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An optimized PSO-ANN model for improved prediction of water treatment desalination plant performance

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ABSTRACT

An accurate prediction of the performance of water treatment desalination plants could directly improve the global socio-economic balance. In this regard, many researchers have been engaged in the various artificial intelligence applied soft computing techniques to predict actual process outcomes. Inspired by the significance of such techniques, an optimized Particle Swarm Optimization based Artificial Neural Network (PSO-ANN) technique has been proposed herewith to predict an accurate performance of the reverse osmosis (RO) based water treatment desalination plants. Literature suggests that the improvements of the soft computing models depend on their modeling parameters. Therefore, we have included an extended list of nine modeling parameters with a systematic indepth investigation to explore their optimal values. Finally, the model's simulations results ($R^2 = 99.1\%$, Error = 0.006) were found superior to the existing ANN models ($R^2 = 98.8\%$, Error = 0.060), with the same experimental datasets. Additionally, the simulation results recommend that among many parameters considered, the number of hidden layer nodes (n), swarm sizes (SS), and the weight of inertia (ω) play a major role in the model optimization. This study for a more accurate prediction of the plant's performance shall pave the way for the process design and control engineers to improve the plant efficiency further.

Key words: artificial neural network, desalination, modeling and simulation, particle swarm optimization, soft computing techniques, water treatment

HIGHLIGHTS

- Proposed parameters to accurately model permeate flux of RO-based desalination plant.
- Rigorous analysis with extended list of nine PSO-ANN parameters to achieve optimal model.
- Model achieved superior results ($R^2 = 99.1\%$, Error = 0.006) than existing models ($R^2 = 98.8\%$, Error = 0.060).

INTRODUCTION

The researchers' interest in optimizing water treatment and desalination plant's performance has significantly increased in the last few decades (Ahmed *et al.* 2019). In this direction, artificial intelligence soft computing techniques such as artificial neural network (ANN), particle swarm optimization (PSO), state vector machines (SVM), genetic algorithm (GA), multi-objective GA (MOGA), etc., have played a vital role in determining the best solutions (Mahadeva *et al.* 2018, 2019, 2020, 2021a, 2021b; Zhang *et al.* 2019; Ghiasi *et al.* 2020; Goel *et al.* 2020; Mohammadi *et al.* 2020; Sit *et al.* 2020; Hejabi *et al.* 2021). An optimization is a systematic approach for locating an optimal solution and maximizing the production performance (Ahmed *et al.* 2019). Therefore, such techniques are finding extensive applications worldwide today.

Sustainable access to clean water leads to healthier people and economic development. Healthier people help preserve a healthy community, and together help build and progress a healthy world (Guterres 2020). However, one in three people across the world do not have access to clean drinking water in the current situation, and >673 million people still defecate outdoors worldwide (Guterres 2020). This leads to a large number of infections and diseases such as diarrhea, cholera,

dysentery, typhoid, and polio that spread through water (Guterres 2020). Therefore, our essential responsibility is to increase clean water availability to people around the world so as to save the planet.

The paper has been organized into four sections. Section 1 gives an essential background for water treatment, artificial intelligence modeling technologies, literature reviews, and significant contributions. The step-by-step proposed methodologies with the block diagram representations are demonstrated in Section 2. Section 3 provides the results and discussion with focus on models optimization, comparative study with existing literature, and significant outcomes. Finally, concluding remarks and future recommendations are presented in Section 4.

For increasing the clean and freshwater access, numerous water treatment and desalination plants have been installed worldwide, supported with many social awareness campaigns to save natural water resources. In this regard, for improving plant efficiency, several researchers have previously developed artificial intelligence models, including PSO-ANN, to predict accurate process outcomes. Literature suggests the use and screening of several models that help improve plant predictions. For instance, Khajeh *et al.* (2013) have presented a PSO-ANN predictive model to remove methylene blue using silver nanoparticles from water samples. The experimental datasets were randomly allocated as: 76% for training, 12% for validation, and 12% for testing the model. The model involved six inputs, one hidden layer with 14 nodes, and one output layer (6:14:1). The modeling parameter values were: swarm size ($SS = 10$), acceleration factors (c_1,$c_2 = 2$), minimum weight of inertia ($\omega_{min} = 0.05$), the maximum weight of inertia ($\omega_{max} = 0.1$), and 10 number of iterations. The correlation coefficients performed superior in PSO-ANN (0.95) than response surface methodology (0.89). Likewise, Ahmadi *et al.* (2014) developed a computational prediction model (PSO-ANN) to predict equilibrium water dew point of natural gas in a triethylene glycol dehydration system. A suitable choice of the number of datasets for training and testing of 130 and 44, swarm size of 22 (*SS*), acceleration factors (c_1,c_2) of 2, and maximum of 200 iterations in their modeling investigations produced more reliable results ($R^2 = 0.998$) than the backpropagation (BP-ANN) model.

Further, Khajeh *et al.* (2017) developed a PSO-ANN predictive model to remove manganese and cobalt from water. The proposed models involved seven inputs, one hidden layer with 13 nodes for manganese and 15 nodes for cobalt separation process, and one output layer (7:13:1 and 7:15:1, respectively). The modeling parameters used in models for manganese and cobalt, respectively, were: ($SS = 15$ and 10), (c_1,$c_2 = 2$), ($\omega_{min} = 0.6$ and 0.05), ($\omega_{max} = 0.8$ and 0.1), and the number of iterations was 10. Zubaidi *et al.* (2018) presented a novel approach for predicting monthly water demand by hybrid PSO-ANN and backtracking search algorithm (BSA-ANN). The datasets were divided into three sets as: training (70%), testing (15%), and validation (15%). Modeling parameters used for PSO-ANN were ($SS =$ ranges from 20 to 50), (c_1,$c_2 = 1.494$), ($\omega = 0.5$), and 100 number of iterations. They observed that the PSO-ANN model performed better than BSA-ANN. On similar lines, Aryafar *et al.* (2019) developed a model to describe process of pollutant adsorption from industrial wastewaters using soft computing techniques (PSO and PSO-ANN). The Institute of Color Science and Technology, Iran, collected 54 industrial wastewater samples for a similar study. The datasets were divided into 75% for training and 25% for testing. The proposed PSO-ANN model exhibited superior results than the PSO or ANN model. Recently, Mahadeva *et al.* (2021a) developed a PSO-ANN and fuzzy-based models to optimize the seawater reverse osmosis desalination plant. The PSO-ANN model performed superior results than the fuzzy based soft computing models.

In summary, the literature appears to suggest usage of the modeling parameters in the following range: 5–50 for *SS*, c_1, $c_2 \leq 2$, $\omega_{max} \leq 1$, and 10–1000 number of iterations. Literature also suggested a choice of dataset division of (75% training, 15% validation and 15% testing) as best suitable for modeling such a system.

Significant contributions

The literature evidently suggests that the PSO-based ANN models are helpful for many desalination and water treatment applications. Therefore, in this paper, the PSO-ANN models have been used to successfully model the desalination system. We also noticed and screened apparent research gaps in the optimization approaches and the number of parameters used in the models in literature (Khajeh *et al.* 2013, 2017; Ahmadi *et al.* 2014; Zubaidi *et al.* 2018; Aryafar *et al.* 2019). Researchers have used a limited number of modeling parameters for their models that tends to reduce the modeling efficiency. Hence, this paper has included an exhaustive list of nine modeling parameters and a step-by-step method for their optimization so as to improve plant performance further. The design approach employed is simple and systematically executed to appropriately model the system. To the best of our knowledge, there is no literature available that proposes the optimized PSO-ANN approach with such an extensive list of nine modeling parameters for water treatment and desalination plants. Thus, this research's significant contribution is to perfectly design PSO-ANN models with nine modeling parameters

and systematically find their optimum solutions. Finally, the results have been compared with the existing ANN models and were found to demonstrate superior performance.

METHODOLOGY PROPOSED

ANN is a widely used soft computing technique that includes a large variety of architectures. In general, the architecture is formulated of three major layers (input, hidden, and output) and the artificial neuron (Mahadeva *et al.* 2019; Mohammadi *et al.* 2021a). These artificial neurons are also called the nodes associated with the layers. Additionally, these nodes form mathematical expressions that modify the incoming signals and pass them further through the network. Also, they have been connected to the weights and biases. The weights and biases play an essential role in the designing of neural network model optimization. Besides, the value of the weights may be calculated by the BP or PSO algorithms (Emamgholizadeh & Mohammadi 2021; Mohammadi *et al.* 2021b). These may be adjusted during the training step according to the error minimization criteria.

In this study, the neural network toolbox of MATLAB 2019a has been used for modeling and simulation. We have employed the PSO algorithm for ANN training, and therefore designated it as the PSO-ANN modeling technique. The PSO algorithm is a multi-agent search technique that finds the optimum solution in the predefined search space. This study has employed reverse osmosis (RO) desalination plant datasets from previous studies (Gil *et al.* 2018) for modeling investigations. The datasets consisted of four input parameters: feed water salt concentration ($S = 35$–140 g/L), condenser inlet temperature ($T_{cond} = 20$–30 °C), evaporator inlet temperature ($T_{evap} = 60$–80 °C), and feed flow rate ($F = 400$–600 L/h) while permeate flux (P_{flux} (L/h.m^2) was the primary output. Further, the data has been divided into three divisions (training, validation, and testing) to train the neural network. In general, the training division is used to obtain the model parameters. The validation division tests the accuracy of ongoing training to avoid overfitting while the testing division validates its performance.

Now, the next task is the optimization of the model. For this, we have included an extended list of nine modeling parameters, such as, the number of hidden layer nodes (n), the number of hidden layers (H), activation functions, training functions, dataset divisions (%), error performance functions, SS, ω and (c_1,c_2) in our modeling investigations. The regression coefficient (R^2) and mean squared error (MSE) have been used to evaluate the model's performances of the plant (Mohammadi *et al.* 2020; Mahadeva *et al.* 2021b). The next task is to find the best modeling parameters for the model. For this, we have followed a systematic and step-by-step approach, described below and represented through block diagram (Figure 1):

Step 1: *Initialization*; Collect the datasets from the literature, arrange them into a suitable format as per the modeling requirements, and then feed them into the model. Later, define the initial and appropriate values of nine modeling parameters according to the literature experiences. The model is now ready for further investigation.

Step 2: *Find best n*; Start initial trials for finding the best value of n. Obtain the best value of n and fix the same in the programming loop.

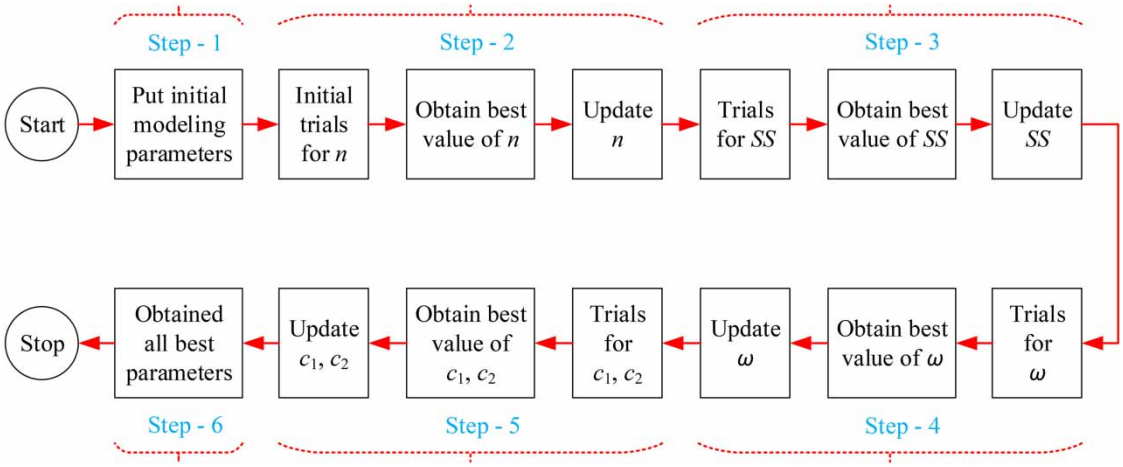

Figure 1 | Block diagram representation to obtain the best modeling parameters and the best performances of the plant using the proposed model.

Step 3: *Find best SS;* With n defined, next start the trials to find the best value of *SS*. This helps complete updation of two essential parameters in our modeling according to their best performances.

Step 4: *Find best* ω; Likewise, further start the trials for finding the best value of ω. Obtain it and update it in the computational program. It is to be noted that the rest of the parameters remain the same.

Step 5: *Find best* (c_1,c_2); In the same manner, start the trials to find the best values of (c_1,c_2). Again, obtain their best values and fix them in the programming loop.

Step 6: *Summarize all best parameters*; Finally, all the best estimates of modeling parameters are noted down. Thus, the best modeling parameters as well as the best performances of the plant using a step-by-step and systematic approach are evaluated.

Table 1 | Best performance results and analysis of the plant using a systematic approach

Step-1	**Model Initialization**	**Screen the initial nine modeling parameters and their initial range and start the model simulations [*H* = 1, Activation function = *logsig-purelin*, Training function = *trainlm*, Dataset divisions (%) = (75–20–5), Error performance function = MSE, *SS* = 25, ω = 0.3, c_1 = 1.5,c_2 = 2.5, and Iterations = 1,000]**					
Step-2	**Finding the best value of *n***			**Step-3**	**Finding the best value of *SS***		
		P_{flux} (L/h.m^2)				P_{flux} (L/h.m^2)	
Trial No.	***n***	**R^2 (%)**	**MSE**	**Trial No.**	***SS***	**R^2 (%)**	**MSE**
1	1	95.9	0.027	**16**	**1**	**98.9**	**0.007**
2	2	98.3	0.011	17	2	98.7	0.009
3	3	97.5	0.016	18	3	97.6	0.016
4	4	97.5	0.016	**19**	**4**	**99.0**	**0.006**
5	5	97.5	0.016	20	5	98.5	0.009
6	6	98.4	0.015	21	6	98.1	0.013
7	7	98.5	0.009	22	7	97.7	0.015
8	8	98.3	0.011	23	8	98.3	0.011
9	**9**	**98.7**	**0.008**	**24**	**9**	**99.1**	**0.006**
10	10	98.6	0.009	25	10	97.7	0.015
11	11	93.3	0.045	26	11	98.6	0.009
12	12	98.7	0.008	27	12	98.3	0.011
13	13	93.8	0.040	28	13	98.0	0.016
14	14	97.6	0.016	29	14	94.1	0.039
15	15	96.3	0.024	30	15	97.7	0.015
Step-4	**Finding the best value of ω**			**Step-5**	**Finding the best value of c_1, c_2**		
Trial No.	**ω**	P_{flux} (L/h.m^2)		**Trial No.**	**c_1,c_2**	P_{flux} (L/h.m^2)	
		R^2 (%)	**MSE**			**R^2 (%)**	**MSE**
31	0.1	98.6	0.009	41	0.8, 3.2	95.7	0.028
32	0.2	98.5	0.010	42	1.0, 1.0	98.5	0.010
33	**0.3**	**99.1**	**0.006**	43	1.5, 1.5	98.6	0.009
34	0.4	91.1	0.058	**44**	**1.5, 2.5**	**99.1**	**0.006**
35	0.5	97.9	0.014	45	2.0, 2.0	98.6	0.009
36	0.6	95.7	0.028	46	2.5, 1.5	98.7	0.009
37	0.7	98.0	0.013	47	3.2, 0.8	98.5	0.010
38	0.8	98.5	0.010	**Step-6**	**Record the all best performances**		
39	**0.9**	**98.8**	**0.008**				
40	1.0	98.7	0.009				

RESULT AND DISCUSSION

Model optimization results

In this work, we have utilized the Neural Network Toolbox of MATLAB R2019a software for model investigations. When we developed the proposed model as per the methodology (explained in the previous section), we noticed some interesting results, which have been tabulated in Table 1. The modeling optimization trials were first performed with the variation of hidden layers nodes ($n = 1$ to 15), as illustrated in Figure 2. Here, we have observed that trial no. 9 (with $n = 9$) achieved the best performance ($R^2 = 98.7\%$, MSE = 0.008). Notably, trial no. 1 (having $n = 1$) and trial no. 11 (having $n = 11$) exhibited larger errors. After screening the model with optimal number of nodes ($n = 9$), the next step was to find the best value of *SS*. In this regard, we observed that trial number 24 ($SS = 9$) achieved superior performance with minimum errors ($R^2 = 99.1\%$, MSE = 0.006), as shown in Figure 3. Once optimal n and *SS* have been determined, we turn optimization with the varying

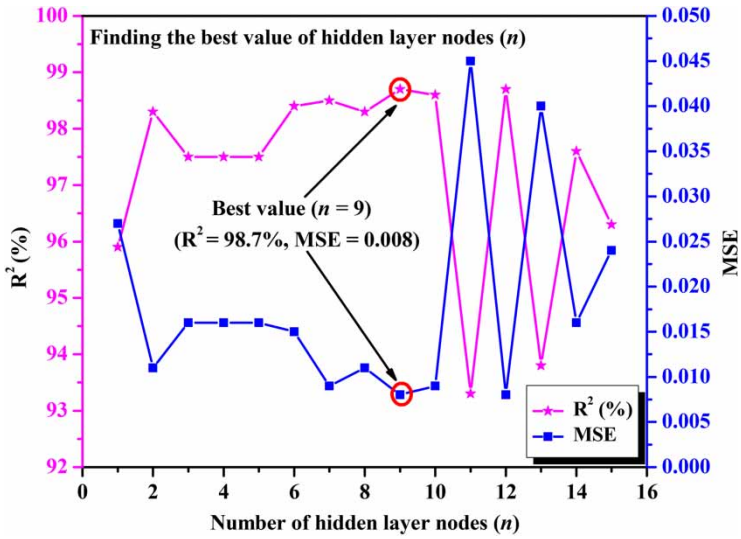

Figure 2 | Illustration of the dependence of modeling performance expressed as R^2(%) and MSE, and screening of the best value of hidden layer nodes (*n*).

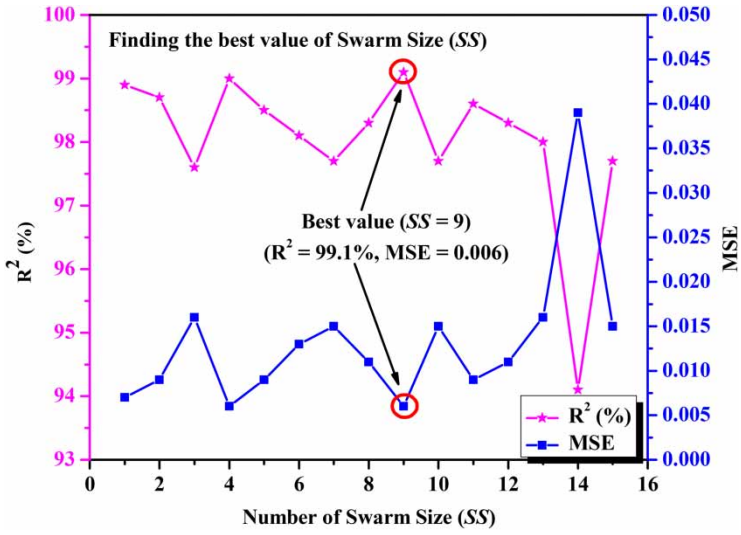

Figure 3 | Illustration of the dependence of modeling performance, expressed as R^2 (%) and MSE, and screening of the best value of Swarm Size (*SS*).

ω. In this analysis, trial number 33 with $\omega = 0.3$ presented with the best results. Literature suggests that the value of ω should be between 0 to 1. Therefore, we have considered varying ω between 0 to 1 with a step of 0.1 in our modeling investigation. The trial number 33 (having $\omega = 0.3$) demonstrated best performance. Likewise, an attempt was made to understand the effect of acceleration factors (c_1,c_2). The trial number 44 (having $c_1 = 1.5$, $c_2 = 2.5$) achieved the best results. The initial assumptions of acceleration factors (c_1,c_2) were considered in this model according to guidance received from the literature. For instance, the literature articles suggest that the acceleration factors should be chosen such that $c_1 + c_2 \leq 4$. The aforementioned protocol helped us to obtain the best performance results of the plant.

A comparative study with existing literature and summary of significant outcomes

A comparative analysis of the four best models from this work versus that of the existing ANN best model (Gil *et al.* 2018) is presented in Table 2. Model - 3 with a *SS* of 9 and nodes distribution of 4:9:1 (other factors same) provided the optimal results. Further, we have also noticed that trial number 16 (Model - 1), trial number 19 (Model - 2), and trial number 39 (Model - 4) detected higher results than the optimal results available in the existing literature achieved with similar datasets utilization for both modeling investigations. We have also noticed that the best modeling performance was achieved with a minimum hidden layer ($H = 1$), while the existing literature used two hidden layers ($H = 2$) in their modeling investigation. It may be that choice of a large number of hidden layers, in this case, unnecessarily increases the complexity of the model. It is also observed that the *logsig* activation function, $\omega = 0.3$, and $c_1 = 1.5$,$c_2 = 2.5$ values are most suitable for optimizing the plant.

The statistical results of the performance evaluations (R^2 and MSE) of the proposed models by different stages (training, validation, testing, and all datasets) are presented in Table 3. As shown in Table 3, Individually, Model - 2 performed best results for training ($R^2 = 99.8\%$, MSE = $\sim$ 0.000), and Model - 1 performed best results for testing ($R^2 = 99.6\%$, MSE =

Table 2 | Comparative analysis of the performance results of proposed models with the existing literature expressed in terms of R^2 (%) and Error

	P_{flux} (L/h.m^2)										
	Parameters used for the optimization									Results	
Model	*n*	*H*	Activation Function	Training Function	Dataset divisions (%)	Error Perfor. Function	*SS*	ω	c_1,c_2	R^2 (%)	Error
Gil *et al.* (2018)	4:7:2:1	2	*logsig-logsig*	*trainlm*	75-20-05	RMSE	–	–	–	98.8	0.060
Model – 1	4:9:1	1	*logsig*	*trainlm*	75-20-05	MSE	1	0.3	1.5, 2.5	98.9	0.007
Model – 2	4:9:1	1	*logsig*	*trainlm*	75-20-05	MSE	4	0.3	1.5, 2.5	99.0	0.006
Model – 3	4:9:1	1	*logsig*	*trainlm*	75-20-05	MSE	9	0.3	1.5, 2.5	99.1	0.006
Model – 4	4:9:1	1	*logsig*	*trainlm*	75-20-05	MSE	9	0.9	1.5, 2.5	98.8	0.008

Table 3 | Statistical results of the proposed models' performance evaluations (R^2 and MSE) for different stages of modeling (training, validation, testing, and all datasets)

	Performance evaluations of the PSO-ANN models by different stages							
	Training (75%)		Validation (20%)		Testing (05%)		All (100%)	
Model	R^2 (%)	MSE	R^2 (%)	MSE	R^2 (%)	MSE	R^2 (%)	MSE
Model – 1	99.0	0.005	98.7	0.014	99.6	0.003	98.9	0.007
Model – 2	99.8	~0.000	98.5	0.016	94.7	0.057	99.0	0.006
Model – 3	99.3	0.004	98.9	0.011	98.6	0.015	99.1	0.006
Model – 4	99.1	0.005	98.6	0.014	96.9	0.024	98.8	0.008

0.006). Moreover, Model – 3 performed best of best results for all datasets. In addition, to better understand the results, Figure 4 illustrates the scatter plots of the predicted permeate flux (P_{flux} (L/h.m^2) of the proposed Model – 3.

CONCLUSION AND FUTURE WORK

The present study proposes a particle swarm optimization-based artificial neural network (PSO-ANN) model to predict the performance of permeate flux (P_{flux} (L/h.m^2) of reverse osmosis (RO) water treatment desalination plant. The model involves the use of an extended list of nine modeling input parameters for optimization, while two output parameters, regression coefficient (R^2) and Error, have been utilized to evaluate the model's performance. Besides, four experimental sets of input (feed water salt concentration, feed condenser inlet temperature, feed evaporator inlet temperature, and feed flow rate) have been considered to accurately predict the permeate flux of the plant in our modeling investigations. Simulation results indicated the superiority of the proposed model in terms of the best-achieved regression ($R^2 = 99.1$) with minimum errors (MSE = 0.006) compared with the existing ANN model ($R^2 = 98.8$, Error = 0.060). The simulations and subsequent analysis also revealed

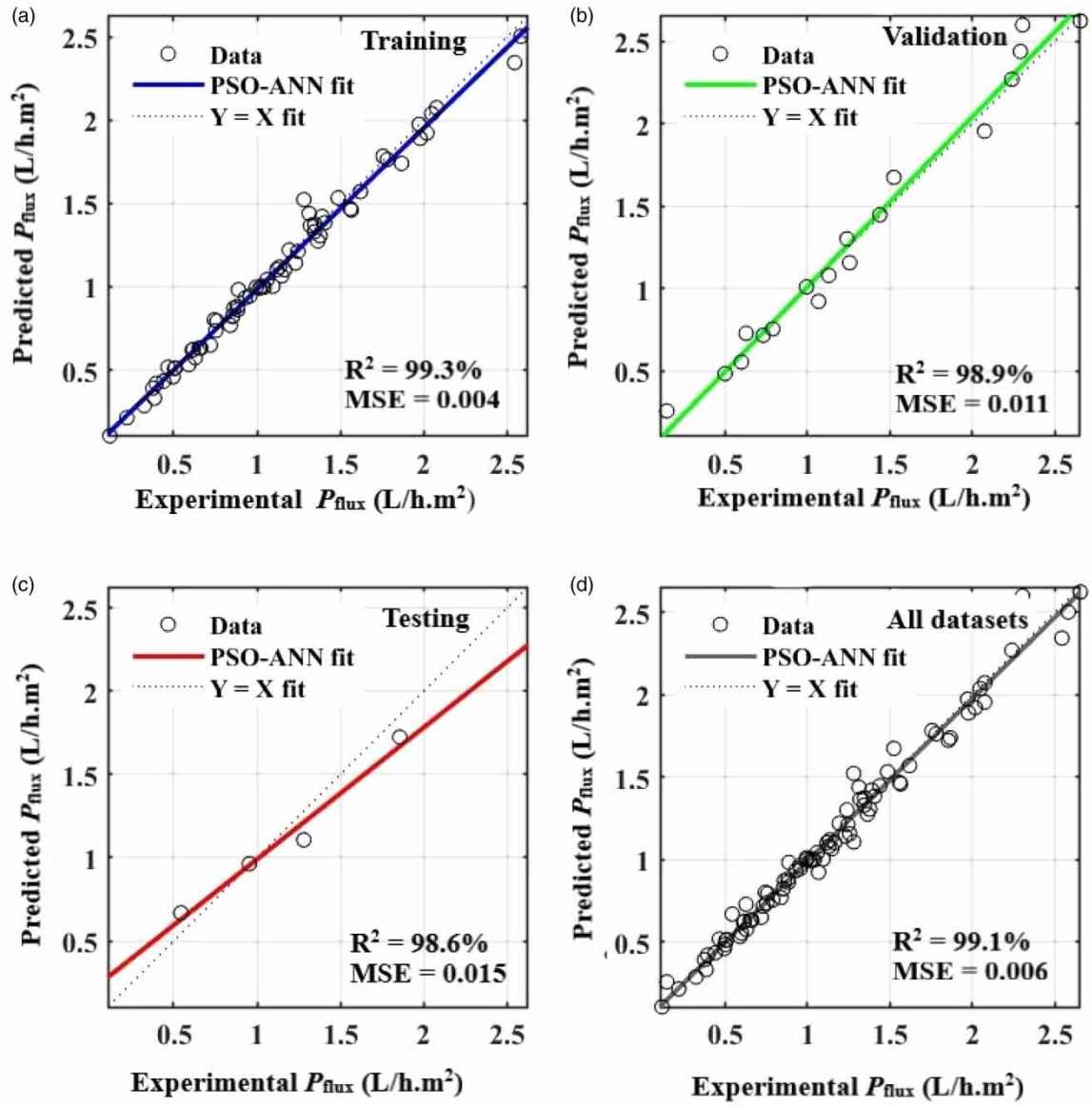

Figure 4 | Scatter plots of the predicted permeate flux (P_{flux} (L/h.m^2) from the PSO-ANN (Model - 3): (a) training (75%), (b) validation (20%), (c) testing (5%), and (d) all datasets (100%).

that the PSO algorithm is the most suitable algorithm to search for an optimum solution for such an ANN problem. The proposed model that exhaustively searches for optimal parameters could be applied to solve many problems in science and engineering applications to ensure the economic and technical sustainability of the processes.

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DATA AVAILABILITY STATEMENT

All relevant data are available from an online repository or repositories.

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