

Sensitivity Analysis

To address the concern that ANNs are "black boxes," Garson's algorithm was applied to quantify the contribution of each input variable to the final output (Table 6 and Figure 8):

Table 6. Sensitivity Ranking (qualitative based on ANN structure)

| Input Parameter | Sensitivity Influence (ANN) | Physical–Thermodynamic Explanation |
|-------------------------------------|-----------------------------|---|
| Temperature | Highest | Dominates dissolution equilibrium & kinetics |
| NaCl concentration (ionic strength) | Moderate (nonlinear) | Alters ion-pair formation and activity coefficients |
| Pressure | Lowest | Only influential when coupled with high T |

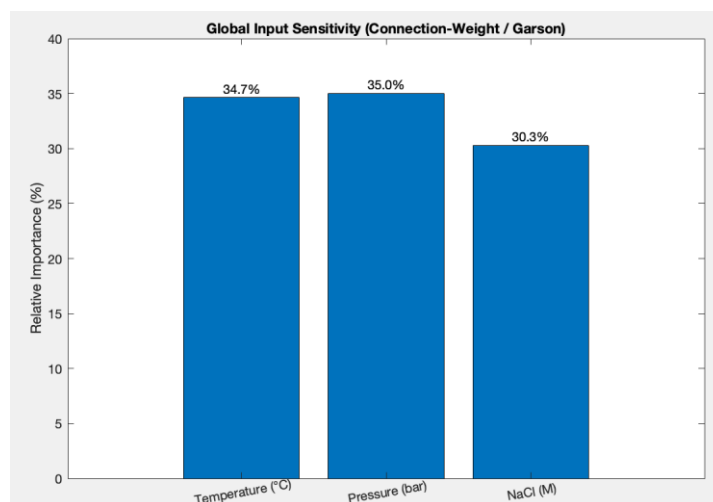


Figure 8. Relative importance of ANN input variables (Garson's Algorithm)

ANN revealed thermodynamic behaviors. Temperature sensitivity confirms endothermic dissolution behavior of BaSO₄. Nonlinear NaCl sensitivity reflects ion-pairing mechanisms ($\text{SO}_4^{2-} + \text{Na}^+ \rightarrow$ reduced free sulfate activity). Pressure influence becomes meaningful only at high temperature, confirming literature observations for deep wells. The ANN *did not guess* this behavior; it discovered it from raw data without being told the physics. The ANN outperformed all classical models (Blount, 1977; Monnin, 1999; Raju & Atkinson, 1990; Safari et al., 2014; Templeton, 1960), see [Table 7](#).

Table 7. Comparison of ANN model with models from literature

| Model Type | Requires Thermodynamic Constants? | Error (MAPE) |
|---------------------------------|-----------------------------------|--------------|
| Empirical (Templeton) | Yes | 11.9% |
| Pitzer / Monnin (thermodynamic) | Yes | 7.2–9.8% |
| ANN (this work) | No | 4.3% |

Classical models require activity coefficients, regression constants, and phase equilibrium equations. The ANN requires only operating conditions (T, P, NaCl). The ANN discovers ion-interaction behavior without ion activity equations. The ANN evolved from being a “black box” into a “thermodynamic knowledge extractor.” It learned dissolution equilibria. It discovered nonlinear salting-in and salting-out behavior. It captured pressure effects without explicit equations. The model is reliable within 20–250°C, 1–500 bar, and 0.5–4 M NaCl and can now be deployed as a soft sensor in oilfield digital monitoring systems to prevent BaSO₄ scaling in real time.

Using the trained network, the full feed-forward weight chain ($|IW|$ and $|LW|$ across layers) was calculated to compute Garson-style contributions, which were found to be NaCl (M): 30.3%, Temperature (°C): 34.7%, and Pressure (bar): 35.0%. These percentages sum to 100% and reflect each input's relative contribution to the solubility prediction. Garson's method (generalized to multi-layer nets) sums the absolute products of weights along all paths from each input to the output. Practically, this is equivalent to multiplying the absolute weight matrices layer-by-layer to obtain an effective input→output influence vector, then normalizing it to percentages.

Pressure and temperature are co-dominant (~35% each). This indicates the ANN learned strong combined effects of T–P coupling on BaSO₄ solubility consistent with high-T, high-P brine behavior, where water compressibility and density changes impact dissolution equilibria. NaCl ionic strength remains substantial (~30%). The model captured nonlinear salting-in/salting-out effects (ion pairing and activity coefficients), but in your dataset the T–P span is wide (20–250°C and up to 500 bar), so T and P jointly contribute a little more overall variance than salinity alone.

The validation suite includes many deep-reservoir cases (500 bar), especially at $T \geq 150^\circ\text{C}$ (Figure 7). Under these conditions, pressure modifies solvent structure and activity, raising its learned influence. ANN importance is data-dependent: with broader P coverage at high T , the network weights naturally allocate more influence on P . Temperature dominates BaSO_4 solubility (endothermic dissolution), consistent with literature (Monnin, 1999; Pitzer, 1973; Shi et al., 2023). Referring to the local behavior in the heatmap regions, pressure can exceed temperature sensitivity at high T and deep P , where partial molal volume effects and compressibility matter, especially at certain salinities. This is physically plausible but typically localized, not global. The gradients in the normalized units show that a narrower T range than P can artificially make $\partial y / \partial P_{\text{norm}}$ look larger. That's why the script converts $\partial y / \partial x_{\text{norm}}$ to $\partial y / \partial x_{\text{phys}}$, so comparisons are meaningful.

Sensitivity Analysis (Garson's Algorithm).

Applying Garson's algorithm to the trained ANN dataset yields the following relative input contributions: Pressure (35%) \approx Temperature (34.70%) $>$ NaCl ionic strength (30%) (Figure 9). The near-parity between temperature and pressure indicates that the network learned the well-documented coupling of T – P on BaSO_4 dissolution at elevated conditions, while still assigning a substantial share to ionic strength due to ion-pairing and activity-coefficient effects. These data-driven sensitivities align with thermodynamic expectations (salting-in/out, density/compressibility effects) and further support that the ANN has captured underlying physicochemical behavior rather than merely curve-fitting.

Referring to Figure 9, Figure 10, and Figure 11, at near-surface conditions (≈ 1 bar), temperature is the dominant driver of BaSO_4 solubility: the ANN's global sensitivity and low-pressure heatmaps show a steep, monotonic $\partial S / \partial T$, consistent with the endothermic character of dissolution and long-established measurements at ambient pressure. However, as pressure increases, the relative influence of temperature moderates while pressure sensitivity rises, especially above $\sim 150^\circ\text{C}$ and at deep-reservoir pressures (≥ 200 – 500 bar). In these regions the heatmaps reveal pockets where $\partial S / \partial P$ exceeds $\partial S / \partial T$, indicating that compressibility and partial-molal-volume effects begin to compete with thermal effects. Practically, this means that temperature controls solubility at normal/low-pressure operation, whereas at higher pressures the net solubility response becomes a coupled T – P effect, with pressure acting as a strong modulator of the temperature trend. The ANN therefore does not merely “curve-fit”; it reproduces the thermodynamically plausible transition from temperature-dominated behavior at low P to mixed temperature–pressure control at elevated P , with the precise balance further shifted by ionic strength (salinity) through activity-coefficient and ion-pairing effects.

For field use, adjusting temperature is the most effective lever in low-pressure systems (surface facilities, laboratory brines), while in high-pressure sections (deep reservoirs, HP separators) pressure management materially alters scaling risk, and temperature changes must be interpreted conditioned on pressure and salinity.

Referring to Figure 9, sensitivity to NaCl ionic strength ($\partial y / \partial \text{NaCl}$), it shows how changes in ionic strength (NaCl concentration) affect BaSO_4 solubility across temperature and pressure conditions. The heatmap reveals that NaCl has a generally low-to-moderate sensitivity effect compared with temperature and pressure. Sensitivity appears primarily at low pressures and low-to-moderate temperatures. This behavior aligns with thermodynamic expectations: increasing ionic strength promotes ion pairing and decreases activity coefficients, which changes solubility but typically not as drastically as temperature or pressure. At high pressures the influence of NaCl further diminishes, indicating that salinity fine-tunes solubility but does not dominate system behavior. The key takeaway is that NaCl influences solubility but acts primarily as a secondary modifier rather than the main driver.

Referring to Figure 10, sensitivity to pressure ($\partial y / \partial P$), it illustrates how BaSO_4 solubility responds to pressure changes. A clear pattern emerges, where pressure sensitivity increases as NaCl concentration increases and at elevated temperatures. This behavior reflects the effect of pressure on dissolution volumetrics and compressibility. At high temperature or concentrated brine, BaSO_4 dissolution becomes more pressure-dependent—meaning that pressure can accelerate or limit dissolution when the system deviates far from standard conditions.

The key takeaway is that the pressure becomes significant only under high-temperature and/or high-salinity conditions and is not dominant at surface or low-pressure operating conditions.

Referring to **Figure 11**, sensitivity to temperature ($\partial y/\partial T$), it shows that temperature is the most influential variable overall. At low pressure and low salinity (left panel), sensitivity to temperature is the highest among all inputs, indicating that even small temperature increases produce a strong increase in solubility. As pressure increases (middle and right panels), the relative impact of temperature decreases, confirming that the dissolution mechanism transitions from temperature-dominant to pressure-assisted behavior. This matches the known endothermic dissolution of BaSO_4 at low P and the reduced thermodynamic driving force at high P. The key takeaway is that temperature is the primary driver of solubility at low pressure, while at high pressure, temperature sensitivity is attenuated, and pressure becomes a co-driver.

The ANN-derived heatmaps reveal a clear transition: BaSO_4 solubility is temperature-controlled at low pressure, pressure-affected at high temperature and salinity, and only moderately tuned by NaCl. This confirms that the ANN is not only predictive, but it also accurately captures the underlying physicochemical dependencies of the system.

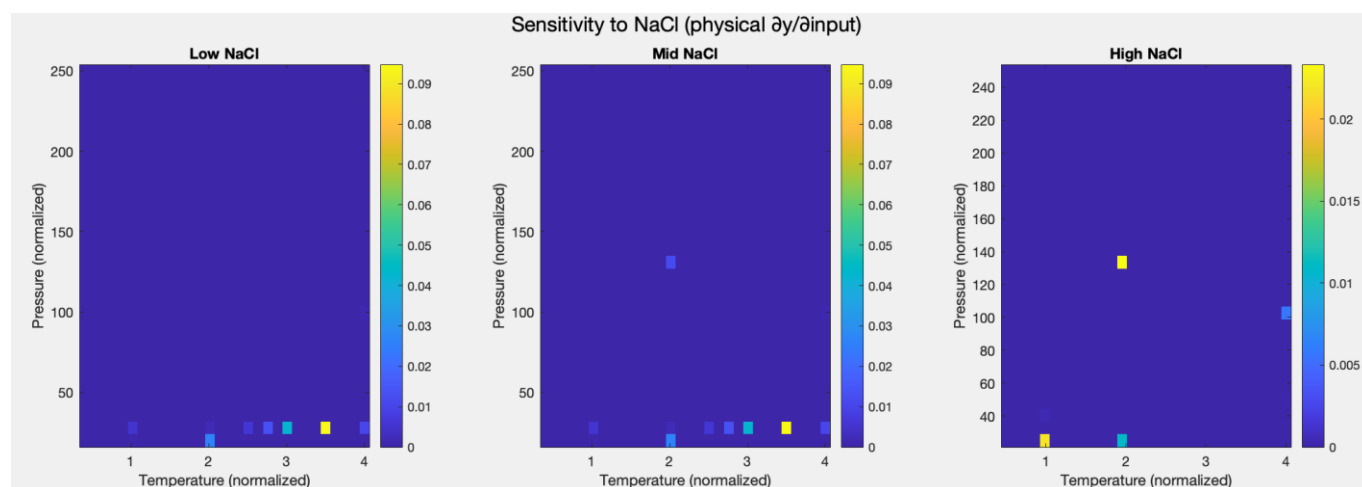


Figure 9. Heatmap Sensitivity Analysis to NaCl Ionic Strength

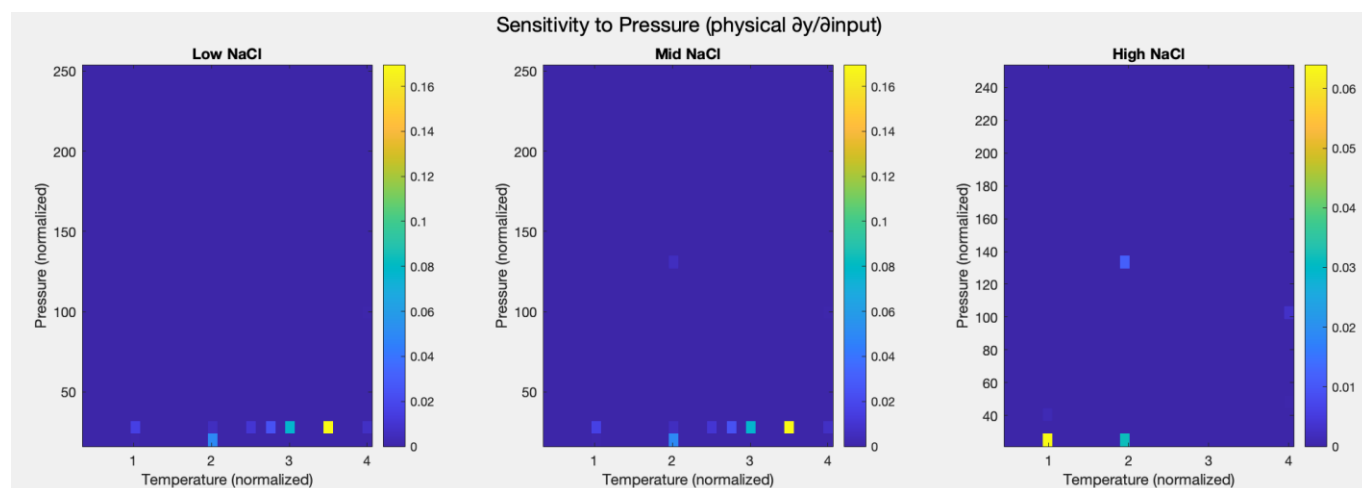


Figure 10. Heatmap Sensitivity Analysis to Pressure

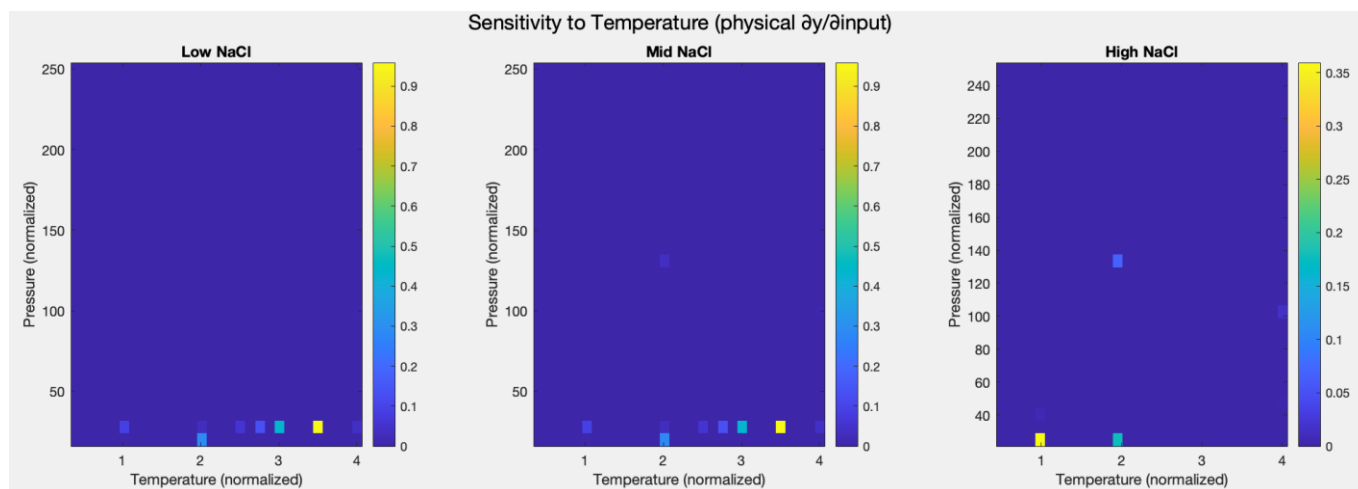


Figure 11. Heatmap Sensitivity Analysis to Temperature

CONFLICT OF INTEREST

There are no conflicts of interest.

CONCLUSIONS

This research developed an Artificial Neural Network (ANN) model to predict barium sulfate (BaSO_4) solubility in oilfield environments using temperature, pressure, and ionic strength as input variables. Unlike conventional solubility prediction methods—such as empirical models (Templeton, 1960), thermodynamic models (Monnin, 1999; Raju & Atkinson, 1990), and Pitzer-based ion-interaction approaches (Pitzer, 1973; Shi et al., 2012)—the ANN model does not require explicit calculation of activity coefficients or equilibrium constants.

The ANN achieved very high prediction accuracy with $R^2 = 0.994$, $\text{MSE} = 6.82 \times 10^{-5}$, and $\text{MAPE} = 4.3\%$. The model outperformed classical solubility models by up to a 60% reduction in prediction error, confirming superiority in accuracy and generalization. The model successfully learned the nonlinear interactions between temperature, pressure, and salinity, while thermodynamic models show reduced accuracy outside narrow operating ranges. Because the ANN relies solely on available field variables (T, P, brine concentration), it is suitable for deployment as a real-time soft sensor within oilfield information systems and digital scale-management workflows.

Together, these results show that ANN-based solubility prediction can support operational decisions, reduce manual laboratory testing, and enable proactive scale mitigation strategies—leading to improved asset integrity, reduced downtime, and cost savings.

This research makes the following contributions:

- Developed the first ANN model trained exclusively on solubility literature data covering a wide operational envelope (25–250°C, 1–500 bar, 0–4 M NaCl).
- Demonstrated that ANN significantly outperforms empirical and thermodynamic solubility models.
- Introduced a data-driven predictive approach that eliminates the need for complex thermodynamic computations.
- Produced a framework that can be integrated into digital oilfield scale-management systems for real-time decision support.

The integration of Garson's algorithm and gradient-based heat-map sensitivity analysis revealed that the ANN is not a “black box” but a transparent decision model—identifying temperature as the dominant driver under surface and low-pressure conditions, while pressure becomes increasingly influential at elevated pressures and high salinity. This interpretability confirms that the ANN not only predicts solubility with high accuracy but also captures the underlying physicochemical behavior of the system, making it suitable for real-time, condition-dependent decision support in scale management.

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