Application of Mixed Kernels Function (MKF) Based Support Vector Regression Model (SVR) for CO₂ – Reservoir Oil Minimum Miscibility Pressure Prediction.

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Abstract

Carbon dioxide (CO₂) injection into oil reservoirs is considered a mature enhanced oil recovery (EOR) technique for conventional reservoirs. The local displacement efficiency of the CO₂-EOR process is highly dependent on the minimum miscibility pressure (MMP), estimating this parameter is critical to design of the CO₂ injection process. Traditional empirical methods to test the CO₂-oil MMP are time consuming and expensive; derived correlations are fast but not accurate. Therefore, an efficient and reliable method to determine MMP is beneficial. In this study, a mixed kernels function (MKF) based support vector regression (SVR) model was developed and used to predict the MMP for both pure and impure CO₂ injection cases. Four parameters were chosen as input parameters: 1) reservoir temperature; 2) average critical temperature; 3) molecular weight of pentane plus (C₅₊) fraction of crude oil, and; 4) the ratio of volatile components to intermediate components in crude oil. MMP was selected as the desired output parameter to train and test this newly developed model. The performance of basic kernels function based SVR model is compared with that of this newly developed MKF-SVR model. The well-trained MFK-SVR was compared with three well-established published correlations, demonstrated the highest correlation coefficient (R of 0.9381), lowest root mean square error (RMSE of 1.9151), smallest average absolute error (AAE

of 1.1406) and maximum absolute error (MAE of 4.6291). We believe that the proposed MFK-SVM model is a more reliable and stable regression model to predict MMP. In addition, a sensitivity analysis was conducted to evaluate the physical correctness. It indicates that the predicted results from the newly developed model are in excellent agreement with previous empirical work.

Keywords: CO₂-oil minimum miscibility pressure, CO₂ enhanced oil recovery, support vector regression, mixed kernels function, particle swarm optimization algorithm

Nomenclature			
AAE	average absolute error	P_i	personal best value
BOPD	Barrels of oil per day	P_b	bubble pressure
C	penalizing parameter in SVM	$P_{m,\min,pure}$	MMP value in pure CO ₂ -oil systems
CO ₂	carbon dioxide	$P_{m,\min,impure}$	MMP value in impure CO ₂ -oil systems
C ₅₊	pentane plus fraction	$\vec{v}_i^{new}$	i^{th} particle's new velocity
d	polynomial degree	$\vec{v}_i^{old}$	i^{th} particle's old velocity
D	architecture space Dimension	PSO	particle swarm optimization
ϵ	insensitivity loss parameter	r	correlation coefficient
ξ_i and ξ_i^*	slack variables	R ²	coefficient of determination
EOR	enhanced oil recovery	RBF	radial basis function
F_{imp}	correction factor for impure CO ₂ stream	RMSE	root mean error
GEP	gene expression programming	SVR	support vector regression
GSA	grid searching algorithm	SVM	support vector machine
Y	RBF kernel parameter	T_{ck}	critical temperature of component k (k = CO ₂ , C ₁ , N ₂ , H ₂ S, and C ₂ –C ₄), °C
K(x _i , x _j)	kernel function	T_{cm}	weight average pseudocritical temperature of the drive gas, °C
m	mixing coefficient	T	reservoir temperature, °C
MAE	maximum absolute error	t _{ite}	current iteration number
MKF	mixed kernels function	t _{max}	maximum iteration number
MKF-SVR	mixed kernels function based support vector regression	x_i	i^{th} particle's position
MMP	minimum miscibility pressure, MPa	$x_{i,j}$	j^{th} value of i^{th} particle
MSE	mean squared error, %	$\vec{x}_i^{old}$	i^{th} particle's old position
MW _{C5+}	molecular weight of C ₅₊ oil fraction, g/mol	$\vec{x}_i^{new}$	i^{th} particle's new position
N	sample number	x_{MED}	mole fraction of intermediate oil components including C ₂ –C ₄ , CO ₂ , and H ₂ S, %
ω_{max}	initial inertia weight	x_k	mole fraction of component k (k = CO ₂ , C ₁ , N ₂ , H ₂ S, and C ₂ –C ₄), %
ω_{min}	final inertia weight	x_{VOL}	mole fraction of volatile oil components including N ₂ and CH ₄ , %
φ_1	cognitive coefficient	Y	Input vector
φ_2	social coefficient	y	output variable
P_g	global best value	$\hat{y}$	estimated output value

1. Introduction

One of the first viable CO₂ commercial EOR applications was started in 1972 in the Kelly-Snyder oil field [1]. Today, CO₂ injection is an established enhanced oil recovery (EOR) technique for recovering residual oil in older and/or mature oil field. In 2014, 136 CO₂-EOR projects were underway in the U.S. and producing approximately 300,000 barrels of oil per day (BOPD) [2]. CO₂ injection can facilitate the reduction of greenhouse gas emissions by storing the CO₂ into geological media, such as depleted oil reservoirs. CO₂ -EOR is a preferred EOR method because CO₂ is miscible with crude oil increasing displacement efficiency, and less expensive than other similarly miscible fluids [3]. The displacement efficiency of CO₂ is highly dependent on the minimum miscible pressure (MMP) [4, 5]. MMP is the minimum pressure at which injected gas can develop multi-contact miscibility with the reservoir oil [6-10]. Above this pressure, interfacial tension between these two phases is zero, and there is no difference between the densities of oil and injected gas [10, 11]. In contrast, at pressure lower than MMP, CO₂ will no longer be miscible with oil and the displacement efficiency decreases. In case of CO₂ injection, the CO₂-oil MMP is of great influence by the CO₂ purity, reservoir temperature and oil composition [12, 13]. The injected CO₂ is not always pure, some impurities such as methane, nitrogen, H₂S, and hydrocarbons, inevitably exist in the CO₂ gas stream. Those impurities bring about large effects on the CO₂-oil MMP. In a dense CO₂ steam, methane and nitrogen impurities substantially increase the MMP, but intermediate hydrocarbons (C₂-C₅) or H₂S impurities decrease the MMP [14]. Accurate CO₂-oil MMP estimation is critical in selecting suitable oil and gas reservoirs for CO₂-EOR processes.

Laboratory empirical methods are commonly used to estimate the MMP [15]. The petroleum industry standard for estimating the MMP is a slim-tube apparatus, because its results are most reliable and comparable with established industry data [16, 17]. In the early 1980s, Christiansen et al. [18] developed a fast experimental method for MMP estimation using a rising-bubble apparatus

(RBA) [19]. Both slim-tube and rising-bubble methods are expensive, time consuming and depend on large amount of data [20, 21]. Rao et al. [22] proposed a fast and simpler experimental method using experimental approach labeled vanishing interfacial tension (VIT) [22-25]. The accuracy of the measurement depends on the composition of the mixture created fluid, and may give a higher MMP result than actual, because the composition cannot be selected in advance [24].

Numerous empirical correlations have been developed to describe the phase behavior of reservoir oil-CO₂ and to minimize the difference between the transformed dependent variable (CO₂-oil MMP) and the sum of the transformed independent variables [4, 12, 16, 26-31]. However each correlation is restricted for specific oil reservoir conditions, such as temperature and oil composition. Where the geological conditions are very complex, empirical correlations cannot meet the various requirements for different oil reservoirs [32]. Thus the application of those techniques is limited, and more adaptable, reliable correlation methods are required to overcome these limitations.

Huang et al. [21] applied an artificial neural network to build up an intelligent model to estimate the pure and impure CO₂-oil MMP value. In order to avoid the disadvantage of overfitting and non-convergence, the artificial neural network was optimized by various evolutionary algorithms (e.g. particle swarm optimization, genetic algorithm) [32-35]. Emera and Sarma [12] developed the genetic algorithm (GA)-based correlation to estimate CO₂-oil MMP value. Asoodeh et al. [36] utilized committee machine, which was based on divide and conquer principle to reap benefits of various regression models to increase the precision of prediction. Kamari, et al. [37] used newly developed gene expression programming (GEP) technique to estimate the CO₂-oil MMP. According Ahmadi, et al. [38], fuzzy logic method was utilized to specify minimum miscible pressure of injected gas and reservoir oil. Support Vector Regression (SVR) is another technique, which is used to estimate CO₂-oil MMP. It is highly effective in representing a system's complexity; it also has a generalizing ability in function approximation [39, 40]. Vapnik and colleagues [41-46] first developed Support Vector Machine (SVM) at AT&T Bell laboratories based on statistical-learning

theory to solve pattern recognitions problems [45]. This algorithm was later extended to solve regression problems [47]. Al-Anazi et al. [48, 49] applied SVR to predict reservoir permeability and porosity. The principle of SVR is to find an optimal hyperplane in which all projected training data from the original data space is located within ε deviation in a high dimensional feature space [45, 50].

The four basic elements of SVR are the separating hyperplane, maximum-margin hyperplane, soft margin and kernel function [51]. The most important part of SVR is the kernel function. There are two different groups of kernels: global kernels and local kernels. Global kernels have stronger extrapolation ability and local kernels have stronger interpolation ability. Standard kernels that can simultaneously extrapolate and interpolate are to some degree inaccurate. In this paper, a process is introduced that uses a mixed kernels function (MKF), which combine the local and global kernel function to overcome this drawback mentioned above [52-54]. Mixing coefficient (m), gamma (γ), penalty parameter (C), polynomial degree (d) and epsilon (ε) are the important parameters in the MKF-SVR model. The determination of these parameters is the key step to achieve high performance from MKF-SVR. A grid searching algorithm (GSA) [40] and particle swarm optimization (PSO) [50, 55] algorithm were applied to optimize these parameters for fast convergence in the training process.

The mixed kernels function (MKF) based support vector regression (SVR) is used to evaluate the pure and impure CO₂/oil MMP in crude oil. Four variable are evaluated: (a) molecular weight of C₅₊ fraction; (b) reservoir temperature; (c) volatile oil fraction (methane and nitrogen gas); and (d) intermediate oil fraction (C₂–C₄ and CO₂, H₂S) in crude oil. The results of MKF-SVR are compared to the results from SVR based on each basic kernel function. Moreover, the result predicted from the MKF-SVM model is compared to calculated values from traditional empirical correlations reported

in the published literature. Sensitivity analysis is conducted to check out the most important input variables.

2. Methodology

2.1 Support vector regression

The support vector machine (SVM) was first introduced in 1960s in Russia [56-58]. Initially it was modified to solve pattern recognitions problems. Later it was extended to the case of nonlinear regression and time series prediction problems [43-45, 59, 60], which is support vector regression (SVR). Using adaptive margin-based loss functions and projecting the learning data (linearly or non-linearly) into higher dimensional feature space, SVR finds the best decision rule that has good generalization ability (Fig. 1a). The projecting functions satisfied with the Mercer's condition are called Kernels – $K(x_i, x_j)$ [61].

For example, assume training data $\{(x^1, y^1), (x^2, y^2), \dots, (x^m, y^m)\} \subset \mathcal{X} \times \mathfrak{R}$, where $\mathcal{X}$ denotes the space of the input parameters (e.g. $\mathcal{X} = \mathfrak{R}^d$). For the case of linear function f takes the form:

$$f(x) = \langle \omega, x \rangle + b, \quad \omega \in \mathcal{X}, b \in \mathfrak{R} \quad \text{Eq. (1)}$$

In the high dimensional feature space, the optimization problem for SVR with ε -insensitive loss function is:

$$\min_{\omega} \quad \frac{1}{2} \|\omega\|^2 + C \sum_{i=1}^m (\xi_i + \xi_i^*) \quad \text{Eq. (2)}$$

$$s.t. \quad \begin{cases} y_i - \langle \omega, x_i \rangle - b \leq \varepsilon + \xi_i, i = 1, 2, \dots, m \\ \langle \omega, x_i \rangle + b - y_i \leq \varepsilon + \xi_i^*, i = 1, 2, \dots, m \\ \xi_i, \xi_i^* \geq 0, i = 1, 2, \dots, m \end{cases} \quad \text{Eq. (3)}$$

The first part of Eq. (2) is the Vapnik-Chervonenkis (VC) confidence interval, whereas the second part is the empirical risk [48]. The regularization constant C in Eq. (2) is used to determine the

complexity of the SVM model. The constant C also makes a compromise between the empirical risk minimization and the confidence degree. The epsilon (ε , essentially controls the complexity of the regression functions mentioned above). The slack variables (ξ_i and ξ_i^*), introduced by Bennett et al. [62], contrast the symmetric boundary produced by the 'hard margin' loss function. Vapnik's ε -insensitivity loss function as illustrated by Fig. 1b and 1c defines a multi-dimensional tube. Only the points outside the ε -tube contribute to the loss, which is equal to the gap between the point values and the radius of the tube. The deviations are penalized in a linear fashion. However, the points inside the ε -tube contribute nothing to the cost, which means the loss (error or cost) is zero.

Figure 1

2.1.1 Kernel function

Kernel functions $K(\vec{x}, \vec{x}^*)$ actually are a projection function. The function projects the original linearly or non-linearly learning data into high dimensional feature space, where all of the data can be presented linearly [63]. A kernel function must meet Mercer's conditions [41, 42, 46, 64, 65], as following:

Suppose $K(\vec{x}, \vec{x}^*) \in L_2(\mathfrak{R}^n) \otimes L_2(\mathfrak{R}^n)$

$$\exists \forall g(x) \in L_2(\mathfrak{R}^n),$$

$$\iint_{L_2 \otimes L_2} K(\vec{x}, \vec{x}^*) g(\vec{x}) g(\vec{x}^*) d\vec{x} d\vec{x}^* \geq 0 \quad \text{Eq. (4)}$$

Based on this theorem, several different types of kernels, which determine the various characteristics of the model, are listed in Table 2. These kernels are two types: local kernels and global kernels [64]. A global kernel allows data points that are far away from each other to have an influence on the kernel values, as shown in Fig. 2a. The polynomial kernel in Eq. (5) is a typical example of a global kernel [52, 66]. The higher the degree of polynomial kernel, the better its

interpolation ability will be. The lower the degree of polynomial kernel function, the better its extrapolation ability will be. In a local kernel only the data that are close to each other have an influence on the kernel values (Fig. 2b). The typical local kernel is the radial basis function kernel (RBF) in Eq. (6). The smaller value of γ is, the worse its interpolation ability will be and vice versa. In other word, no single value of kernel parameter γ or polynomial degree will provide a model with both interpolation and extrapolation properties [52].

$$K_{poly}(x_i, x_j) = (\langle x_i, x_j \rangle + 1)^d \quad \text{Eq. (5)}$$

$$K_{rbf}(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|^2) \quad \text{Eq. (6)}$$

Figure 2

Based on the Mercer's conditions, there is one corollary. Assuming $K_1(\vec{x}, \vec{x}^*)$, $K_2(\vec{x}, \vec{x}^*)$ are admissible support vector kernels and $C_1, C_2 \geq 0$,

$$K(\vec{x}, \vec{x}^*) = C_1 K_1(\vec{x}, \vec{x}^*) + C_2 K_2(\vec{x}, \vec{x}^*) \quad \text{Eq. (7)}$$

$K(\vec{x}, \vec{x}^*)$ is an admissible kernel [55]. The mixed kernels function $K(\vec{x}, \vec{x}^*)$, which combines the good characteristics of both $K_1(\vec{x}, \vec{x}^*)$ and $K_2(\vec{x}, \vec{x}^*)$, has been proposed by numerous investigators [52-54, 61, 65, 67].

The mixtures of the RBF and polynomial kernels can be defined as Eq. (8, 9)

$$K_{mix} = mK_{poly} + (1-m)K_{rbf} \quad 0 \leq m \leq 1 \quad \text{Eq. (8)}$$

$$K_{mix}(x_i, x_j) = m(\gamma_1 \langle x_i, x_j \rangle + 1)^d + (1-m)\exp(-\gamma_2 \|x_i - x_j\|^2) \quad 0 \leq m \leq 1 \quad \text{Eq. (9)}$$

Where K_{poly} is a polynomial kernel and K_{rbf} is a radial basis function kernel, m is the mixing coefficient. If $m=0$, then the mixed kernels function will equal the RBF kernel, which means $K_{mix} = K_{rbf}$. If $m=1$, then the mixed kernels function will become the polynomial kernel, which means $K_{mix} = K_{poly}$. The effect of the mixing a polynomial kernel with a RBF kernel is shown in Fig. 3, where $x_i = 0.2, \gamma = 0.1, d = 1$. The mixed kernels function has characteristics of both the polynomial kernel and the RBF kernel, and improves fitting and generalizing ability.

Figure 3

2.2 Particle swarm optimization

Based on stochastic search and optimization processes, Eberhart et al. (1995) [55] first developed the particle swarm optimization algorithm (PSO), which is an evolutionary algorithm and imitated human (or insects) social behaviour. Individuals interact with one another while learning from their own experience, and gradually the population member move into better regions of the problem space [55]. Particles, indicating the potential solution, randomly locate in the architecture space (like birds or fish randomly distributed in a specific open environment), and are utilized to calculate the global optima of the fitness function. Assuming D -dimensional architecture space, population $x = \{x_1, x_2, x_3, \dots, x_n\}$ is composed by n particles (x_i). Each $x_i = \{x_{i1}, x_{i2}, x_{i3}, \dots, x_{iD}\}$ is indicating its position, and is also representing a potential solution. A global best value is $p_g = \{g_1, g_2, g_3, \dots, g_D\}$ and personal best value is $p_i = \{p_{i1}, p_{i2}, p_{i3}, \dots, p_{iD}\}$. The velocity for particle x_i , representing the rate of position change, is written as $v_i = \{v_{i1}, v_{i2}, v_{i3}, \dots, v_{iD}\}$.

Figure 4

In PSO, each particle updates its position by velocity adjustment and fluctuates between p_i and p_g .

The process for velocity adjustment is presented in Fig.4. When the particle swarm algorithm is running without restraining velocities, it rapidly increases to unacceptable levels within a few iterations. Some form of damping of the dynamics of particles (e.g., $v_{\max}$) is necessary. To better allow an elegant and well-explained method for preventing explosion, ensuring convergence, reducing and eliminating the importance of $v_{\max}$, Shi et al. [68] introduced the inertial weight.

$$\vec{v}_i^{new} = \omega_t \vec{v}_i^{old} + \phi_1 \otimes (\vec{p}_i - \vec{x}_i) + \phi_2 \otimes (\vec{p}_g - \vec{x}_i) \quad \text{Eq. (10)}$$

$$\vec{x}_i^{new} = \vec{x}_i^{old} + \vec{v}_i^{new} \quad \text{Eq. (11)}$$

$$\omega_t = \omega_{\max} - (\omega_{\max} - \omega_{\min}) * t_{ite} / t_{\max} \quad \text{Eq. (12)}$$

Where $\omega_{\max}$ is initial inertia weight, $\omega_{\min}$ is the final inertia weight, ϕ_1 is cognitive coefficient and ϕ_2 is social coefficient, t_{ite} is current iteration number, $t_{\max}$ is maximum iteration number.

3. Model Development

Because of strong interpolation and extrapolation capability, the new MKF-SVR was chosen to build the model for CO₂-oil MMP prediction. This model was optimized by PSO. The existing SVR for comparison was also chosen because of its many advantages over the traditional methods and empirical correlations; these include fast convergence to the global optimum, high generalization performance, and less probability for over-fitting. The construction of the MKF-SVR model was undertaken with the LIBSVM toolbox developed by Chang et al. [69]; the optimization process was based on the MATLAB software. The design process for this model involves three parts: data acquisition, data normalization and model optimization and validation.

3.1 Experimental Dataset

The accuracy and stability of the developed model is largely dependent on the training data's reliability and comprehensiveness. Based on a review of recent research, reservoir temperature, oil composition, purity of injected gas play an important role in CO₂-oil MMP values [4, 29, 70-72]. Thus, input data sets used in this model include average critical temperature of the drive gas ($T_{cm} = \sum Z_i \times T_{ci}$), reservoir temperature (T), molecular weight of the C₅₊ fraction (MC₅₊), and the ratio of volatile (C₁ and N₂) to intermediate (C₂-C₄, H₂S and CO₂) components in crude oil, Pure and impure CO₂-oil MMP is the desired output. In this work, all of the experimental data used were collected from existing published literature [20, 29, 36, 70, 71, 73-98]. Details of datasets are presented in Table 1. Normally, all data for the training of a supervised machine-learning algorithm are divided into three parts: training data, validation data and testing data. This paper combines the validation data and training data. The combination is used as training dataset. A V-fold cross-validation method was used as resampling method during the training process. The purpose of training and validation process is to find the best parameters for MKF-SVR model and to ensure accurate prediction performance. The goal of the testing process is to evaluate the accuracy and stability of the well-trained MKF-SVR model [30]. Of the 147 data samples collected, 90% (133) were used for training and validation, and the remaining 10% (14) were used for testing.

Table 1

3.2 Data Normalization

According [99], adequate normalization of input data prior to a training process can reduce the estimation errors and calculation time during training process. Thus, dataset normalization is an important step during dataset preparation. In this study, absolute scale is used. The normalized formula is chosen as following:

$$Y_i^{normalized} = \left[\frac{Y_i^{old} - Y_{\min}}{Y_{\max} - Y_{\min}} \right] \quad \text{Eq. (13)}$$

where $Y_i^{normalized}$ is the normalized input vector, Y_{min} and Y_{max} are the minimum and maximum and value respectively, Y_i^{old} are the original input vector. The normalized input vector ranges from 0 to 1. When training and testing process are completed, predicted MMP values by well-trained MKF-SVR model also ranges from 0 to 1. In order to project the predicted MMP value into original order, data renormalization is necessary. The renormalization formula is following:

$$Y_i^{renormalized} = (Y_{max} - Y_{min})Y_i^{predicted} + Y_{min} \quad \text{Eq. (14)}$$

Where $Y_i^{renormalized}$ is the renormalized output, $Y_i^{predicted}$ is predicted output by well-trained MKF-SVR model.

3.3 Parameters optimization based on improved PSO

As discussed, the final performance of the MKF-SVR is strongly dependent on the parameters of the mixed kernels function. After dataset was normalized, control parameters of PSO including maximum velocity, minimum velocity, initial inertia weight, final inertia weight, cognitive coefficient, social coefficient and population size should be randomly initialized. The parameters of MKF-SVR including mixing coefficient (m), penalizing coefficient (C), RBF kernel parameter (γ), polynomial degree (d) and (ϵ) in ϵ -insensitivity function are set up randomly. In order to search the global optimum reasonably and to convergent quickly, the parameter m is limited in $[0, 1]$, γ in $[10^{-3}, 10^4]$, d in $[1, 4.5]$, C in $[10^{-2}, 10^5]$ and ϵ in $[10^{-4}, 10^{-1}]$. During the process of searching best parameters by PSO, particles update their positions by changing velocity and converge finally at a global optimum within the searching space. In this study, the particles' positions are the vectors of $m, \gamma, d, C, \epsilon$, which are denominated as $P(m, \gamma, d, C, \epsilon)$. Then v -fold ($v=4$) cross-validation resampling method is applied to validate the performance of searched best parameters until criterions are met. To evaluate the performance of training process, mean square error (MSE) is chosen as the fitness function, which is formulated as:

$$F_{Fitness} = \frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2 \quad \text{Eq. (15)}$$

where $\hat{y}_i$ is the predicted value, y_i is the true value and n is the number of samples. Fig. 5 shows the workflow to find the optimum values of each parameter in the mixed kernels function

Figure 5

3.4 Testing of the MKF-SVR model

After the training and validation processes were completed, all of the parameters were optimized and the expected regression model was established. In order to verify its generalization capability and stability, the well-trained model is tested by using the testing data set (10% data), which were not used in the training and validation process.

4. Results and Discussion

Asoodeh et al. [36] used the original SVR model to estimate the CO₂-oil MMP; Shokrollahi et al. [15] applied the adapted LS-SVM model to estimate the CO₂-oil MMP. Detailed difference between SVR and LS-SVM refers to reference [100]. Although both models have relatively good prediction performance, the generalization ability of these models can be improved by the MKF-SVR model, because of the limitation of applied kernel function. In this study, the result of the original SVR is compared with different basic kernel functions and that of the adapted SVR with mixed kernels function in order to demonstrate improved performance of the MKF-SVR model than the traditional correlations. The results are compared to those produced by four numerical correlations proposed in the work of Alston et al. [29], Sebastian et al. [70], Yelling et al. [16] and Emera [12].

4.1 Results

There are four different kernel functions as listed in Table 2: each has different parameters that should be optimized separately. The grid searching algorithm was applied to find the best

parameters of each basic kernel function. PSO algorithm is applied to optimize the five parameters for the mixed kernels function. Table 3 shows the range of parameters for PSO algorithms.

Table 2

Table 3

The well-trained MKF-SVR model is applied to estimate the MMP value of crude oil. In order to verify the reliability and accuracy of the model [49, 101], five statistical parameters were introduced as evaluation indexes to test the performance of the model. These parameters include coefficient of determination (R^2), correlation coefficient (r), root mean error (RMSE), average absolute error (AAE), and maximum absolute error (MAE), as defined in Table 4. An R^2 (Coefficient of Determination) of 1 indicates a perfect model, while an R^2 of 0 indicates an inaccurate model [48, 102]. Moreover, R and RMSE are used to evaluate overall performance, while AAE and MAE are used to determine the error range of the predicted results [30].

Table 4

With the aid of PSO, the optimal parameters in the MKF-SVR model were determined to be $C=955.0476$, $\gamma=144.3693$, $m=0.3435$, $d=3.935$, $\epsilon=0.0804$.

The training and testing performance of the SVR model with mixed kernels function and other basic kernel functions are listed in Table 5. The performance of the MKF-SVR model improves the accuracy and stability as indicated by the decreased RMSE and AAE, and increases in the correlation coefficient and coefficient of determination. The process of searching for best gamma and penalize parameter is shown in Fig. 6, using grid searching algorithm for the SVR with linear kernel, polynomial kernel, RBF kernel, sigmoid kernel and n-fold of 4. The cross-validation mean square errors are 8.4967, 9.2179, 6.1250 and 8.4766 respectively. The process of searching for best

parameters in MKF-SVR model by particle swarm optimization (PSO) is shown in Fig. 7. A comparison of Figs. 6 and 7 shows that the MKF-SVR model has the smallest cross-validation mean square error (4.0012). The MFK-SVR model has the highest training and testing coefficient of determination (0.8767) as shown in Fig. 8. Compared with other kernel functions, the MKF-SVR model provides more accurate predictions as demonstrated by Fig.9 showing the comparison of actual values and forecasted values.

Figure 6

Figure 7

Figure 8

Figure 9

Table 5

4.2 Comparison of MKF-SVR model with empirical correlations

In order to further evaluate the model accuracy and stability, the comparison between some well-known empirical correlations with the predicted results calculated from the newly MKF-SVR model is necessary. The empirical correlations selected for the comparisons include correlations by Yelling et al. [16](corrected with Sebastian et al. [70]impurity correction factor), Yelling et al. [16](corrected with Alston et al. [29] impurity correction factor), Emera et al. [12](corrected with Sebastian et al. [70]impurity correction factor), Emera et al. [12](corrected with Alston et al. [29] impurity correction factor), Alston et al. [29], and Sebastian et al. [70]. Detailed descriptions of each correlation are given in Appendix. The correlations consider the pure CO₂ injection case and also investigate the impact of an impure CO₂ drive gas stream. The Alston et al. [29] and Sebastian et al. [70] correlations were developed for both pure and impure CO₂-drive stream, while the Yelling et al.

[16] and Emera et al. [12] correlations were developed only for a pure CO₂-drive stream; thus they need impurities correction factors to correct for impure CO₂ data samples. The Alston et al. [29] and Sebastian et al. [70] impurity correction factors are summarized in the Appendix.

Table 6

A scatter diagram (Fig. 10) illustrates the comparison between the laboratory experimental MMP values and the predicted values. The cross-plots visualize the accuracy of proposed model and available correlations. The diagonal line in each figure represents the theoretical equality between predicted and experimental values. Tightness of the points to the diagonal line directly expresses the agreement level between the simulated and experimental values. The MKF-SVR results show a total coefficient of determination of 0.87, and the majority of data points for the training and testing process lie on a 45° line, indicating that the newly developed MKF-SVR model is robust and stable (Fig. 10a). There is an excellent agreement between the experimental data and the predictions of newly developed MKF-SVR model indicating that this model can be successfully applied to predicting MMP for both pure and impure CO₂ injection cases. As Fig. 10b-f illustrates, the best fit lines of predicted results of correlations deviate from the diagonal line, which indicate that the agreement between the experimental data and value predicted by mixed kernel based SVR model is improved among the selected correlations. The simulation results of classic correlations and newly developed model (in terms of R, RMSE, AAE, MAE) were also compared and presented in Table 6. The MFK-SVR model has the smallest RMES (of 1.9151), AAE (of 1.1140) and MAE (of 4.6291); and highest R (of 0.9381). In terms of results, it is clearly seen that MFK-SVR model have high performance compared with other correlations. To prove the strong generalization ability of MKF-SVR model, the performance of different machine learning-based model on train, test and total data are evaluated by R² and RMSE (Table 7). As Table 7 listed, the total R² of LS-SVM [15] is higher than that of MKF-SVM, however the performance of LS-SVM in the testing process is not good (R² is

0.8070). Testing process reflect the generalization ability of a model. Compared with LS-SVM, MKF-SVR has high R^2 and low RMSE in training and testing process, this newly developed model has strong generalization ability.

Table 7

Figure 10

4.3 Sensitivity analysis

In order to further investigate the relationship between the influence factor (i.e. reservoir temperature, average critical temperature, molecular weight of C_{5+} fraction and volatile to intermediate ratio) and CO_2 -oil MMP, a sensitivity analysis was conducted. This process is executed by changing one studied variable gradually, while holding the other variables constant [37]. As Fig. 11a shows, the increase of reservoir temperature will increase MMP, as the solubility of CO_2 into oil is decreases [103-105], which means the CO_2 is less miscible with oil, an increase in CO_2 -oil MMP. When reservoir temperature decreases, the interfacial tension between oil and CO_2 also declined [22, 23], therefore the MMP decreased correspondingly. This model results are in agreement with previous work [5, 15, 106].

The purity of the injection gas stream has significant and complex impacts on CO_2 -oil MMP. Generally, the presence of H_2S or intermediate hydrocarbon components will decrease the CO_2 -oil MMP, while the presence of C_1 or N_2 will increase the CO_2 -oil MMP [29, 70, 83]. In order to describe the impact of purity of injection gas stream on CO_2 -oil MMP simply and concisely, the average critical temperature is the best reasonable parameter. As Fig. 11b shows, the increase of average critical temperature will decrease the CO_2 -oil MMP.

As Fig. 11c illustrates, the MMP increases as the average molecular weight of pentane plus fraction increases. Pentane plus fraction, the major component of crude oil indicates an increase of the

average molecular weight of C_{5+} and the percentage of heavy oil molecules [107, 108]. The increase in average molecular weight of C_{5+} is less miscible with CO_2 , thus MMP increases.

The evaporation property of volatile components may increase the gas phase during the multi-contact of CO_2 and oil, decreasing the oil miscibility with CO_2 [10, 73], while the intermediate components are easy to mix with CO_2 due to their inter-solubility into each other [20, 73], thus the increase of volatile to intermediate ratio will increase the MMP [29], as shown in Fig. 11d.

Figure 11

5. Conclusions

A hybrid model of mixed kernels function (MKF) based support vector regression (SVR) model was developed to predict pure and impure CO_2 -oil minimum miscibility pressure (MMP) during a CO_2 -EOR process. In this MKF-SVR model, four factors (i.e. reservoir temperature, average critical temperature, molecular weight of C_{5+} fraction of crude oil, and the ration of volatile components to intermediate components in crude oil) representing the most comprehensive and robust set were selected as the input variables while MMP was considered as output variable. Through the foregoing analysis and discussions of the simulation results, several conclusions are drawn:

- (1) The mixed kernel function based support vector regression (SVR) model was successfully applied to predict the CO_2 -oil MMP value for both pure and impure CO_2 gas.
- (2) Different kernel functions affect the final performance of SVR significantly. Mixed kernel function, which combines the advantages of global radial basis function (RBF) and local (Polynomial) kernel functions, increases the applicability of SVR dramatically.
- (3) The comparison of traditional correlations with the mixture kernel based SVR model shows excellent performance and greater generalization ability with higher correlation coefficient ($R =$

0.9381), smaller average absolute error (AAE = 1.1406), maximum absolute error (MAE = 4.6291) and the reduced root mean square error (RMSE = 1.9151).

(4) Based on the sensitivity analysis, reservoir temperature, molecular weight of C_{5+} fraction and volatile/intermediate ratio of crude oil positively influence the CO_2 -oil MMP, while average critical temperature has a negative impact on CO_2 -oil MMP. Moreover the impacts of all factors towards the CO_2 -oil MMP is nonlinear.

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Appendix A

In this Appendix, totally nine correlations used for MMP prediction in pure CO₂-oil systems are summarized and presented. All of the correlations are converted to consistent units.

A.1. Correlation proposed by Yelling et al.

Yelling [16] correlation correlates CO₂-oil MMP only with the reservoir temperature. This correlation only can be used when T (reservoir temperature) ranges from 35.8 to 88.9 °C, which is given by:

$$P_{m,\min,pure} = 12.6472 + 0.01553(1.8T + 32) + 1.24192 \times 10^{-4}(1.8T + 32)^2 - \frac{716.9427}{(1.8T + 32)} \quad \text{Eq. (A1)}$$

If $MMP < P_b$ (P_b is the bubble pressure), then P_b is taken as MMP.

A.2. Correlation proposed by Emera et al.

A new correlation modified from the Alston correlation by Emera et al. [12]. When $P_b \geq 0.345 \text{ MPa}$, this correlation is presented as follows:

$$P_{m,\min,pure} = 5.0093 \times 10^{-5} (1.8T + 32)^{1.164} (M_{C_{5+}})^{1.2785} \left(\frac{x_{VOL}}{x_{MED}} \right)^{0.1073}, \quad \text{Eq. (A2)}$$

otherwise, when $P_b < 0.345 \text{ MPa}$

$$P_{m,\min,pure} = 5.0093 \times 10^{-5} (1.8T + 32)^{1.164} (M_{C_{5+}})^{1.2785}, \quad \text{Eq. (A3)}$$

where T is reservoir temperature, P_b is bubble pressure, MC_{5+} is the fraction of C₅₊ molecular weight; x_{vol} is the volatile components and x_{med} is the intermediate components.

However, those correlations can be used only when special conditions are satisfied: (i) the test temperature should range from 40.8 to 112.2°C; (ii) the MMP ranges between 8.28 and 30.2 MPa;

(3) the C_{5+} molecular weight ranges from 166.2 g/mol to 267.5 g/mol. If the calculated MMP is smaller than P_b (bubble pressure), then P_b is taken as MMP.

A.3. Correlation proposed by Alston et al.

The correlation developed by Alston et al. [29] for the pure CO_2 injection case is represented as a function of reservoir temperature, oil pentane and heavier molecular weight, and the ratio of volatile to intermediate mole fractions in the reservoir oil. When the bubble pressure of reservoir oil in pounds per square inch absolute (psia) is greater than 50 psia (0.345MPa), the influence of the volatile/intermediate ratios is important, and the correlation can be written as:

$$P_{m,min,pure} = 6.0536 \times 10^{-5} (1.8T + 32)^{1.06} (M_{C_{5+}})^{1.78} \left(\frac{x_{VOL}}{x_{MED}} \right)^{0.136}. \quad \text{Eq. (A4)}$$

However, when the bubble pressure of reservoir oil is smaller than 50 psia (0.345MPa), it contains relatively small or zero quantities of volatile and intermediate components, and the MMP is not affected significantly by these components. Thus the influence of the volatile/intermediate ratios is not significant, and the correlation is:

$$P_{m,min,pure} = 6.0536 \times 10^{-5} (1.8T + 32)^{1.06} (M_{C_{5+}})^{1.78}, \quad \text{Eq. (A5)}$$

where T is reservoir temperature, $M_{C_{5+}}$ is the fraction of C_{5+} molecular weight; x_{vol} is the volatile components and x_{med} is the intermediate components.

For the impure CO_2 stream injection case, contaminants have the adverse or positive effects on MMP. Thus a correction factor F_{imp} is introduced. It was calculated based on the critical temperature of each component in the stream. The pseudo-critical temperature (T_{cm}) of the solvent stream was calculated using a weight-fraction mixing rule as follows:

$$F_{imp} = (87.8/T_{cm})^{1.935 \times 87.8/T_{cm}} \quad \text{Eq. (A6)}$$

$$T_{cm} = \sum_{k=1}^n w_k (1.8T_{ck} + 32) \quad \text{Eq. (A7)}$$

where T_{cm} is the weight average critical temperature of the solvent stream, w_k is the weight fraction of component k ($k = \text{CO}_2, \text{C}_1, \text{N}_2, \text{H}_2\text{S}$, and $\text{C}_2\text{--C}_4$), and T_{ck} is the critical temperature of component k . Then the impure CO_2 -oil MMP was calculated as:

$$P_{m,\text{min},\text{impure}} = P_{m,\text{min},\text{pure}} \times F_{\text{imp}}. \quad \text{Eq. (A8)}$$

A.4. Correlation proposed by Sebastian et al.

Based on the Sebastian and co-worker's research [70], combined with previous study, Sebastian et al. proposed a new correlation to predict the change in MMP value resulting from the impurities (i.e. $\text{C}_1, \text{H}_2, \text{O}_2, \text{CO}_2, \text{N}_2, \text{H}_2\text{S}$, and $\text{C}_2\text{--C}_5$ hydrocarbons) in the CO_2 drive gas. The relationship between impure and pure CO_2 -oil MMP was described as:

$$F_{\text{imp}} = 1.0 - 0.0213(1.8T_{cm} - 31) + 2.51 \times 10^{-4}(1.8T_{cm} - 31)^2 - 2.35 \times 10^{-7}(1.8T_{cm} - 31)^3, \quad \text{Eq. (A9)}$$

where T_{cm} is the mole average pseudocritical temperature of the gas stream, and can be expressed as:

$$T_{cm} = \sum_{k=1}^n x_k T_{ck} \quad \text{Eq. (A10)}$$

where x_k is the mole fraction of component k ($k = \text{CO}_2, \text{C}_1, \text{N}_2, \text{H}_2\text{S}$, and $\text{C}_2\text{--C}_4$), and T_{ck} is the supercritical temperature of each component k .

The MMP pure was calculated use the following formula:

$$P_{m,\text{min},\text{pure}} = 12.6472 + 0.01553(1.8T + 32) + 1.24192 \times 10^{-4}(1.8T + 32)^2 - \frac{716.9427}{1.8T_R + 32}, \quad \text{Eq. (A11)}$$

and the impure CO₂-oil MMP was calculated as:

$$P_{m,mim,impure} = P_{m,min,pure} \times F_{imp} . \quad \text{Eq. (A12)}$$

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Figure captions

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Tables

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Table 1 Literature experimental data that used for MMP prediction

Reference	Dataset	Training Dataset		Testing Dataset	
	Type of CO ₂ stream	Pure	Impure	Pure	Impure
Rathmell et al. (1971) [73]		3			
Jacobson, (1972)[74]		1	3		
Dicharry et al. (1973) [75]		1			
Holm et al. (1974) [76]				1	
Shelton et al. (1977) [77]				1	
Spence et al. (1980) [78]		1		1	
Graue et al. (1981) [79]			2		
Metcalfe (1982) [20]		5	20	1	2
Frimodig (1983) [80]		3	18		2
Henry et al. (1983) [81]		1			
Thakur et al. (1984) [82]		2			
Alston et al. (1985) [29]		11	12	1	1
Sebastian et al. (1985) [70]		1	6		
Harmon et al. (1988) [84]		1			
Eakin et al. (1988) [83]		1	7	1	1
Chaback (1989) [85]		4			
Khan et al. (1992) [86]		2			
Zuo et al. (1993) [71]		1	1		
Dong (1999) [87]			2		
Srivastava et al. (2000) [88]					
Dong et al. (2001) [89]		1	1		1
Jaubert et al. (2002) [90]		1			
Bon et al. (2005) [91]		3			
Bon et al. (2006) [92]		1			
Sun et al. (2006) [93]		2			
Zhou et al. (2008) [94]		1			
Al-Ajmi, et al. (2009) [95]		1	2		
Li et al. (2012) [97]		4			
Cao (2012) [96]		1			
Zhang et al. (2015) [98]		6		1	
Total		59	74	7	7

Table 2 Common Kernel function, corresponding mathematical expressions and parameters ranges.

Kernel Function		C	Y	d	ε	m
Linear Kernel	$K(x_i, x_j) = \langle x_i, x_j \rangle + c$	$2^0 \sim 2^7$	$\times$	$\times$	5×10^{-4}	$\times$
Polynomial Kernel	$K(x_i, x_j) = (\gamma \langle x_i, x_j \rangle + c)^d$	$2^{-4} \sim 2^4$	$2^{-3} \sim 2^3$	2	10^{-4}	$\times$
Radial Basis Function Kernel	$K(x_i, x_j) = \exp(-\gamma \ x_i - x_j\ ^2)$	$2^{-3} \sim 2^3$	$2^{-15} \sim 2^{15}$	$\times$	10^{-3}	$\times$
Sigmoid Kernel	$K(x_i, x_j) = \tanh(\gamma \langle x_i, x_j \rangle + c)$	$2^{-0} \sim 2^{10}$	$2^{-6} \sim 2^1$	$\times$	10^{-1}	$\times$
Mixture Kernel	$K_{mix} = \rho K_{poly} + (1 - \rho) K_{rbf}$	$10^{-2} \sim 10^5$	$10^{-3} \sim 10^4$	1~4.5	$10^{-4} \sim 10^{-1}$	0~1

Table 3 Typical parameters used for training SVR model with PSO algorithms.

Parameter	Value	Parameter	Value
Maximum Generation	150	Population size	50
Cognitive efficient (φ_1)	1.5	Social efficient (φ_2)	1.5
Initial inertia weights $\omega_{\max}$	0.9	Final inertia weight $\omega_{\min}$	0.4

Table 4 Error measures for accuracy assessment [48]

Accuracy measure	Mathematical expression
Coefficient of Determination, R^2	$R^2 = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)}{\sum_{i=1}^N (y_i - \text{aver}(y_i))}$
Correlation coefficient, r	$r = \frac{\sum_{i=1}^N (y_i - \bar{y}_i)(\hat{y}_i - \bar{\hat{y}}_i)}{\sum_{i=1}^N (y_i - \bar{y}_i)^2 \sum_{i=1}^N (\hat{y}_i - \bar{\hat{y}}_i)^2}$
Root mean square error, RMSE	$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2}$
Average absolute error, AAE	$AAE = \frac{1}{N} \sum_{i=1}^N y_i - \hat{y}_i $
Maximum absolute error, MAE	$MAE = \max y_i - \hat{y}_i , i = 1, 2, 3, \dots, N$

Table 5 The training and testing performance of SVR model with linear, polynomial, RBF, sigmoid and mixed kernels function.

Data Set	Statistical Parameters	Kernel Function				
		Linear	Polynomial	RBF	Sigmoid	MKF
Training Set	RMSE	2.9220	3.0128	2.4558	2.9181	2.0111
	AAE	2.1244	2.0668	1.7852	2.2223	1.1659
	MAE	5.8374	6.3763	4.8271	5.9940	5.1228
	r	0.8531	0.8415	0.8989	0.8528	0.9365
	N ^e	133				
Test Set	RMSE	2.2851	1.9760	1.4670	2.2667	1.204
	AAE	1.7873	1.3221	1.0862	1.8198	0.8814
	MAE	4.7201	3.9290	1.4040	2.5362	2.4607
	r	0.8395	0.8717	0.9274	0.8386	0.9503
	N ^e	14				
Total	RMSE	2.8675	2.9299	2.3794	2.8625	1.9151
	AAE	2.0923	1.9959	1.7186	2.1840	1.1406
	MAE	5.8374	6.3763	4.8271	5.9940	4.6291
	r	0.8411	0.8695	0.9099	0.8420	0.9381
	N ^e	147				

Table 6. The comparison of MFK-SVR and five correlations statistical results

Model	R	RMSE	AAE	MAE	N
MFK-SVR	0.9381	1.9151	1.1140	4.6291	147
Alston et al. [26]	0.7826	5.5644	6.5647	19.3981	141
Yelling et al. [24](Sebastian et al. [83] correction)	0.2145	7.0807	3.5881	21.0441	147
Yelling et al. [14](Alston et al. [26] correction)	0.3429	7.4034	5.9779	16.5373	143
Emera et al. [28](Sebastian et al. [62]correction)	0.5001	6.6600	5.8539	23.4808	146
Emera et al. [28](Alston et al. [26]correction)	0.7407	5.7220	6.4173	18.2914	142

Table 7 The comparison of different machine learning-based model on train, test and total datas statistical results

Model	Training		Testing		Total	
	R ²	RMSE	R ²	RMSE	R ²	RMSE
MKF-SVR	0.8770	2.0111	0.9031	1.0240	0.8800	1.9151
SVR (RBF kernel) [14]	0.8080	2.4558	0.8601	1.4670	0.8279	2.3794
LS-SVM (RBF kernel) [15]	0.9180	1.6400	0.8070	1.6800	0.9030	1.6900
GEP [37]	0.8350	2.3470	0.8720	1.7490	0.8280	2.2550

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