ME597 Artificial Intelligence in Thermal Systems

Artificial neural networks for performance prediction of membrane distillation desalination systems

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Abstract:

Depleting freshwater reserves are becoming a global concern and the thermal desalination of alternative water sources like seawater presents a possible solution. AI and machine learning can capture the complex physics involved in these systems and present an easy way for estimating their performance for informed decision making. We used simple regression tools and an advanced ANN model to analyse the performance of membrane distillation (MD) desalination systems from a comprehensively developed dataset. Neural networks are significantly accurate in predicting the overall performance of MD systems and can facilitate better decision making for adopting desalination technologies.

Introduction:

The lack of access to drinking water for billions of people across nations is increasingly becoming an issue of global importance [1]. The limited availability of freshwater sources and harvesting techniques has led to the development of effective desalination strategies for treating the abundant saline water from oceans [2-4]. In most water treatment methods, the salinity of the feed (saline water) rises as pure water is extracted from the solution and so desalination plants have to be efficient across a wide range of salinities (from seawater levels to saturation levels) [5-7]. Filtration techniques and pressure based processes like reverse osmosis are often energy intensive when treating highly saline waters and can be rendered impractical. Thermal desalination systems have shown consistent performance with variations in feed salinity and large scale processes like multi-effect distillation (MED), thermal vapor compression (TVC) among many others can meet the increasing water demand [8].

Energy costs in thermal desalination systems often govern their feasibility and in some cases can be as high as about two-thirds of the total operating expense [9-11]. This presents a major limitation of using large scale thermal desalination plants in developing and under-developed nations which are usually the ones hardest hit in terms of pure water supply. Low temperature thermal desalination processes like membrane distillation (MD) can be used a cost effective method in these countries to achieve energy efficient desalination [12]. The performance of MD systems is governed by numerous parameters like the feed salinity, feed inlet temperature, system length scales and configurations to name a few [13-15]. Accurately predicting the performance of MD systems across these varied conditions presents a major challenge in their design and optimization. Over the years, numerous studies have examined the performance of MD resulting in comprehensive datasets that can be fed into machine learning algorithms to facilitate a future pathway for the technology [16-18].

The idea of using machine learning and artificial intelligence in desalination has gained momentum over the recent years with studies considering membrane fouling, flux production, energy efficiency and even parameter optimization [19]. Supervised ML regression tools and artificial neural networks (ANN) have been used to predict the productivity of solar stills [20,21]. Artificial intelligence has been used to understand the mass transfer in desalination membranes and to optimize the membrane parameters using methods like genetic algorithms (GA) and ANNs [22-24]. However, very few studies have been aimed at predicting the system scale performance of desalination systems in general. Tashvigh et al. [25] used a GA approach to determine the optimal system parameters for maximizing pure water flux instead of actually predicting the performance at various salinities and top temperature. Yang et al. [26] adopted ANNs to predict the performance of a VMD system with varying temperature, flow rate and module lengths but their experiments dealt with low salinity feeds which are seldom observed in practical scenarios. Furthermore, both of these studies used a relatively small experimental dataset (154 and 36 respectively) to train and test their models which does not give an overall estimation of the diverse conditions. Thus, a comprehensive study on the performance prediction of MD systems using critical input parameters and extensive datasets is missing in the literature and efforts need to be directed towards producing well defined datasets and reliable predictive models.

In the present study, we developed a multivariable regression model to predict the energy efficiency and flux production of air gap membrane distillation (AGMD) systems. In conjunction, exploratory analysis was done to formulate an ANN algorithm for accurate prediction of system performance based on the learning of a comprehensive dataset. The feed salinity, inlet temperature, flow rate and module length were chosen as the input parameters for the models and the output variables were the energy efficiency (GOR) and permeate flux (LMH). The dataset was developed from numerous runs of an in-house well validated numerical code investigating the heat transfer and thermodynamics of practical AGMD systems. This work marks the first comprehensive performance prediction and data analysis of MD with variations in feed inlet salinity. The groundwork laid for developing ANN algorithms can facilitate reliable predictions across varied operating conditions and as a consequence formulating a complete ANN method would be the next step.

Dataset description:

Input parameters for the data set are chosen to be the feed inlet salinity which is a measure of salt concentration, feed inlet temperature which represents the temperature after the top heater, feed mass flow rate and module length which is the net channel length across the entire module array. The output parameters are energy efficiency, which in MD is described by gained output ratio (GOR) defined as heat of vaporization of permeate divided by the heat input required for the MD system.

$$GOR = \frac{\dot{m}_p h_{fg}}{\dot{Q}_h}$$

$\dot{m}_p$ [kg/s] represents the permeate flux, h_{fg} [kJ/kg] is the latent heat of vaporization and $\dot{Q}_h$ [kW] is the thermal energy input required. The second output parameter is the permeate production measured in litres per meter square membrane area per hour (LMH).

The data set is developed from a well validated numerical code [27-29] capturing the heat, mass -transfer and thermodynamics of MD systems. The computational MD model was based on one-dimensional finite difference method, where properties varied along the length and were assumed to be constant along the width. Mass and energy conservation equations were solved for each discretized control volume (shown in Figure 1) using the built-in property evaluation functions of engineering equation solver (EES) [30]. Span-wise property variations were accounted for using thin temperature and concentration boundary layers.

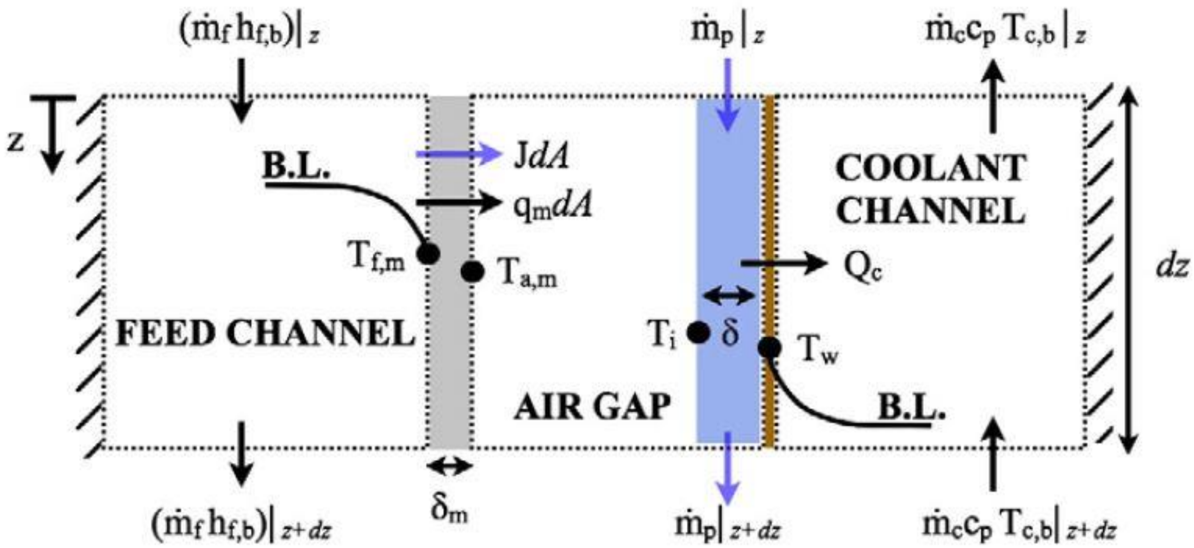

Figure 1: *A computational element used for developing the numerical code capturing the heat transfer and thermodynamics of MD systems [29].*

Methodology:

A comprehensive dataset is developed for training the polynomial regression and ANN models using an in-house code modelling MD systems. The range of input parameters is chosen as follows: Feed salinity is varied from 35 g/kg to 175 g/kg in 35 g/kg intervals, feed inlet temperature on the hot side is varied from 40ºC to 80ºC in intervals of 10ºC, the feed flow rate is varied from 0.25 kg/s to 1 kg/s in intervals of 0.25 kg/s and finally the module length is varied from 0.5 m to 20 m using 20 equal partitions. In total, the dataset consists of nearly 2,000 data points which are then used for training and testing the learning models.

In the first phase of this study, polynomial multivariable regression is carried out to develop a simple model that can help in understanding the correlation between the input variables and the desired outputs of permeate flux and efficiency. The performance of the resulting regression model is judged based on the R2 score obtained in predicting the test data points and the relative losses incurred in training and validation of the model. Eventually, a sensitivity analysis is carried out to determine the optimal learning rate for the regression algorithm by plotting the losses with a set of learning values. These performance metrics and parametric analysis build the foundation for developing an ANN model and tuning the associated hyper parameters for optimization.

An ANN based on feed forward neural network is formulated in the second phase using the comprehensive data points available for training. Model specific hyper parameters are initialized using the activation function ReLU, random allocation for weights and the number of hidden layers and neurons within each layer are optimized from an initial state of 1 and 16 respectively. The SGD optimizer is used with a suitable learning rate and the loss function is set as mean squared error (common for regression problems) in the algorithm. Mini-batch size for data analysis and the number of epochs are initialized using appropriate values with the early stopping method being used for regularization to avoid overfitting (reducing the number of hyper parameters). The resulting model is trained on the dataset and the results are compared to those from the polynomial regression model. Finally, hyper parameter optimization is carried out to determine the optimal values of learning rate, number of hidden layers, batch size and the type of activation function that leads to better predictions. These optimal values complete the ANN model and results from the regression model and ANN algorithm are compared and validated for unseen operating conditions generated using the thermodynamic MD code.

Results and Discussions:

1. Losses and R2 value for multivariable regression

Multivariable regression was carried out using the developed data set and a second order polynomial was fitted for energy efficiency and flux estimation of MD systems. The model accurately captures the variation of efficiency (R2 score > 0.95) with the input parameters and does a decent job of predicting the permeate production. In conjunction, the training and validation losses are very small for both estimations of efficiency and flux as seen in Table 1.

Table 1: *Performance metrics for the multivariable regression model predicting the performance of MD systems*

Parameter	**R2 score**	**Training Loss**	**Validation Loss**
Energy Efficiency	0.9566	0.0002764	0.001007
Flux	0.8046	0.0003301	0.000917

2. Artificial neural networks for predicting energy efficiency and flux

An ANN model was developed to accurately predict the performance of MD for unseen conditions with respect to the model. The model specifications are detailed as follows: the number of hidden layers are set as 5, number of hidden neurons are 64, the activation function for hidden and output layers is ReLU with random weight initialization. The SGD optimizer is used with mean squared loss function, batch size of 4 and 30 epochs. The resulting ANN model exhibits an accuracy of 0.94207 and the losses in training and testing are plotted with the number of epochs as shown in Figure 2 and 3.

Hyper-parameter optimization was carried out using the grid search method to determine the optimal activation function and SGD batch size for the ANN model. The best function was found to be ReLU among other tanh, sigmoid and Leaky ReLU options and the optimal value for batch size was found to be 4. Thereafter a manual search was carried out to determine the optimal number of hidden layers and the learning rate for the neural network as shown in Figure 4 and 5.

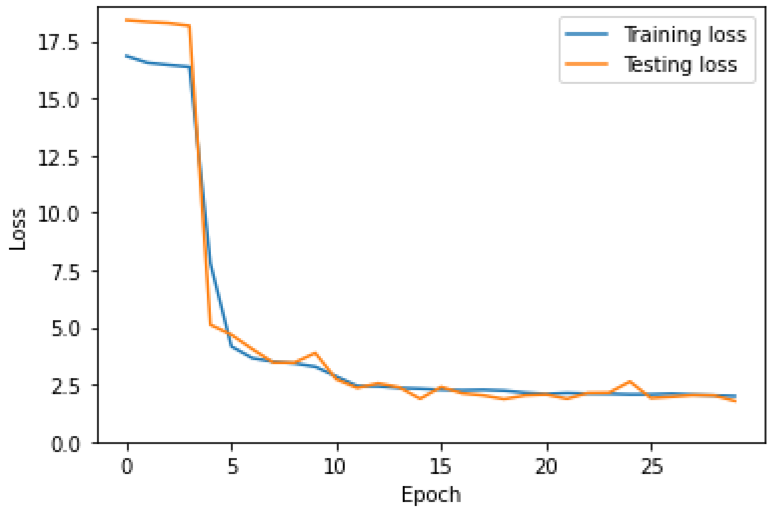

Figure 2: *Training and testing losses with number of epochs for the ANN model with the specifications mentioned in this section.*

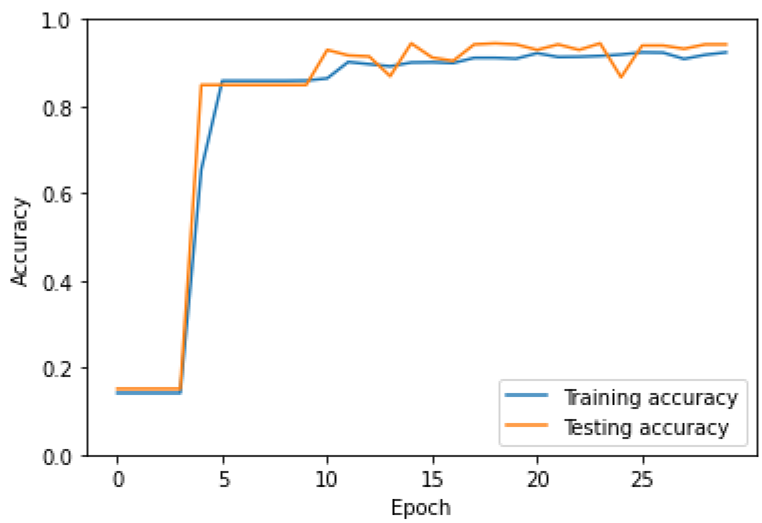

Figure 3: *Training and testing accuracy with number of epochs for the ANN model with the above outlined specifications.*

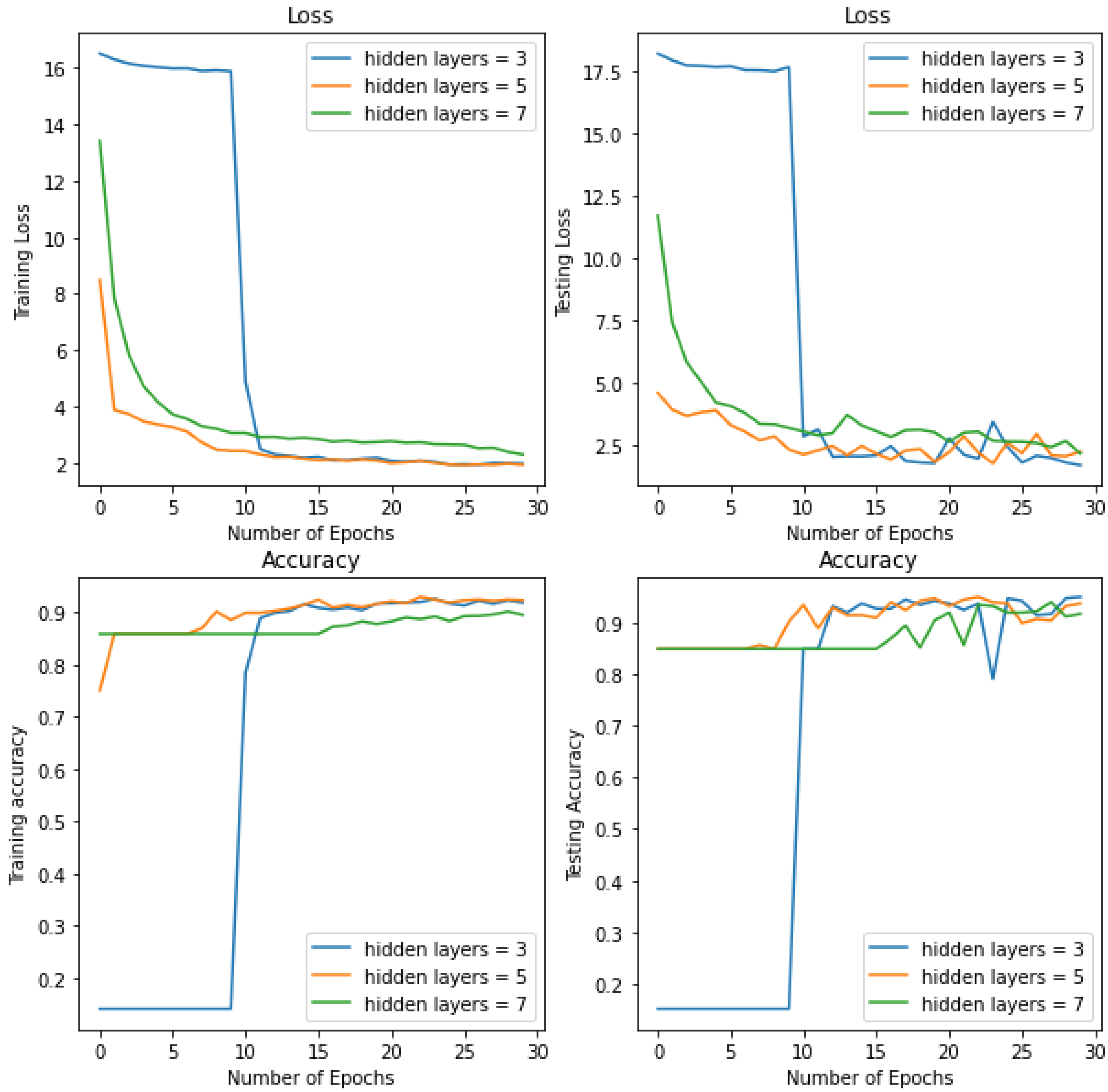

Figure 4: *Training and testing losses, accuracy with number of epoch for varying number of hidden layers (3,5 and 7 hidden layers are considered here). The performance for all the three cases are similar with 5 hidden layers showing slightly better results.*

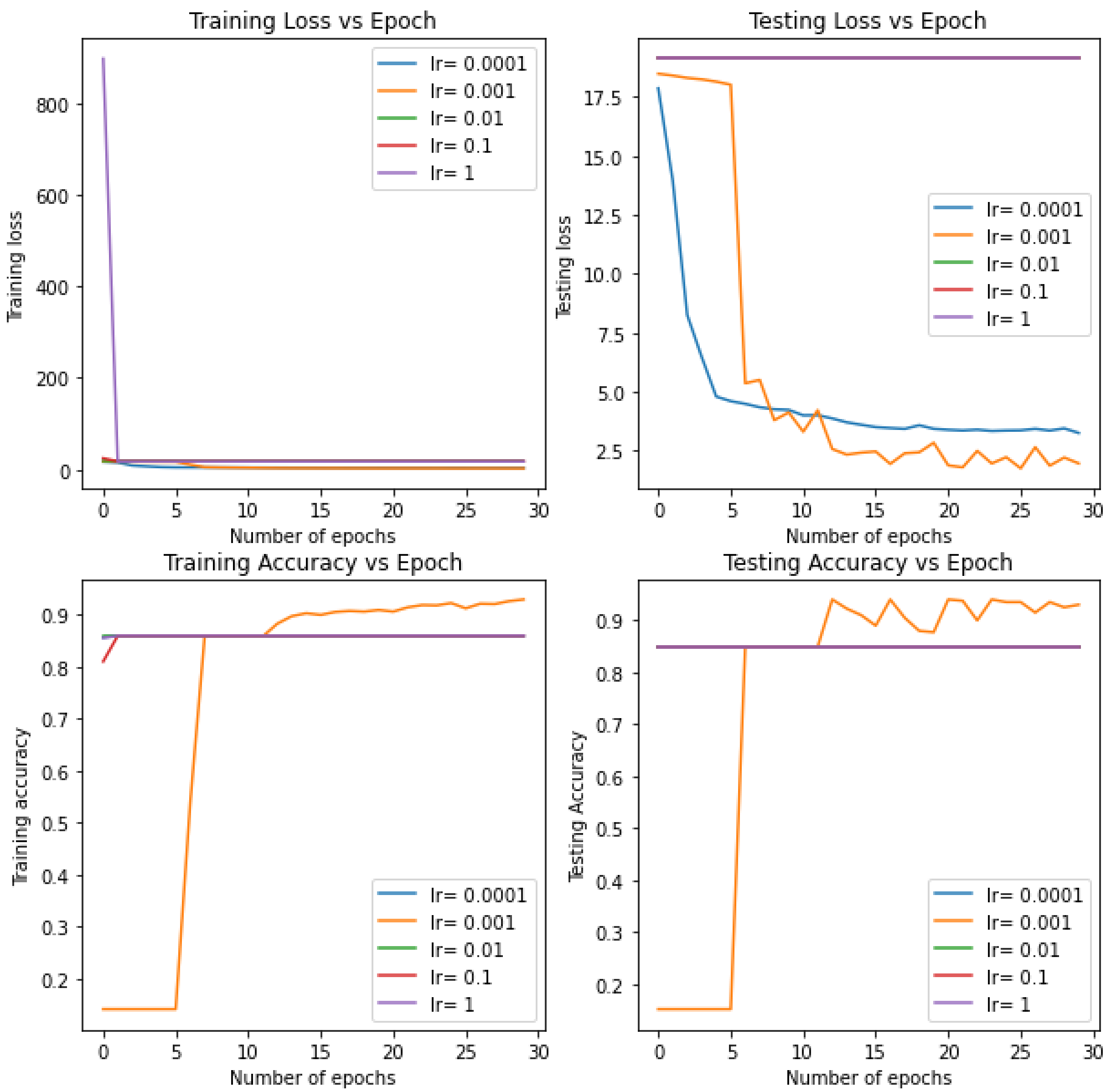

Figure 5: *Training and testing losses, accuracy with number of epoch for varying learning rates. The performance at larger learning rates (1, 0.1 and 0.01) is poor with high losses and low accuracies. The learning rate of 0.001 is found to give the most acceptable results with low losses and higher accuracies.*

3. Performance of the models on novel input conditions

The optimized ANN model and multivariable regression model were used to predict the energy efficiency and permeate production of MD systems under novel conditions shown in Table 2 (not included in the data set used). The results from these models were compared to the numerical algorithm output and they were found to be closely correlated as shown in Table 3. We observe, that the multivariable regression model does a great job in predicting the energy efficiency for the test cases but is significantly off in predicting the permeate production. This was expected since the R2 value was lower when fitting the flux values from the data set and a closer look reveals an exponential relation between flux and the input parameters. The ANN model is consistent in predicting both the energy efficiency and flux of MD as seen in Table 3, but in some cases is a bit off compared to the regression model. This can be rectified by including more data points in the data set so that the model can learn effectively. Accurate prediction of flux values shows the benefits of using an ANN model which can capture the complex relations between permeate flux and the input parameters.

Table 2: *Test case conditions for the ANN and multivariable regression models*

Index	**Salinity [g/kg]**	**Feed Inlet Salinity [ºC]**	**Feed Mass Flow Rate [kg/s]**	**Module Length [m]**
1	90	55	0.8	6
2	115	75	0.6	2
3	40	65	0.55	5.5
4	65	70	0.7	8.5
5	145	58	0.9	12

Table 3: *Comparison of MD performance for the above mentioned test cases with numerical solutions, ANN and regression model solutions. The index represents the respective test cases with conditions outlined in Table 2.*

Index	**Computational Results**		**ANN Results**		**Regression Results**	
	Efficiency [GOR]	**Flux [litres/m^{2}hr]**	**Efficiency [GOR]**	**Flux [litres/m^{2}hr]**	**Efficiency [GOR]**	**Flux [litres/m^{2}hr]**
1	2.533	1.146	3.320	1.017	2.640	1.430
2	1.774	4.005	1.434	5.078	1.948	4.309
3	4.193	1.405	3.854	1.809	4.850	2.016
4	5.103	1.308	5.276	1.197	5.374	1.635
5	3.540	0.679	3.889	0.495	3.747	0.333

Conclusions:

Artificial intelligence and machine learning can be used to accurately capture the heat transfer and thermodynamics of MD desalination systems. Simplistic tools like multivariable regression can be adopted to accurately predict the energy efficiency of MD (R2 score of 0.96) but they suffer from inaccuracies in estimating the permeate production (R2 score of 0.80). A complete performance description can be obtained by training artificial neural networks (Accuracy of 0.94) on comprehensive datasets so as to capture the involved relationship between performance metrics and input parameters. This work shows that AI tools can be used for accurately predicting the performance of desalination systems and can help decision making in under-developed and developing countries.

References

[1] - Alabastri, A., Dongare, P. D., Neumann, O., Metz, J., Adebiyi, I., Nordlander, P., & Halas, N. J. (2020). Resonant energy transfer enhances solar thermal desalination. Energy & Environmental Science, 13(3), 968-976.

[2] - Wenten IG. Reverse osmosis applications: prospect and challenges. Desalination. 2016 Aug 1, 391:112-25.

[3] - Elimelech M, Phillip WA. The future of seawater desalination: energy, technology, and the environment. science. 2011 Aug 5, 333(6043):712-7.

[4] - Werber JR, Osuji CO, Elimelech M. Materials for next-generation desalination and water purification membranes. Nature Reviews Materials. 2016 Apr 5, 1(5):1-5.

[5] - Li J. F., Guan Y. S., Cheng F. Q., Liu Y. Treatment of high salinity brines by direct contact membrane distillation: Effect of membrane characteristics and salinity. Chemosphere 2015, 140, 143-149.

[6] - Leitch, M. E., Li, C. K., Ikkala, O., Mauter, M. S., Lowry, G. V. Bacterial Nanocellulose Aerogel Membranes: Novel High-Porosity Materials for Membrane Distillation. Environ. Sci. Technol. Lett. 2016, 3 (3), 85-91.

[7] - Swaminathan J, Chung HW, Warsinger DM, Lienhard V JH. Energy efficiency of membrane distillation up to high salinity: Evaluating critical system size and optimal membrane thickness. Applied Energy 2018, 211:715-734.

[8] - Chiavazzo E, Morciano M, Viglino F, Fasano M, Asinari P. Passive solar high-yield seawater desalination by modular and low-cost distillation. Nature Sustainability. 2018 Dec, 1(12):763-72.

[9] - Dongare PD, Alabastri A, Pedersen S, Zodrow KR, Hogan NJ, Neumann O, Wu J, Wang T, Deshmukh A, Elimelech M, Li Q. Nanophotonics-enabled solar membrane distillation for off-grid water purification. Proceedings of the National Academy of Sciences. 2017 Jul 3, 114(27):6936-41.

[10] - Goh, P.S., Matsuura, T., Ismail, A.F. and Hilal, N. Recent trends in membranes and membrane processes for desalination. Desalination 2016, 391, pp.43-60.

[11] - Al-Obaidani S., Curcio E., Macedonio F., Di Profio G., Ai- Hinai H., Drioli E. Potential of membrane distillation in seawater desalination: Thermal efficiency, sensitivity study and cost estimation. J. Membr. Sci. 2008, 323 (1), 85-98.

[12] - Lin S., Yip N.Y. and Elimelech M. Direct contact membrane distillation with heat recovery: Thermodynamic insights from module scale modeling. Journal of membrane science 2014, 453, pp.498-515.

[13] - Swaminathan J, Chung HW, Warsinger DM, Lienhard V JH. Membrane distillation model based on heat exchanger theory and configuration comparison. Applied Energy 2016, 184:491-505.

[14] - Camacho LM, Dum Lee L, Zhang J, Li J-D, Duke M, Gomez J, et al. Advances in membrane distillation for water desalination and purification applications. Water 2013, 5(1):94-196.

[15] - Khayet M, Matsuura T. Membrane distillation principles and applications. Elsevier, 2011.

[16] - Warsinger DEM, Swaminathan J, Lienhard V JH. Effect of module inclination angle on air gap membrane distillation. In: Proceedings of the 15th international heat transfer conference, IHTC-15, paper no. IHTC15-9351, Kyoto, Japan, August 2014.

[17] - Warsinger DM, Swaminathan J, Maswadeh L, Lienhard V JH. Superhydrophobic condenser surfaces for air gap membrane distillation. J Membr. Sci. 2015, 492:578-87.

[18] - Swaminathan J, Chung HW, Warsinger D, Al-Marzooqi F, Arafat HA, Lienhard V JH. Energy efficiency of permeate gap and novel conductive gap membrane distillation. J Membr. Sci. 2016, 502:171-8.

[19] - Al Aani S, Bonny T, Hasan SW, Hilal N. Can machine language and artificial intelligence revolutionize process automation for water treatment and desalination?. Desalination. 2019 May 15, 458:84-96.

[20] - Wang Y, Kandeal AW, Swidan A, Sharshir SW, Abdelaziz GB, Halim MA, Kabeel AE, Yang N. Prediction of tubular solar still performance by machine learning integrated with Bayesian optimization algorithm. arXiv preprint arXiv:2002.03886. 2020 Feb 10.

[21] - Maddah HA, Bassyouni M, Abdel-Aziz MH, Zoromba MS, Al-Hossainy AF. Performance estimation of a mini-passive solar still via machine learning. Renewable Energy. 2020 Dec 1, 162:489-503.

[22] - Chamani H, Yazgan-Birgi P, Matsuura T, Rana D, Ali MI, Arafat HA, Lan CQ. CFD-based genetic programming model for liquid entry pressure estimation of hydrophobic membranes. Desalination. 2020 Feb 15, 476:114231.

[23] - Dudchenko AV, Mauter MS. Neural networks for estimating physical parameters in membrane distillation. Journal of Membrane Science. 2020 May 25:118285.

[24] - Jing C, Shin S, Yoon T. Developing The Optimized Ocean Current Strengthening Desalination Semi-permeable Membrane Distillation Based On Decision.

[25] - Tashvigh AA, Nasernejad B. Soft computing method for modeling and optimization of air and water gap membrane distillation—A genetic programming approach. Desalination and Water Treatment. 2017 May 1, 76(1):30-9.

[26] - Yang C, Peng X, Zhao Y, Wang X, Fu J, Liu K, Li Y, Li P. Prediction model to analyze the performance of VMD desalination process. Computers & Chemical Engineering. 2020 Jan 4, 132:106619.

[27] - Swaminathan, J., Chung, H. W., & Warsinger, D. M. (2018). Energy efficiency of membrane distillation up to high salinity: Evaluating critical system size and optimal membrane thickness. Applied Energy, 211, 715-734.

[28] - Warsinger, D. M., Swaminathan, J., & Morales, L. L. (2018). Comprehensive condensation flow regimes in air gap membrane distillation: visualization and energy efficiency. Journal of membrane science, 555, 517-528.

[29] - Summers, E. K., & Arafat, H. A. (2012). Energy efficiency comparison of single-stage membrane distillation (MD) desalination cycles in different configurations. Desalination, 290, 54-66.

[30] - S.A.Klein. Engineering Equation Solver Version 10.