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EVALUATION OF MACHINE LEARNING ASSISTED PHASE BEHAVIOR MODELLING OF CO_2-OIL SYSTEMS

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This study evaluates machine learning (ML) methodologies in the pursuit of advancing thermodynamic flash calculations that are vital for carbon dioxide storage applications and for the oil and gas industry in general. We generated a dataset for training machine learning algorithms using a traditional physics-based model. This developed hybrid model incorporated into the machine learning model underlying physical constraints. While preliminary results from training and numerical matching were promising, the hybrid model's real-world application revealed non-trivial shortcomings. Specifically, mismatch in the multiphase region was observed during compositional space testing. Such subtle but significant flaws in machine learning methods have profound implications for the accurate physics of carbon storage projects. This article, therefore, presents advantages and disadvantages of employing ML for thermodynamic calculations, emphasizing the intricate balance between computational efficiency and representative physics.

KEY WORDS: *carbon dioxide, phase equilibrium, machine learning, hybrid model*

CO_2-МҰНАЙ ЖҮЙЕСІНІҢ ФАЗАЛЫҚ АУЫСУЛАРЫН МАШИНАЛЫҚ ОҚЫТУ АРҚЫЛЫ МОДЕЛЬДЕУ

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Бұл жұмыс көмірқышқыл газын сақтауға және мұнай-газ саласына қажетті көпкомпонентті қоспаның құрамының термодинамикалық есептеулерін жақсарту үшін машиналық оқыту (МО) әдістерін бағалайды. Дәстүрлі физика моделін пайдалана отырып, біз машиналық оқыту алгоритмдерін үйретуге арналған деректер жинағын жасадық. Біз машиналық

оқытуды модельдің негізгі физика шектеулерімен біріктіретін гибридті модельді жасадық. Алдын ала оқыту және сандық салыстыру нәтижелері перспективалы болғанымен, гибридті модельді нақты әлемде қолдану елеулі кемшіліктерді анықтады. Атап айтқанда, композициялық кеңістікті сынау кезінде біз көпфазалы модель пішінінің сәйкессіздігін анықтадық. Машиналық оқыту әдістеріндегі мұндай кемшіліктер, байқалмайтын, бірақ көміртекті сақтау жобаларының нақты физикасына үлкен әсер етеді. Бұл мақала термодинамикалық есептеулер үшін МО пайдаланудың мүмкіндіктерін мен кемшіліктерін бағалайды, есептеу тиімділігі мен физиканың репрезентативтілігі арасындағы күрделі теңгерімді көрсетеді.

ТҮЙІН СӨЗДЕР: *көмірқышқыл газы, фазалық тепе-теңдік, машиналық оқыту, гибридті модель.*

ОЦЕНКА МОДЕЛИРОВАНИЯ ФАЗОВОГО ПОВЕДЕНИЯ СИСТЕМ CO_2-НЕФТЬ С ПОМОЩЬЮ МАШИННОГО ОБУЧЕНИЯ

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В данной работе оцениваются методики машинного обучения (МО) в целях совершенствования термодинамических расчетов состава многокомпонентной смеси, необходимых для хранения углекислого газа, а также для индустрии нефти и газа в целом. Используя традиционную физическую модель, мы создали набор данных для обучения алгоритмов машинного обучения, разработали гибридную модель, объединяющую машинное обучение с физическими ограничениями, лежащими в основе модели. Несмотря на то, что предварительные результаты обучения и численного сопоставления оказались многообещающими, применение гибридной модели в реальном мире выявило значительные недостатки. В частности, при тестировании композиционного пространства мы обнаружили несоответствие формы многофазной модели. Подобные недостатки методов машинного обучения, малозаметные, но существенные, оказывают серьезное влияние на точную физику проектов по хранению углерода. В данной работе оцениваются возможности и «подводные камни» использования МО для термодинамических расчетов, подчеркивается сложный баланс между эффективностью вычислений и репрезентативностью физики.

КЛЮЧЕВЫЕ СЛОВА: *углекислый газ, фазовое равновесие, машинное обучение, гибридная модель.*

Introduction

Carbon dioxide is widely acknowledged as the primary cause of observed global warming. Concerns are growing due to increased CO_2 emissions. The carbon capture, utilization, and storage (CCUS) strategy of capturing large amounts of CO_2 from emission sources and subsequently utilizing or long-term storing in underground reservoirs has emerged as a proven and effective approach to mitigating the impact of CO_2 emissions on climate change [1].

During the geologic carbon sequestration, injection of CO_2 into oil and gas reservoirs exhibit significant variations in their compositions because of CO_2 partitioning into liquid and gas phases and solubility in oil. Compositional modeling is required to capture the CO_2-hydrocarbon phase equilibria and the flow of multiple phases in order to accurately model complex phase behavior. The phase split calculations, which provide the number and composition of the equilibrium phases assuming instantaneous mass transfer between phases, are essential to this modeling approach. Determining phase equilibria for each simulation grid element at each time step is crucial because it directly affects the accuracy of fluid property prediction.

Peng-Robinson (PR) [2] and the Soave-Redlich-Kwong (SRK) [3] cubic equations of state (EoS) are commonly used approaches for compositional simulations along with the Rachford-Rice flash equation [4] to compute phase equilibrium [5]. The phase behavior calculation is directly related to the equilibrium ratio, or K-value, which is expressed as the ratio of molar fractions in the vapor phase to molar fractions in the liquid phase [6]. The primary unknown in the phase split calculation is the K-value [7], which is determined through an iterative process of trial and error until solution convergence is reached. Empirical correlations based on investigating experimental data are used to determine an initial K-factor to start the iterative process [8]. The accuracy of this initial guess is critical because the convergence of the final solution is sensitive to the initial input [9].

Complex calculations of phase equilibrium cause high computation costs in compositional models. According to research, phase flash calculations account for a significant portion of the total simulation time. This can limit the feasibility of applying for long-term, field-scale CO_2 injections, primarily due to rigorous iteration calculations [10]. In response to these challenges, various methods for accelerating phase equilibrium calculations have been proposed. K-value calculation techniques, reduction methods, precalculated tie-lines methods, and the incorporation of machine learning are among these approaches.

The initial K-value is commonly calculated using the Wilson correlation [11]. Improving the accuracy of this initial K-value can significanlty speed up phase calculations. Notably, Ghafoori et al. (2012) and Vatandoost et al. (2016) achieved more precise prediction of K-values related to reservoir fluid composition [12]. The latter research focused on heavy hydrocarbon and volatile oil systems, developing distinct correlations to forecast K-value. Furthermore, Michelsen (1998) and Wang (1994) demonstrated that using initial flash calculation estimates obtained from the previous time step can considerably speed up the phase equilibrium calculation when coupled with the full Newton's method [13, 10].

The conventional reduction method entails lumping the reservoir fluid composition into a reduced set of pseudo-components [14], while maintaining the accuracy of the equation

of state model. Michelsen (1986) introduced a method to reduce the computational cost with the primary concept being to neglect binary interaction parameters (BIP) originally determined by fitting the equation of state to experimental data [15]. Hendriks et al. (1992) and Firoozabadi and Pan (2002) extended the reduction method and demonstrated dimensionality reduction in various phase equilibrium problems without neglecting BIP [16].

Voskov and Tchelepi (2009) [17] demonstrated an acceleration in phase split calculations by utilizing precalculated tie-lines generated using the negative flash method proposed by Whitson and Michelsen (1989) [18]. The Compositional Space Adaptive Tabulation (CSAT) technique further optimized the displacement path along tie-lines during gas injection processes, reducing simulation time by eliminating the need for redundant stability checks. Belkadi et al. (2011) expanded on this by introducing Tie-line Distance Based Approximation, a method designed to accelerate tie-line search [19].

Machine learning techniques have recently emerged as useful tools for addressing computational time challenges in phase equilibrium calculations. Notably, artificial neural networks (ANNs) have been used successfully to calculate oil properties, such as bubble point pressure, gas-oil ratio, and formation volume factor. This advancement eliminates the necessity for iterative computations [20]. Furthermore, the support vector machine (SVM) technique based on kernel neuron functions has demonstrated its effectiveness in predicting complex nonlinear problems relating to crude oil PVT properties [21].

While machine learning techniques have shown promise in significantly reducing computational time, questions about the accuracy and feasibility of a data-driven approach remain. Magzymov et al. (2021) highlighted the inaccuracies in a purely data-driven machine learning technique [22]. They proposed incorporating physics principles into the machine learning algorithm to capture flow in porous media. Recent scientific interest has been drawn to physics-informed machine learning, which has applications to a variety of physics problems, such as Navier–Stokes, Poisson, Burgers equations, and other partial differential equations. This hybrid approach allows the industry to avoid relying solely on data-driven machine learning algorithms.

Gaganis and Varotsis (2012) presented the physics-machine learning coupling by introducing discriminating functions for non-iterative phase stability calculations [23]. These discriminating functions utilized the tangent plane distance criteria [7] and identified stable conditions. Furthermore, Gaganis and Varotsis (2014) applied the regression model to derive the reduced variables for two-phase split calculations [24]. They also used Support Vector Machine (SVM) to distinguish between stable and unstable conditions. Kashinath et al. (2018) employed Relevance Vector Machines (RVM) for classifying the supercritical one-phase region, while using another classifier to determine the phases in the sub-critical region. Finally, ANNs were used to predict the K-values for phase splitting [25].

In this study, we utilized a negative flash calculation method based on the Peng-Robinson EoS and Rachford-Rice flash equations to generate a set of synthetic data that included compositions of liquid and vapor phases within CO_2-hydrocarbon mixtures. We could effectively avoid potential issues with experimental data quality by generating data using the physics-based negative flash method. Subsequently, we applied the synthetic data to train the hybrid physics-based machine learning model and compared it to a pure data-driven machine learning model.

Methodology

Phase equilibrium calculations and construction of machine learning algorithm

This section describes a procedure for negative flash calculations with further construction and training of the corresponding machine learning models. We generate a training dataset by using the negative flash calculation approach based on the Peng-Robinson equation of state (1978) to determine phase equilibrium of CO_2-hydrocarbon system. The machine learning models are then trained on the synthetic dataset to predict the equilibrium ratio. Finally, we validate machine learning results with the physics-based calculations. Integrating machine learning technique for predicting K-values shortens the computational time while maintaining phase equilibrium physics.

2.1. Negative flash calculation

We solve two-phase isothermal negative flash problems over the range of composition containing CO_2 and hydrocarbon mixture, pressure and temperature. Advantage of the negative flash procedure is the simultaneous calculation of phase split (number of phases) and phase equilibrium (liquid and gas phase composition).

Negative flash is based on the common approach requiring the chemical potential of each component i=1,2,…,n in each coexisting phases to be equal. Chemical potential is expressed in terms of fugacity:

$$f_i^L = f_i^V \tag{1}$$

or in terms of fugacity coefficients:

$$x_i \phi_i^L P = y_i \phi_i^V P \tag{2}$$

where L and V corresponds to the liquid and vapor phase, x_i and y_i – component i mole fractions ϕ_i^L and ϕ_i^V are the fugacity coefficients of component i in liquid and vapor phases, P is pressure. Fugacity coefficient can be expressed in terms of the measurables values of pressure, temperature and volume:

$$ln\phi_i = \frac{1}{RT}\int_V^\infty \left[\left(\frac{\partial P}{\partial n_i}\right)_{T,V,n_j \neq i} - \frac{RT}{V}\right] dV - lnZ, \qquad i = 1, 2, \ldots N \tag{3}$$

Peng-Robinson Equation of state (Peng and Robinson, 1978) is applied to determine fugacity coefficient, where the general form of the equation (4) is transformed to eq. (5) expressed in terms of compressibility factor Z, and then substituted to eq. (3) and finalized in eq. (6).

$$P = \frac{RT}{v-b} - \frac{a_c \alpha}{[v(v+b)+b(v-b)]} \tag{4}$$

$$Z^3 - (1-B)Z^2 + (A - 2B - 3B^2)Z - (AB - B^2 - B^3) = 0 \tag{5}$$

$$ln\phi = (Z-1) - \ln(Z-B) + \frac{A}{2B\sqrt{2}} ln\frac{Z+(1-\sqrt{2})B}{Z+(1+\sqrt{2})B} \tag{6}$$

Material balance for each component i must be satisfied:

$$z_i = x_i n^L + y_i n^V, \qquad i = 1,2,\ldots N \tag{7}$$

Where n^L and n^V are the fraction of moles in liquid and vapor phases. Introducing equilibrium coefficient, or K-value: $K=y_i/x_i$, phase mole fractions can be expressed:

$$x_i = \frac{z_i}{1 + (K_i - 1)n^V} \tag{8}$$

$$y_i = \frac{K_i z_i}{1 + (K_i - 1)n^V} \tag{9}$$

The straightforward approach of solving x_i, y_i, and n^V is based on the trial-and-error successive substitution method. The constraint of the x_i and y_i mole fraction summation to unity can be solved by Rachford-Rice relation [4]:

$$f(n^V) = \sum_{i=1}^{N}(y_i - x_i) = \sum_{i=1}^{N}\frac{z_i(K_i - 1)}{1 + (K_i - 1)n^V} = 0 \tag{10}$$

We use Wilson's correlation to specify initial K-value (Wilson, 1969). The first guess of n^V is reasonably set to 0.5. Further solution of K-value and n^V is iterative successive substitution starting with updating n^V at the fixed K-value followed by further updating K-value. Function $f(n^V)$ decreases monotonically with asymptotes $1/(1\text{-}K_i)$. Non-negative phase composition occurs at the n^V between asymptotes $\frac{1}{1-Kmax} < n^V < \frac{1}{1-K_{min}}$. Final convergence is agreed to be achieved when K-value error is in the range of the accepted tolerance.

2.2 Physics-informed ML construction framework

We designed a hybrid framework that incorporates machine learning techniques to perform negative flash calculations to replace computationally expensive physical models while preserving physics-based workflow. The *Figure 1* depicts the schematic workflow of a physically representative model of flash calculations compared to a hybrid model.

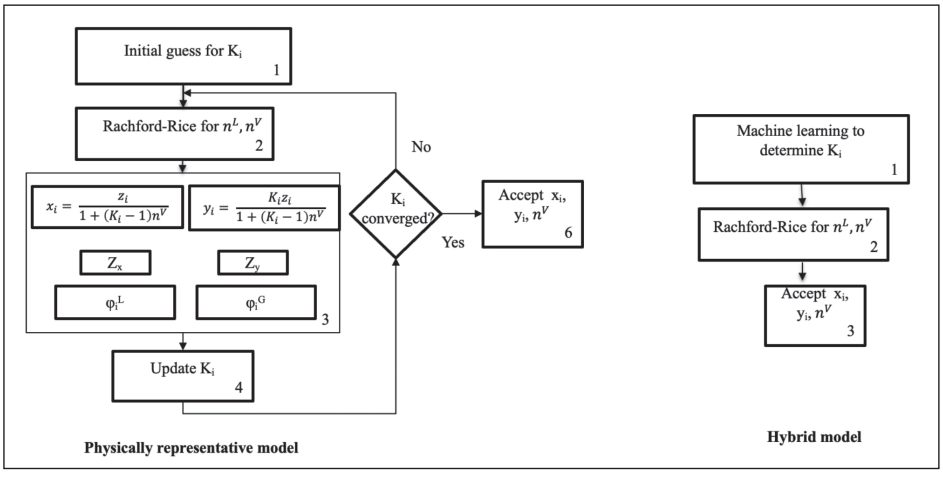

Figure 1 - **Comparison of physically representative model with the hybrid model**

Both models use the fluid composition (0 to 1), pressure (40 to 70 atm) and temperature (330 to 370 K) as inputs to produce outputs that include negative flash phase compositions. Carbon dioxide (CO_2), butane (C_4), and decane (C_{10}) were used. To generate synthetic data, physics-based flash calculations were conducted on a random sample of input parameters within a reasonable range that represented hydrocarbon reservoirs and CO_2 injection scenarios. This paper focuses on two phase regions. A total of 7000 data points were generated within the domain of interest. These data points were divided into three sets: 80% for machine learning model training, 10% for validation, and 10% for testing.

For implementation of machine learning algorithms in a hybrid model we applied physical constraints (see *Figure 2*). Raw machine learning implementation may result in unphysical modelling and predictions. For example, unconstrained machine learning can produce results that violate mass balance, where sum of all component fractions does not equal unity for each phase. Moreover, the boundary of two-phase compositional space may have an irregular shape.

We build the hybrid model that incorporates the computational efficiency of machine learning with the underlying physics. The hybrid model consists of a series model in which machine learning was used to find Ki equilibrium constants for each component instead of focusing on individual components. Following that, we use Ki equilibrium constants in one-time Rachford-Rice calculations. The final step ensures that we respect mass balance and phase amounts by using negative flash calculation. It is worth noting that the choice of target variables is important. We selected to predict ln(xi) and ln(yi) of each component. Then, Ki values were calculated externally based on neural networks output as Ki=yi/xi.

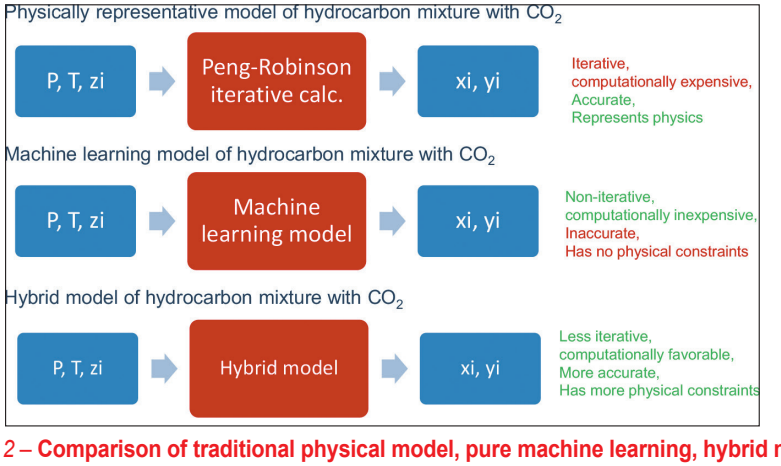

Figure 2 – **Comparison of traditional physical model, pure machine learning, hybrid model**

Results and Discussions

We tested several machine learning algorithms to evaluate the accuracy of matching the set of synthetic data (see *Figure 3*). We evaluated linear regression, decision tree, support vector machine, Gaussian process regression, and neural network (deep learning). For fair comparison we tested how well the models can match a single parameter $\ln(y_c10)$ vapor composition of decane. Based on the evaluation we selected neural network model for further implementation in the hybrid model, because neural networks have demonstrated accuracy, flexibility to incorporate multiple input/output features, and flexibility to alter internal architecture of the model.

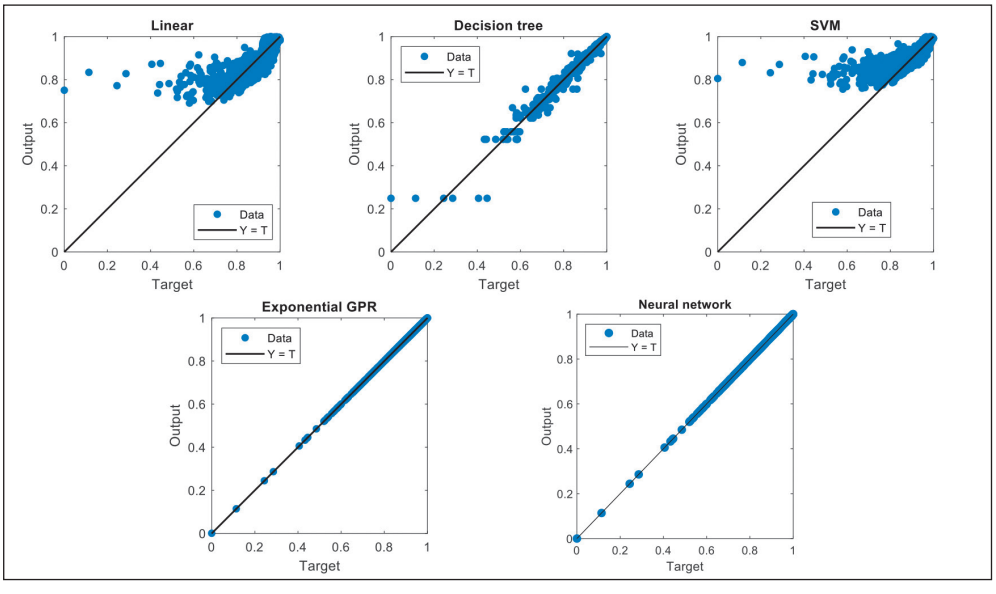

Figure 3 – **Comparison of machine learning algorithms ability to match vapor phase composition of decane in CO2-hydrocarbon systems**

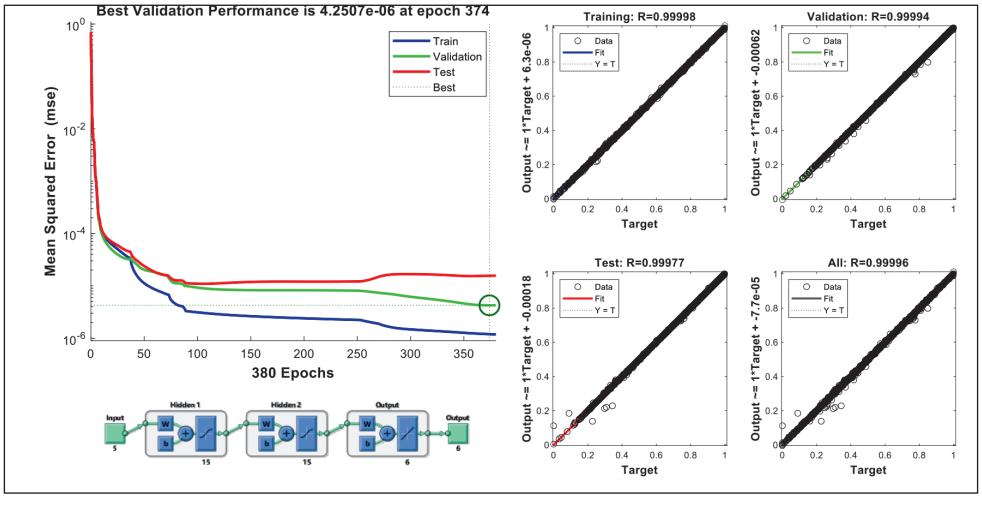

Figure 4 – **Hybrid model of hydrocarbon mixture with CO2: training, validation, and testing**

Figure 4 shows tuning of neural network as well as model fitting, validation, and testing performance. As demonstrated by the match, the neural network is capable of capturing essential features of component compositions. Then, based on the overall composition, we perform one-time Rachford-Rice calculations to obtain final equilibrated phases as well as phase saturation. The results are shown in *Figure 5* for 40 atm and 335 K. *Figure 5a* depicts physical equation-of-state results, with blue lines representing tie-lines in the two-phase region. *Figure 5b* shows outputs of the hybrid model proposed in this

paper. When compared, both results are very close. *Figures 5c* and *5d* show Ki matching. It is worth noting that even though the hybrid model matches target values in *Figures 4, 5c* and *5d*, we can observe that two phase regions differ noticeably in compositional space. *Figure 6* depicts similar results for different conditions (55 atm and 350 K). Again, we see that the overall size of the two-phase zone generated by the hybrid model is similar to the physical model, but the size is noticeably different. A difference in the two-phase region size has significant implications for reservoir simulation efforts and carbon capture project design. For example, the red circle in the compositional space in *Figure 5a* and *5b* is single-phase versus two-phase predicted by the hybrid model. The presence or absence of two phases has important implications for flow modeling in porous media, including relative permeability effects, trapping, capillary forces. Thus, numerical match of hybrid model does not imply that machine learning or hybrid models can completely replace physical models. Depending on the application, hybrid models can provide significant computational benefits; however, a comprehensive evaluation of hybrid and physics-informed models is required before wide-scale implementation.

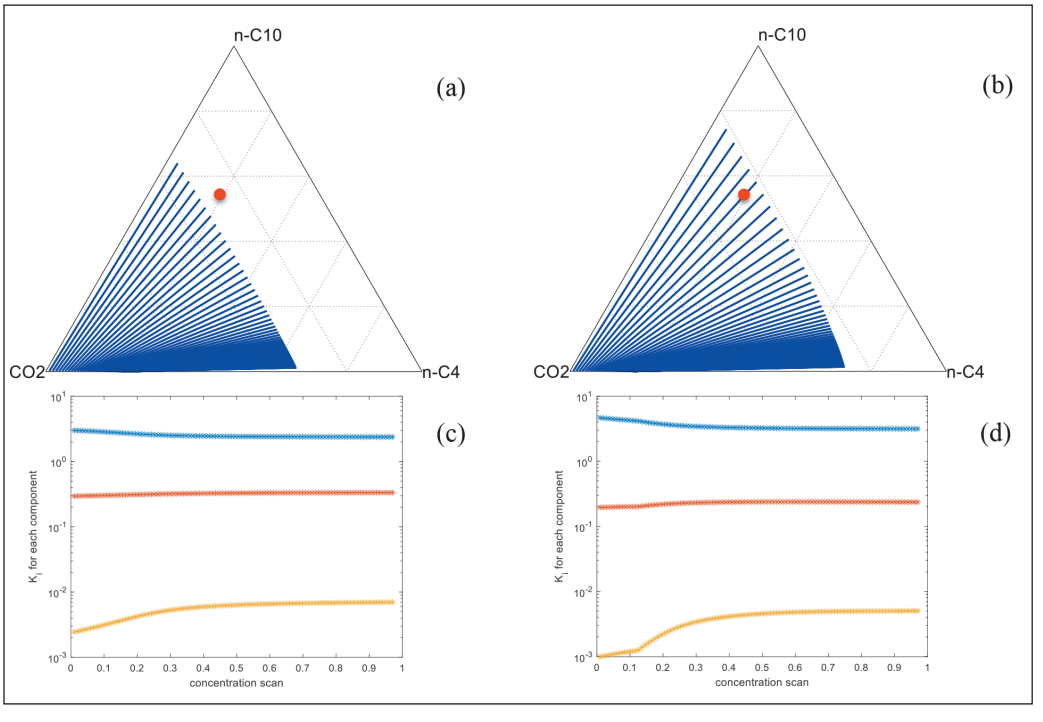

Figure 5 – **Results for flash calculations at 40 atm, 335K**

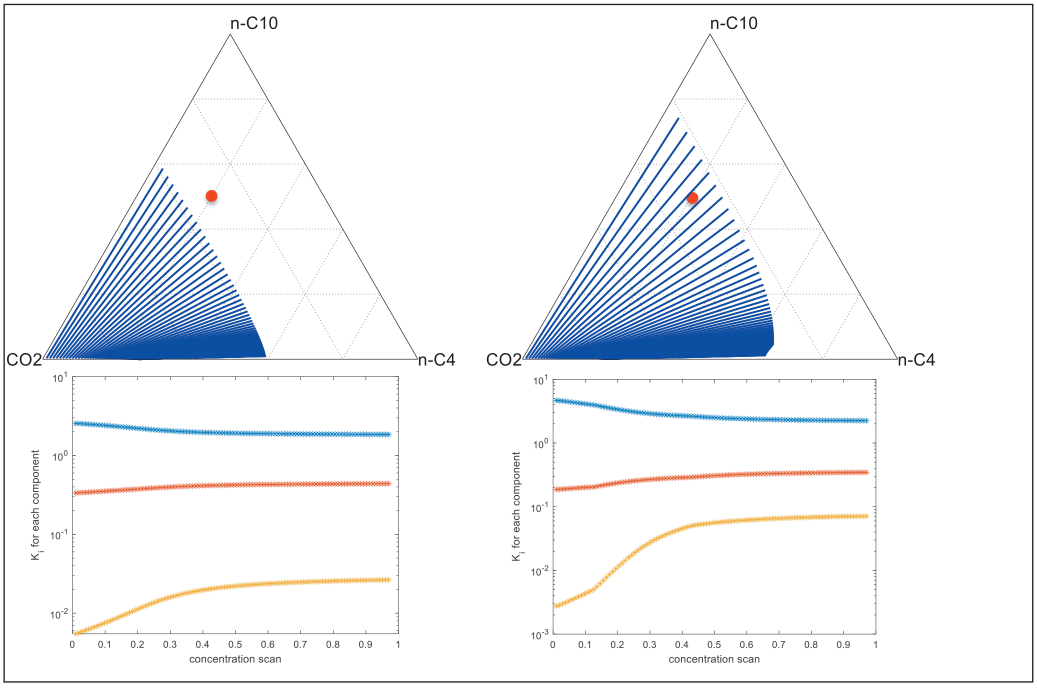

Figure 6 – **Results for flash calculations at 55 atm, 350 K**

Conclusions

In this paper, we presented the hybrid approach to thermodynamic flash calculations that combines traditional physical models and machine learning algorithms. We developed the framework for training neural networks with data generated by physical models. The hybrid model was tested for the ability to capture physical phenomena. According to the results, the hybrid model is capable of capturing the essential physics of phase behavior. The initial results of training and numerical analysis appeared promising, but the hybrid model had some limitations. During compositional space tests, there was a noticeable difference in the shape of the multiphase region. These minor but significant differences in machine learning approaches can have a great impact on the precision required in carbon storage project design. This study examined the benefits and challenges of using machine learning for thermodynamic computations, highlighting the delicate balance between potential computational efficiency gain and accurate physical representation.

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REFERENCES:

1 Metz B., Davidson O., De Coninck HC., Loos M., Meyer LA. IPCC special report on carbon dioxide capture and storage: prepared by working group III of the intergovernmental panel on climate change. IPCC, Cambridge University Press. – 2005.

2 Robinson D.B., Peng D.Y., The characterization of the heptanes and heavier fractions for the GPA Peng–Robinson programs. Gas processors association. – Research report RR-28. – 1978.

3 Soave, G. Equilibrium constants from a modified Redlich-Kwong equation of state // Chemical Engineering Science. – 1972. – v. 27. – no. 6. – p. 1197–1203.

4 Rachford H. H., Rice J. D. Procedure for Use of Electronic Digital Computers in Calculating Flash Vaporization Hydrocarbon Equilibrium // Journal of Petroleum Technology. – 1952. – v. 4. – no. 10. – p. 19–3.

5 Li Y-K., Nghiem L. X. Effect of Phase Behavior on CO2 Displacement Efficiency at Low Temperatures: Model Studies with an Equation of State // SPE Reservoir Engineering. – 1986. – pp. 414-422.

6 Souders M. Jr., Selheimer C.W., Brown G.G. Hydrocarbon vapor–liquid equilibria // Industrial and Engineering Chemistry. – 1932. – p. 24-517.

7 Michelsen M. L. The isothermal flash problem. Part I. Stability // Fluid Phase Equilibria. – 1982. – v. 9. – no. 1. – p. 1–19.

8 Katz DL., Hachmuth KH. Vaporization equilibrium constants in a crude oil– natural gas system // Industrial Engineering Chemistry. – 1937. – no.29.

9 Danesh A. PVT and Phase Behavior of Petroleum Reservoir Fluids. Elsevier Science Ltd. – 1998.

10 Wang P., Stenby E.H. Non-iterative flash calculation algorithm in compositional reservoir simulation // Fluid Phase Equilibrium. –1994. – no.96. – p. 93–108.

11 Wilson G.M. A modified Redlich-Kwong equation of state, application to general physical data calculations // 65th National AIChE Meeting. – Cleveland, OH. – 1969.

12 Ghafoori M. J., Aghamiri S. F., Talaie M. R. A new empirical K-value equation for reservoir fluids // Fuel. – 2012. – v. 98. – p. 236–242.

13 Michelsen M. L. Speeding up the two-phase PT-flash, with applications for calculation of miscible displacement // Fluid Phase Equilibria. – 1998. – v. 143. – no. 1–2. – p. 1–12.

14 Whitson C. and Brule M. Phase behavior. SPE Monograph series. – 2000.

15 Michelsen M. L. Simplified Flash Calculations for Cubic Equations of State // Industrial and Engineering Chemistry Process Design and Development. – 1986. – v. 25. – no. 1. – p. 184–188.

16 Hendriks E.M., van Bergen A.R.D. Application of a reduction method to phase equilibria calculations // Fluid Phase Equilib. – 1992. – no.74. – p. 17–34.

17 Voskov D., Tchelepi H. Tie-simplex based mathematical framework for thermodynamic equilibrium computations of mixtures with an arbitrary number of phases // Fluid Phase Equilib. – 2009. – p.1–11.

18 Whitson C., Michelsen, M.L., The negative flash // Fluid Phase Equilib. – 1989, – no.53. – p.51–71.

19 Belkadi A., Michelsen M.L., Stenby E.H. Comparison of two methods for speeding up flash calculations in compositional simulations // SPE Reservoir Simulation Symposium. – 2011. (SPE 142132-MS)

20 Al-Marhoun M. A., Osman E. A. Using artificial neural networks to develop New PVT correlations for saudi crude oils // Society of Petroleum Engineers - Abu Dhabi International Petroleum Exhibition and Conference ADIPEC. – 2002 (doi:10.2523/78592-MS)

21 Gaganis V., Varotsis N. Machine learning methods to speed up compositional reservoir simulation // 74th European Association of Geoscientists and Engineers Conference and Exhibition Incorporating SPE EUROPEC 2012: Responsibly Securing Natural Resources. –no. 1992. – p. 3220–3231. (SPE 154505)

22 Magzymov D., Ratnakar R. R., Dindoruk, B., Johns, R. T. Evaluation of Machine Learning Methodologies Using Simple Physics Based Conceptual Models For Flow in Porous Media // SPE Annual Technical Conference and Exhibition. – 2021.

23 Gaganis V., Varotsis N. Non-iterative phase stability calculations for process simulation using discrimination functions // Fluid Phase Equilib. – 2012. – v. 314. – p.69–77.

24 Gaganis V., Varotsis N. An integrated approach for rapid phase behavior calculations in compositional modeling // Journal of Petroleum Science and Engineering. – 2014. – v. 118. – p. 74–87 (doi:10.1016/j.petrol.2014.03.011).

25. Kashinath A., Szulczewski M. L., Dogru A. H. A fast algorithm for calculating isothermal phase behavior using machine learning // Fluid Phase Equilibria. – 2018. – v. 465. – p. 73–82 (doi:10.1016/j.fluid.2018.02.004).