https://doi.org/10.15255/KUI.2020.073
KUI-35/2021
Original scientific paper
Received November 10, 2020
Accepted February 24, 2021

Dragonfly Support Vector Machine Modelling of the Adsorption Phenomenon of Certain Phenols by Activated Carbon Fibres

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Abstract

The objective of this research was to build a mathematical model based on a Support Vector Machine (SVM) capable of predicting the amount adsorbed at equilibrium (q_e). Activated carbon fibres (ACF) were used for the adsorption of certain phenols (phenol, 2-chlorophenol, 4-chlorophenol, 2,4,6-trichlorophenol, 4-nitrophenol, and 2,4-dinitrophenol). An experimental dataset of 129 points was collected from previously published papers. The inputs considered for modelling were temperature (T), concentration at equilibrium (c_e), and two descriptors (boiling point (BP) and density (d)) to differentiate between the pollutants studied. The data used were pre-processed by the statistical analysis to ensure that they were adequate for modelling. The results showed a superiority of the Gaussian kernel function DA-SVM model demonstrated by its determination coefficient ($R^2 = 0.997$) and root mean squared error (RMSE = 0.027 mmol l^{-1}).

Keywords

Adsorption, phenols, support vector machine, dragonfly algorithm, activated carbon fibre, amount adsorbed at equilibrium

1 Introduction

Water pollution is an alteration in its quality and nature that makes its use dangerous and/or disrupts the aquatic ecosystem. It concerns surface water (rivers, bodies of water) and/or groundwater. Its main origins are human activity, industries, agriculture, and domestic and industrial waste landfills.[1–3] Phenol and its derivatives are used in a number of applications such as the chemical, pharmaceutical, petroleum, paper, wood, rubber, dyes, and pesticide industries. Phenols are classified as priority pollutants because of their toxicity to organisms, even at low concentrations.[4,5] Their adverse effects on the environment and public health have been demonstrated by growing evidence, such as the death of aquatic life, inhibition of normal activities of the microbial community, and carcinogenicity in animals.[6] Due to the high toxicity, high prevalence and poor biodegradability of phenols, it is necessary to remove them from wastewater before discharging them into water bodies.

The adsorption treatment process is one of the most important technologies today. It is widely used for pollution control and purification in a wide variety of fields, for example, the petroleum, petrochemical and chemical industries, environmental, and pharmaceutical applications.[7,8]

Activated carbon fibres (ACF) are generally microporous, with a large surface area and a narrow pore distribution. The microporous nature gives ACFs adsorption advantages because the adsorption energy is increased in small pores. In addition, ACFs have a large external surface area and their micropores are directly exposed to the surface, resulting in a rapid rate of adsorption.[9]

Machine learning (ML) is a type of artificial intelligence (AI) that allows software applications to be more precise in predicting outcomes without being explicitly programmed to do so.[10–15]

Support Vector Machine (SVM) is a machine learning or statistical technique defined for the prediction of variables. Generally, this technique is employed to avoid the overfitting and convex optimisation problems (no local minima), and it runs well on smaller databases. This research consists of studying the data of the adsorption of phenols with ACFs, and of modelling by the machine learning technique (DA-SVM).

2 Support vector machines (SVM) technique

The SVM is based on a statistical learning theory. This method was introduced by *Vapnik*.[16–18] The architecture of SVM model is not determined *a priori*. The mathematical expression of the output estimation of the SVM is given as follows:

$$f(x) = w \cdot \varnothing(x) + b \tag{1}$$

where w is a weight vector, b is a bias, denotes the dot product, and $\varnothing$ is the non-linear transfer function that maps

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the input vectors into a high-dimensional feature space, in which theoretically a simple linear regression can cope with the complex non-linear regression of the input space. *Vapnik* introduced the following convex optimisation problem with a ε-insensitivity loss function to obtain the solution to Eqs. (2) and (3):[19]

$$\text{minimize}: \frac{1}{2}w^2 + C\sum_{K=1}^{N}\left(\xi_k^+ + \xi_k^-\right) \tag{2}$$

$$\text{subject to} \begin{cases} y_k - \left(w \cdot \varnothing\left(x_k\right) + b\right) \le \varepsilon + \xi_k^+ \\ -y_k + \left(w \cdot \varnothing\left(x_k\right) + b\right) \le \varepsilon + \xi_k^- \quad k = 1,2,\ldots\ldots,N \\ \xi_k^+, \xi_k^- \ge 0 \end{cases} \tag{3}$$

where ξ_k^+ and ξ_k^- are slack variables that penalize training errors by the loss function over the error tolerance ε, and C is a positive trade-off parameter or capacity parameter that determines the degree of the empirical error in the optimisation problem and determines the trade-off between the flatness of the function and the amount to which deviations larger than (ε) are tolerated.

Eqs. (4) and (5) can be solved using the Lagrangian multipliers and the Karush-Kuhn-Tucker (KKT) optimality conditions, as follows:[20]

$$f\left(x, \alpha_i, \alpha_i^*\right) = \sum_{i=1}^{N}\left(\alpha_i - \alpha_i^*\right) \cdot K\left(x, x_i\right) + b \tag{4}$$

where α_i and α_i^* are the Lagrangian multipliers, K is a kernel function defined by an inner product of the nonlinear transfer functions:[19]

$$K\left(x, x_i\right) = \exp\left(-\frac{x - x_i^2}{\sigma^2}\right) \tag{5}$$

3 SVM optimisation with Dragonfly algorithm (DA) technique

The chosen methodology can be schematised in accordance with the flowchart in Fig. 1, which includes the following steps:

The program shown in Fig. 1 depends on the technical SVM and the method of optimisation by the Dragonfly algorithm (DA) proposed by *S. Mirjalili*.[21] The DA initially feeds the SVM with a random combination of hyperplane parameters in their previously defined ranges. In five iterations, the steps starting with the data division and up to the development of the SVM model are repeated, and the minimum value of RMSE obtained is saved as the best value.[23–26]

The DA then generates a new population of parameter hyperplanes for the SVM algorithm, and the same set of steps is repeated in order to obtain a new best RMSE, among which the minimum RMSE corresponds to the DA-SVM model optimal result.

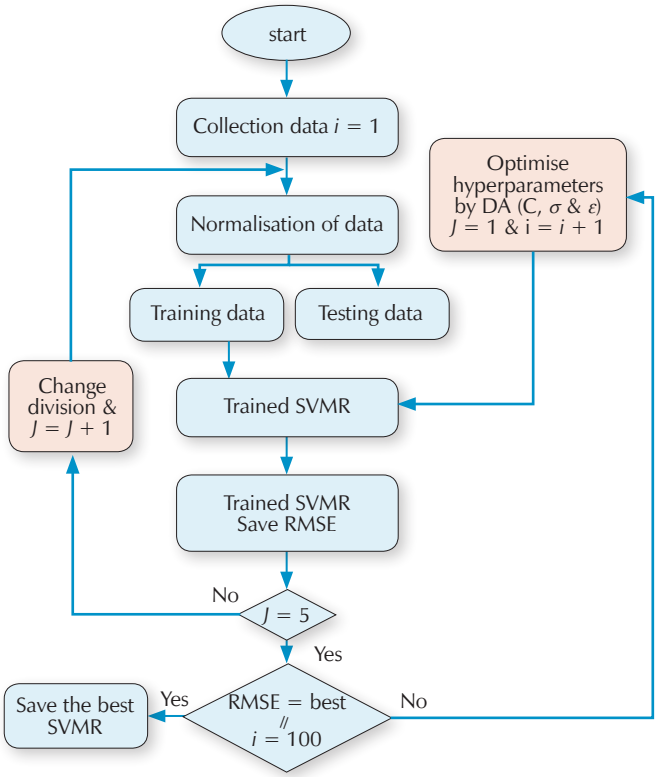

Fig. 1 – DA-SVM technique[12]

Numeric values in the input data matrix have been normalised to improve the optimisation and speed convergence. The normalisation function is expressed by the following Eq. (6)

$$X_n = X^{0.09} \tag{6}$$

To assess the predictive power of the DA-SVM model, a root mean squared error (RMSE) Eq. (7) and coefficient of determination (R^2)) Eq. (8) were used as evaluation criteria.

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(q_{ei}^{\text{exp}} - q_{ei}^{\text{cal}}\right)^2}{n}} \tag{7}$$

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} = 1 - \frac{\sum_{i=1}^{n}\left(q_{ei}^{\text{exp}} - q_{ei}^{\text{cal}}\right)^2}{\sum_{i=1}^{n}\left(q_{ei}^{\text{exp}} - q_{e(\text{moy})}\right)^2} \tag{8}$$

4 Data collection, pre-treatment, and analysis

The modelling data was collected from the literature,[22] the database must be analysed statistically. Table 1 summarises the values of some statistical parameters, such as standard deviation, variance, and KURTOSIS. The database contains 21 adsorption systems (seven phenols multiplied by three temperature changes). The amount adsorbed at equilibrium is predicted by the following variables: temperature

Table 1 – Statistical criteria

			Unit	Min	Max	STD	KURTOSIS
input	molecular weight	M_w	g mol^{-1}	94.11	197.45	31.84	−0.94
	density	d	g cm^{-3}	1.07	1.68	0.20	−1.00
	boiling point	BP	°C	113.00	279.00	47.66	−0.35
	temperature	T	°C	25.00	55.00	12.36	−1.52
	concentration at equilibrium	c_e	mmol l^{-1}	0.01	1.12	0.19	3.89
output	amount adsorbed at equilibrium	q_e	mmol g^{-1}	0.42	2.68	0.54	−0.78

and concentration at equilibrium as operating conditions, and molecular weight, density, and boiling point as descriptors to differentiate between the phenols.

Fig. 2 represents the multicollinearity test of the input variables. The test is a plot of the Kendall rank correlation coefficients between all pairs of variables, indicating a hypothesis test to determine which correlations are significantly different from zero.

5 Results and discussion

SVM was optimised by the dragonfly method. In a hybrid program called DA-SVM, the iterations were set at 30, and the number of search agents at 10. The program controls the hyperplane parameters (C, ε, n, and σ), in the domains following C ∈ [1e-3,1e3], σ ∈ [1e-3,1e3], ε ∈ [0,1], polynomial order « n » [2,5] and the 'Gaussian' (Eq. 9) and 'polynomial' (Eq. 10) kernel functions.

$$\text{Gaussian} = \exp\left(-x_j - x_k^{\,2}\right) \tag{9}$$

$$\text{Polynomial} = \left(1 + x_j^{'} x_k\right)^n \tag{10}$$

The database was randomly divided by the Holdout Partitions method into two sets: one for the learning (train), and another for validation, consisting of 80 % and 20 %, respectively.

5.1 Polynomial kernel function results

Fig. 3 displays the linear regression curve of the amount adsorbed at equilibrium ($q_{e(cal)}$) estimated by the DA-SVM optimised with the experimental amount adsorbed at

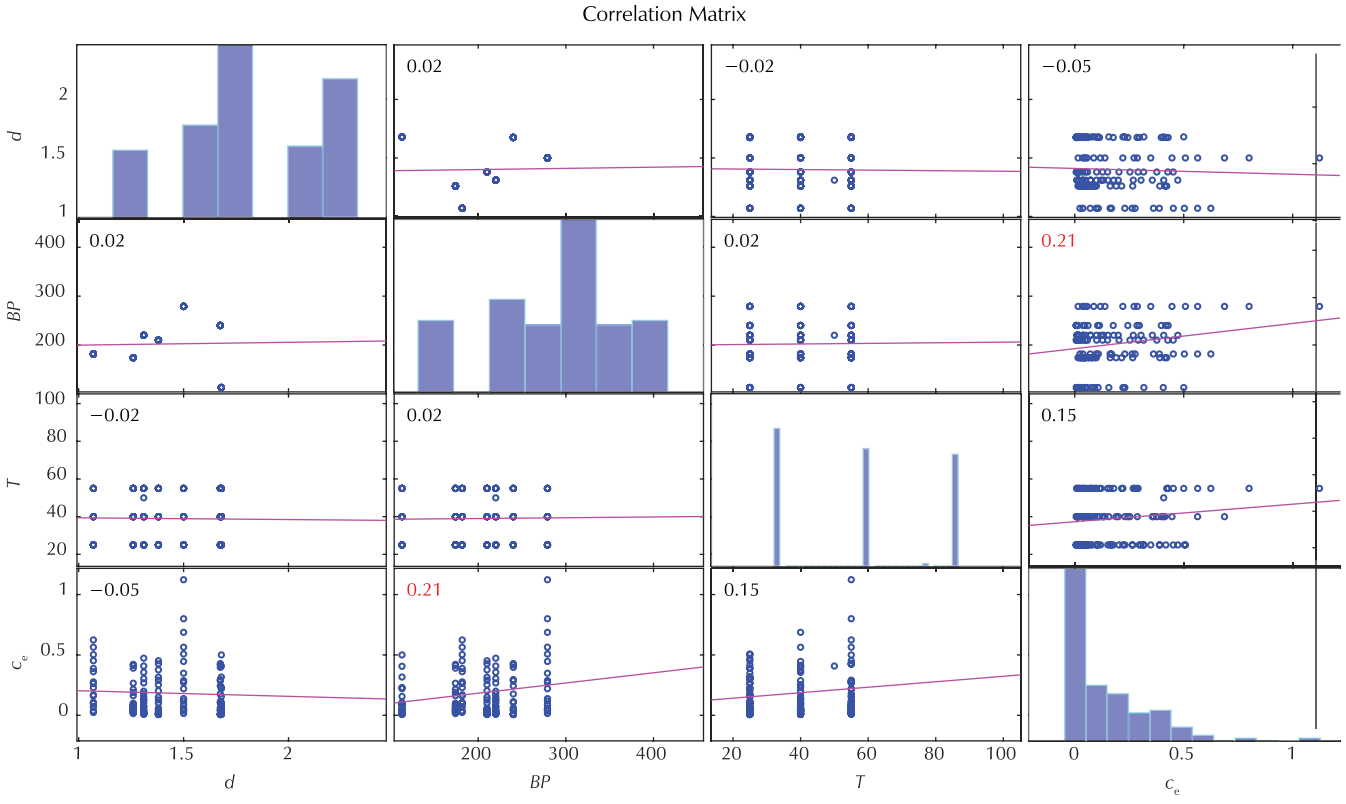

Fig. 2 – Multicollinearity test

equilibrium ($q_{e(exp)}$) for the two phases: learning (train) and validation, in using the polynomial kernel function with a regression vector [α (slope), β (y-intercept), R (correlation coefficient)] = [0.95, 0.015, 0.974], and Table 4 summarises the parameters of the model.

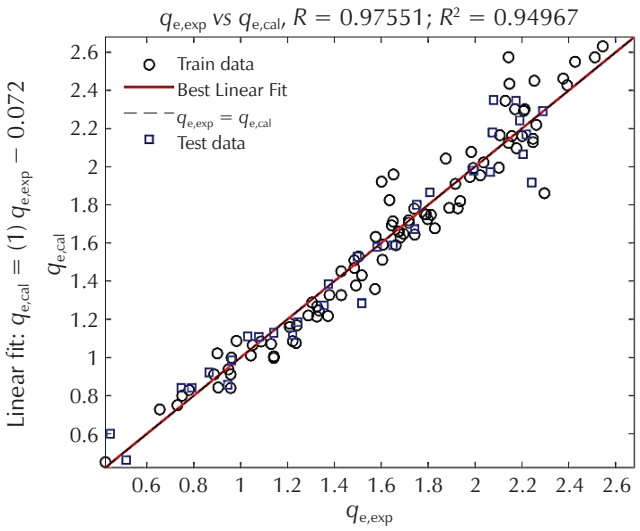

Fig. 3 – Linear regression between the experimental q_e and q_e calculated by the DA-SVM model using the polynomial kernel function

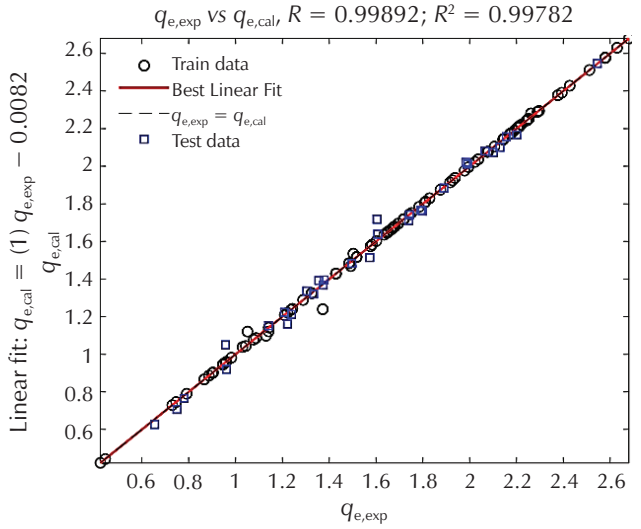

Fig. 4 – Linear regression between the experimental q_e and q_e calculated by the DA-SVM model using the Gaussian kernel function

To this end, two approaches, among which a polynomial kernel function DA-SVM model and a Gaussian kernel function DA-SVM model, were evaluated in terms of correlation performance and prediction accuracy (Fig. 5).

5.2 Gaussian kernel function results

The linear regression curve of the (q_e) calculated by DA-SVM optimised with the (q_e) experimental for the two phases (learning and validation) using the Gaussian kernel function is represented in Fig. 5 with a vector regression [α (slope), β (y-intercept), R (correlation coefficient)] = [1.00, 0.0017, 0.998], and Table 3 summarises the model parameters.

5.3 Comparative study of the results of the two approaches

The performances of the models developed in this work were compared to the statistical criterion (Eqs. 7 and 8).

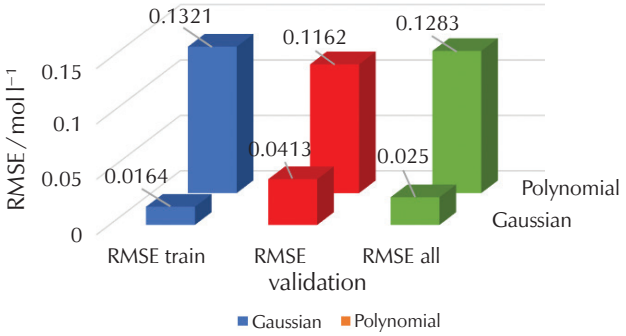

Fig. 5 – Comparison of the Gaussian kernel function DA-SVM model and polynomial kernel function DA-SVM model

Table 2 – Model parameters (Polynomial kernel function)

C	Polynomial order	Epsilon ε	Function	Amount of support vectors	RMSE learning	RMSE validation	RMSE ALL
85	2	0.0015	Polynomial kernel	97	0.1321	0.1162	0.1283

Table 3 – Model parameters (Gaussian kernel function)

C	Sigma σ	Epsilon ε	Function	Amount of support vectors	RMSE train	RMSE validation	RMSE ALL
44	1.75	$4.15 \cdot 10^{-04}$	Gaussian kernel	92	0.0164	0.0413	0.0250

For more details, it was noticed that the error of learning Gaussian kernel function DA-SVM model is eight times less than the error of learning polynomial kernel function DA-SVM model, and the Gaussian kernel function DA-SVM model test error three times less than the polynomial kernel function DA-SVM model test error. In general, it can be concluded that the prediction capacity of Gaussian kernel function DA-SVM model is five times better than the prediction capacity of polynomial kernel function DA-SVM model.

5.4 Graphical representation of the Gaussian kernel function DA-SVM model

Figs. 6–12 represent the adsorption kinetics of certain substituted phenols (phenol, 2-chlorophenol '2-CP', 4-chlorophenol '4-CP', 2,4,6-trichlorophenol '2,4,6 TCP', 4-nitrophenol '4-NP', and 2,4-dinitrophenol '2,4DNP') experimental and calculated by optimal Gaussian kernel function DA-SVM model.

Fig. 6 shows a projection of the experimental values of the phenol adsorption at 25, 40, and 55 °C by ACFs on the predicted values by the Gaussian kernel function DA-SVM model. The results indicate the ability of the model to predict with high accuracy.

Fig. 7 proves the large amplitude of the Gaussian kernel function DA-SVM model for the prediction of the amount adsorbed at equilibrium of 2-chlorophenol at temperatures 25, 40, 55 °C.

Results in Fig. 8 indicate the ability of the model to predict with high accuracy. In addition, the projection of the experimental values of the 4-chlorophenol adsorption at 25, 40, and 55 °C by ACFs on the predicted values by the Gaussian kernel function DA-SVM model was perfect.

The experimental data of 2,4-dichlorophenol adsorbed amount at equilibrium at 25, 40, and 55 °C, and the data calculated by the Gaussian kernel function DA-SVM model are shown in Fig. 9. It can be observed that the model has excellent prediction.

Projecting experimental values of 2,4,6-trichlorophenol adsorbed at 25, 40, and 55 °C by ACFs over the values predicted by a Gaussian kernel function DA-SVM model demonstrates the model's ability to predict with high accuracy (Fig. 10).

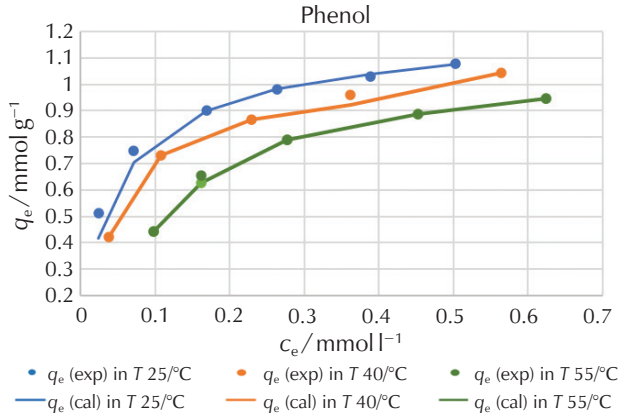

Fig. 6 – Phenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C).

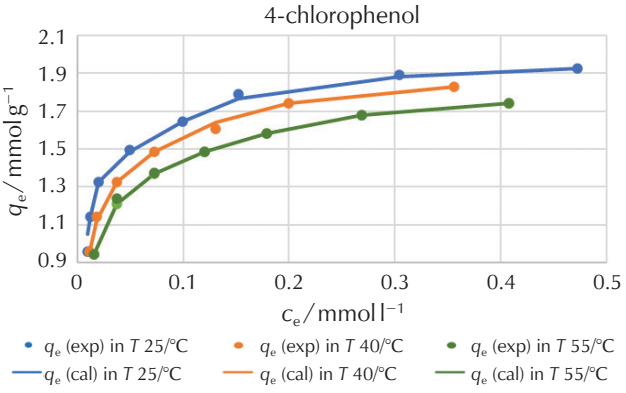

Fig. 8 – 4-chlorophenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C)

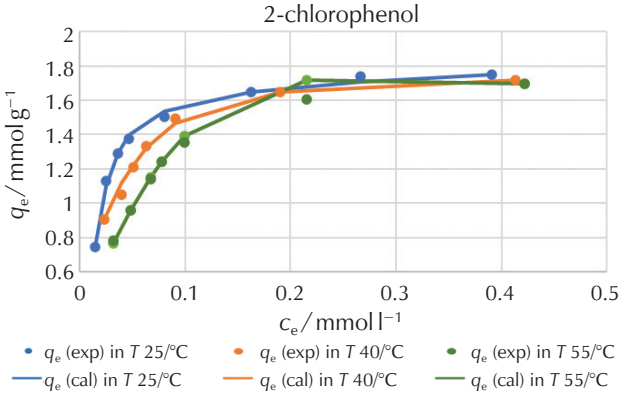

Fig. 7 – 2-chlorophenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C)

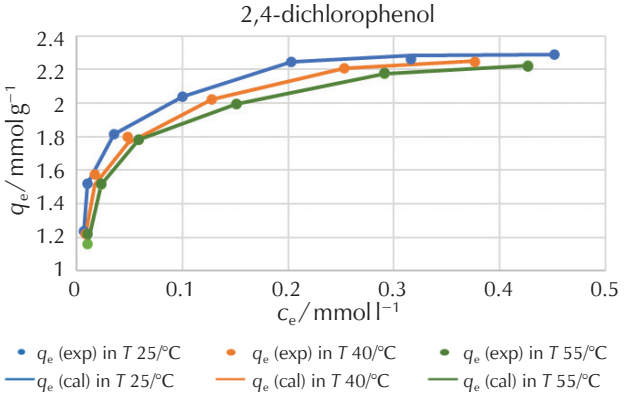

Fig. 9 – 2,4-dichlorophenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C)

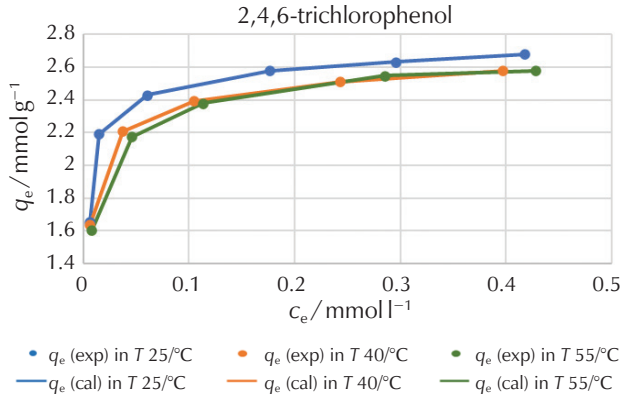

Fig. 10 – 2,4,6-trichlorophenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C)

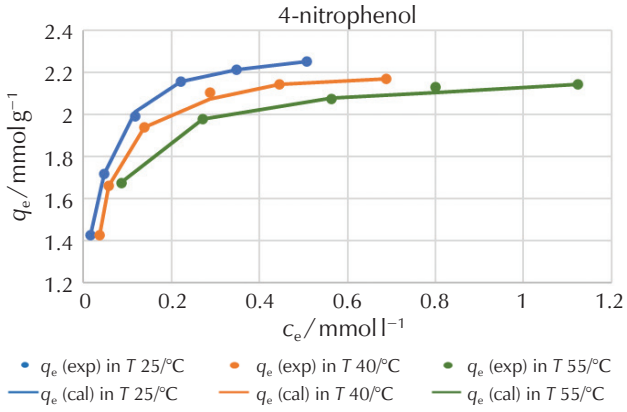

Fig. 11 – 4-nitrophenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C)

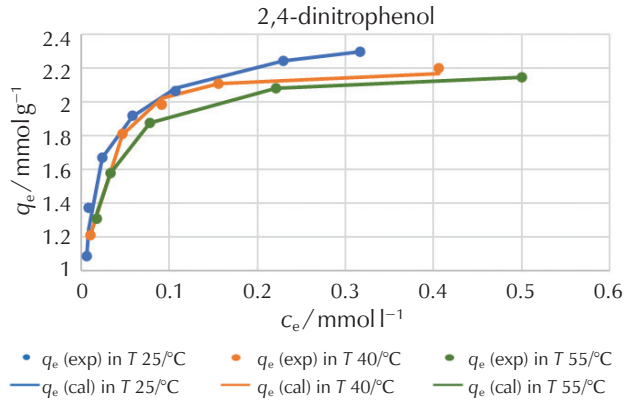

Fig. 12 – 2,4-dinitrophenol adsorption kinetics by ACF at different temperatures (25, 40, and 55 °C)

The Gaussian kernel function DA-SVM model demonstrated its great ability to predict the amount adsorbed at equilibrium of 4-nitrophenol at 25, 40, and 55 °C, as shown in Fig. 11.

The results (Fig. 12) indicate the ability of the Gaussian kernel function DA-SVM model to predict with high accuracy the values of adsorption of 2,4-dinitrophenol at 25, 40, and 55 °C by ACFs.

From the results of R^2 and *RMSE* of 21 systems mentioned in Table 4, it was observed that Gaussian kernel function DA-SVM model had a great capacity to predict the values related to the amount adsorbed at equilibrium with a confined RMSE error between [0.014–0.051]/mmol l^{-1} and adjustment capacities R^2 between [0.991–1.000].

6 Conclusion

In this research, a Dragonfly Algorithm-based Support Vector Machine (DA-SVM) mathematical model was constructed to predict the amount adsorbed at equilibrium of phenol, 2-chlorophenol, 4-chlorophenol, 2,4,6-trichlorophenol, 4-nitrophenol, and 2,4-dinitrophenol by the ACFs at three temperature levels (25, 40, and 55 °C).

The amount adsorbed at equilibrium (q_e) was studied with a database containing the experimental conditions (temperature (T) and concentration at equilibrium (c_e)), and three descriptors to distinguish phenols (molecular weight (M_w), density (d), and boiling point (BP) to differentiate the phenols. The inputs and output were statistically studied, and the analysis results proved their ability to predict with no multicollinearity.

Table 4 – Statistical criteria modelling by Gaussian kernel function DA-SVM model

	Phenol			2-CP			4-CP			2,4-DCP			2,4,6-TCP			4-NP			2.4-DNP		
T/°C	25	40	55	25	40	55	25	40	55	25	40	55	25	40	55	25	40	55	25	40	55
R^2	0.998	0.995	0.997	0.996	0.991	0.990	0.994	0.998	0.999	1.000	0.997	0.998	1.000	1.000	1.000	0.999	0.999	0.996	0.991	0.996	0.996
RMSE / mmol l^{-1}	0.0423	0.0181	0.0124	0.0201	0.0287	0.0457	0.0341	0.0138	0.0106	0.0075	0.0281	0.0251	0.0014	0.0016	0.0014	0.0080	0.0120	0.0125	0.0504	0.0225	0.0144

The q_e modelled was by the SVM technique, the Dragonfly optimisation algorithm (DA) was used to assist SVM to refine its hyperplane parameters, and Gaussian kernel function and polynomial kernel function were tested. The Gaussian kernel function DA-SVM model showed an advantage by giving more accurate values related to a global determination coefficient ($R^2 = 0.997$) and a global root mean squared error (RMSE = 0.027 mmol l^{-1}).

ACKNOWLEDGEMENTS

The authors acknowledge the Directorate-General for scientific research and technological development (DGRSDT)-MESRS, Algeria. The authors acknowledge Mr. Houssam Eddine Slama.

Notes

Authors declare that there is no conflict of interest.

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SAŽETAK

Modeliranje adsorpcijskog fenomena određenih fenola metodom potpornih vektora Dragonfly pomoću vlakana aktivnog ugljena

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Cilj ovog istraživanja bio je izraditi matematički model zasnovan na metodi potpornih vektora (SVM) koji može predvidjeti količinu adsorbiranu u ravnoteži (q_e). Vlakna s aktivnim ugljenom (ACF) upotrijebljena su za adsorpciju određenih fenola (fenol, 2-klorofenol, 4-klorofenol, 2,4,6-triklorofenol, 4-nitrofenol i 2,4-dinitrofenol). Eksperimentalni skup podataka od 129 bodova prikupljen je iz prethodno objavljenih radova. Ulazi parametri koji su uzeti u obzir za modeliranje bili su temperatura (*T*), koncentracija u ravnoteži (c_e) i dva deskriptora (točka vrenja (*BP*) i gustoća (*d*)) za razlikovanje ispitivanih onečišćujućih tvari. Korišteni podatci prethodno su obrađeni statističkom analizom da bi se osigurala njihova primjerenost za modeliranje. Rezultati su pokazali superiornost modela DA-SVM Gaussove kernel funkcije demonstriranog njegovim koeficijentom determinacije (R^2 = 0,997) i srednjom kvadratnom pogreškom (RMSE = 0,027 mmol l^{-1}).

Ključne riječi
Adsorpcija, fenoli, metoda potpornih vektora, Dragonfly algoritam, vlakno aktivnog ugljena, količina adsorbirana u ravnoteži

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Izvorni znanstveni rad
Prispjelo 10. studenoga 2020.
Prihvaćeno 24. veljače 2021.