Journal of Engineering and Sustainable Development
Vol. 30, No. 04, July 2026
https://jeasd.uomustansiriyah.edu.iq/index.php/jeasd
ISSN 2520-0917
Research Article
https://doi.org/10.31272/2686

Neural Network Prediction of Mass Transfer Coefficients in Distillation Columns Using Aspen Hysys

Shahad Z. Al-Najjar[1*], Hayder A. Alhameedi[2], Salih A. Rushdi[2], Zainab T. Al-Sharify[3,4], Helen Onyeaka[4] and Suzanne Alsamaq[5]

[1]Department of Chemical Engineering, College of Engineering, Al-Nahrain University, Baghdad, Iraq
[2]Chemical Engineering Department, College of Engineering, University of Al-Qadisiyah, Al-Qadisiyah, Iraq
[3]Environmental Engineering Department, College of Engineering, Mustansiriyah University, Baghdad, Iraq
[4]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom
[5]Faculty of Business and Annotation, Arden University, Birmingham, United Kingdom

[*]Email: shahad.z.atta@nahrainuniv.edu.iq

Article Info

Received	**13/05/2024**
Revised	**09/05/2026**
Accepted	**11/06/2026**

Abstract

Predicting the mass transfer coefficient (K) is one of the most important parameters in industrial separation processes, as it greatly determines the efficacy of distillation in separating components between the liquid and vapor phases. Traditional approaches find it difficult to model K dependence on operational factors such as reflux ratio, molar feed flow rate, and feed composition. This research combines the Aspen Hysys simulation and artificial neural networks (ANNs) to write K as a function of these variables in a benzene-toluene binary system. Aspen Hysys was used to simulate a continuous distillation column that produced K values under different conditions. This data was used to train an ANN (3:4:1 multilayer perceptron) to predict K. The ANN's training performance was 95.3%, and its predictive accuracy was high. This composite method can improve predictive performance in the optimization of distillation column design and operation. It can be effectively used as a tool in industrial practice.

Keywords: Aspen Hysys, Distillation, Mass Transfer Coefficient, Neural Network, Simulation.

1. Introduction

The most significant thermal separation method of the chemical processing industry is distillation. However, in spite of all known benefits and wide use, the main disadvantage of traditional distillation is the heavy energy consumption. This is on account of the fact that the distillation columns can take up more than half of the operational costs in an industrial chemical facility. Distillation is a very common separation process used in the petrochemical and chemical industries. It capitalizes on the component mixtures, varying the volatility of component mixtures [1], [2]. The refining part has to be streamlined to satisfy the growing necessity of higher energy efficiency criteria and the quest to achieve greater yields and purity in most areas. Accordingly, major initiatives are underway to create more efficient systems with reduced dimensions and higher energy efficiency. The idea of cycle heightening is interesting, mechanically speaking, because it implies the use of small volumes, which leads to significant improvements in safety and, consequently, the downsizing of separation measures. These properties are achieved through the use of falling film technology, which has been well recognized and studied for a long time [2].

Distillation and Absorption share a common physical basis: the transfer of mass between the gas and liquid phases at the interface. This process is characterized by a volumetric mass transfer coefficient on both the vapor/gas side (kVa) and the liquid side (kLa). However, designing distillation columns based on absorption mass transfer data is not successful due to considerable inaccuracies in estimating the peak-like theoretical plate for distillation (HETP) [3].

Simulation has been extensively utilized in practical applications for cluster and persistent substance measurement activities over the past two decades. Over the past two decades, there has been a remarkable increase in the use of readily available computational techniques by engineers. Based on these choices, experts can easily employ more substantial methods of analysis and synthesis.

Aspen HYSYS is a cycle reproduction condition intended to serve many training ventures. It is an intelligent, natural, open,

and extensible program. It likewise has many extra choices to expand its abilities into specific industries. With this program, thorough, consistent, state- and dynamic models of plant configuration can be developed. Aside from that, checking, investigating, operational improvement, business planning, and resourcing can be performed with the guidance of the cycle test system. Through its intuitive interface, measurement factors and unit activity geography can be controlled without any problem [4], [5].

The mass transfer coefficient is determined by many variables derived from the simulation process in the Aspen Hysys program. Yongli et al [6] adopted a correlation to predict the mass transfer coefficient based on the Sherwood number and Reynolds number by utilizing various binary systems.

$$Sh_G = 1.01\, Re_G^{0.7}\, We_G^{0.4}\, Sc_G^{0.5} \quad (1)$$

Where:

- **Sh$_G$** - *Gas-side Sherwood number*, a dimensionless number representing the ratio of convective mass transfer to diffusive mass transfer on the gas phase.
- **Re$_G$** - *Gas-side Reynolds number*, which indicates the flow regime of the gas; it depends on gas density , gas velocity, characteristic length or hydraulic diameter, and gas viscosity .
- **We$_G$** - *Gas-side Weber number*, which describes the ratio of inertial forces to surface tension forces; it uses gas density, velocity, characteristic length, and surface tension.
- **Sc$_G$** - *Gas-side Schmidt number*, which represents the ratio of momentum diffusivity to mass diffusivity; it depends on gas viscosity, density, and gas diffusivity.

Radev et.al. [7] proposed the use of the penetration model to determine the gas-side mass transfer coefficient. This coefficient is tested in a laboratory column with sieve trays under atmospheric pressure, specifically in a methanol-water mixture.

But Stefanov and Ivanov [8] proposed predicting the volumetric gas-side mass transfer coefficient KOGa from measurements conducted in binary systems consisting of methanol-ethanol, n-propanol-water, and methanol-ethanol. Hence, the predictive model established in this study can be effectively implemented in a glass laboratory column equipped with a single filter tray [9].

Shahana et.al. [10] focused on using artificial neural networks for the identification of heat-integrated distillation columns, specifically modeling the dynamic nature of the process. However, it does not address the prediction of mass transfer coefficients in distillation columns. Neural Network for Identification of Heat-Integrated Distillation Column.

Singh et al. [11] focused on developing theoretical and ANN-based models for a binary distillation column, validated against experimental data. They found that the Neural network model predicts top product composition accurately and developed models that align well with experimental data.

In 2022, Osman and El Arabi [12] focused on utilizing an artificial neural network (ANN**)** to model a distillation column, with the goal of optimizing product purity through Model-Based Predictive Control. They successfully implemented the ANN to develop a realistic model based on data from an Aspen HYSYS simulation. Additionally, the integration of Dynamic Matrix Control (DMC) optimized with the NSGA-II algorithm demonstrates effective, offset-free dynamic control.

2. Methodology

This study explores the potential of artificial neural networks (ANNs) to predict the mass transfer coefficient (K) in a tray distillation column. The mass transfer coefficient is a critical parameter that directly impacts separation efficiency, making its accurate prediction essential for optimizing column design and operation. To achieve this, the research adopted a two-pronged approach, combining Aspen HYSYS simulation and ANN modeling, as illustrated in the process flow diagram in Fig. 1. We provide a detailed explanation of the methodology, focusing on the highlighted steps shown in the diagram, along with the relevant equations as shown in Table 1.

The process flow diagram (Fig. 1) outlines the workflow of the study, which consists of the following key stages:

- A high-fidelity simulation of the tray distillation column was performed using Aspen HYSYS.
- Operational data, such as liquid and vapor flow rates, tray geometry, temperature profiles, and compositions, were generated.

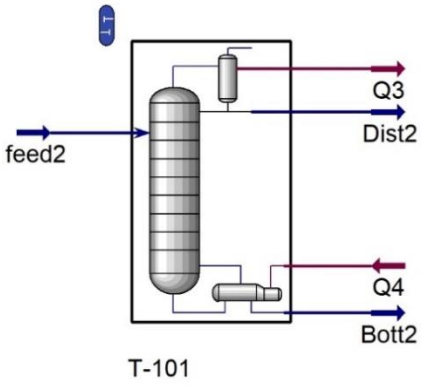

Figure 1. PFD for the process.

2.1. Aspen HYSYS Simulation

The study employed the Aspen HYSYS process simulator to create and simulate models of the separation process using both traditional and integrated (continuous distillation) methods. The diagram in Fig. 1 illustrates the model created for the traditional separation process using Aspen HYSYS. According to the illustration, the procedure utilized a single piece of equipment, specifically a distillation column. The distillation process began with a feed stream consisting of a mixture of benzene and toluene. This mixture entered the distillation unit at a temperature of 70 ^{o}C and a pressure of 1.5 bar. The mixed feed had a flow rate ranging from 1000 to 5000 kmole /hr. The mole percentage of benzene varied between 0.3 and 0.8, while the

reflux ratio ranged from 1.36 to 2.51. The NRTL fluid package (Non-Random Two-Liquid), a fluid package in Aspen HYSYS, refers to a thermodynamic model used for predicting the behavior of non-ideal liquid mixtures. was utilized for simulating the conventional process [13], [14].

The molar flow rates of the components involved in the distillation model are presented in Fig. 2. The feed material is introduced into the distillation device, which has two fundamental components: benzene and toluene. Pressure and temperature remain constant throughout the simulation process.

Table 1. Inlet and Outlet Conditions for Distillation Column.

	Column: T-101/ COL1 Fluid Pkg: Basis-1 /NRTL - Ideal			
Conditions	**Name**	**Feed2 @COL1**	**Dist @COL1**	**Bott2 @COL1**
	Vapor	0.000	0.000	0.000
	Temperature [°C]	70.00	79.25	135.4
	Pressure[bar]	1.500	1.000	2.000

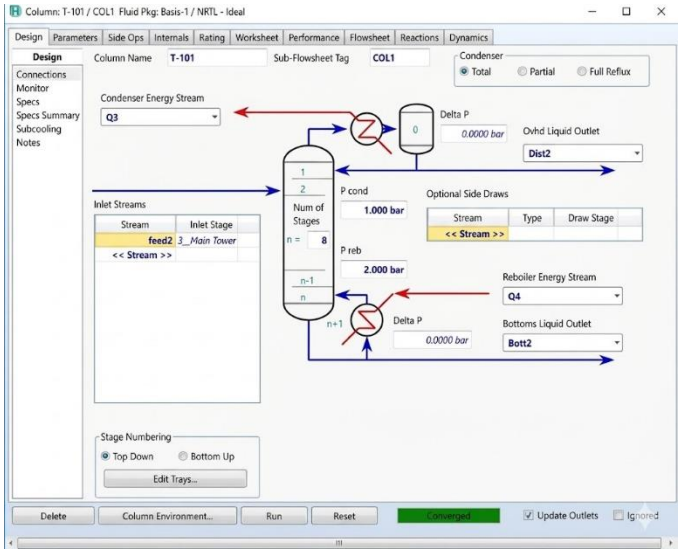

Figure 2. Aspen Hysys configuration.

The overall volumetric gas-phase mass transfer coefficient, $K_{OG}a$, is calculated from equation (2) [8]**:**

$$K_G a = \frac{u_G \rho_G N_{OG}}{h_f M} \qquad (2)$$

Where:

- $K_G a$ - Overall gas-phase volumetric mass transfer coefficient, u_G Superficial gas velocity, the gas flow rate per unit cross-sectional area of the column.
- ρ_G - Gas density.
- N_{OG} - Number of overall gas-phase transfer units (NOG), a dimensionless measure of mass transfer difficulty across the gas–liquid interface.
- h_f- Height of a transfer unit (HTU) or height factor.
- M -*Molar mass of the transferred component*, used to convert mass flux into molar flux.

To anticipate the $K_{OG}a$ value, it is necessary to have knowledge of how to estimate the vapor-side mass transfer coefficient K_{OG} and the interfacial area separately.

2.2. Artificial Neural Network (ANN) Modeling

K is crucial to the separation efficiency, and its correct prediction makes the design and operation of the column optimal. The ANN model took reflux ratio, feed flow rate, and benzene mole fraction in the feed as the input variables, which reflect the intricate interdependence existing between the operating variables and K. The model was trained using a large amount of experimental data obtained under different conditions. The ANN, with the advanced optimization algorithms of STATISTICA 12, carefully learned the complex associations of the data and was able to eventually provide high prediction accuracy of K. Such data-driven methodology can be of great benefit, versus the classical empirical correlations, which usually have difficulties with complex mixtures and operating regimes. The resulting ANN model can be useful to distillation engineers and scientists, as it can help them forecast K with high confidence and optimize the distillation processes to be more efficient and sustainable [15] [16]. The neural network is a complicated network in which the nodes perform calculations, guided by an activation function, and the links transfer signals among nodes, and each link is allocated a weight that identifies the extent to which it magnifies the signal. In the current research, neural networks are applied to perfectly fit a set of experimental data points to create a pure empirical model. Individual data points that are experimented with are known as training cases or learning cases and collectively form the training set or learning set. They include input vectors, the values of the input variables, which are related to the experimental output value of the particular neural network. It has been proposed that to avoid the premature convergence of the algorithm, periodic mutation operations might be applied [17] [18].

Lastly, an Artificial Neural Network (ANN) model was created using the Neural Network Toolbox of the STATISTICA software. Reflux ratio, feed flow rate, and benzene mole

fraction were used as input variables in the model, and the normalized K was the output variable [19].

The artificial neural network (ANN) was extensively trained to use data obtained through Aspen Hysys simulations. After 1000 iterations, five Artificial Neural Network (ANN) models were generated. The most effective of these models was that with a 3:4:1 structure (the 3 input neurons, four hidden neurons, and one output neuron), which had a training accuracy of 95.3%

3. Results and Discussion

The results are shown in Figs. 3 to 5. It is clear that the relationship between operational factors and the difficult-to-measure mass transfer coefficient (K_{OG}.a) on the elusive gas-side is complex. Fig. 3 presents the elegant pirouette of K_{OG}.a when it reaches its most impressive performance with a reflux ratio of 1.36 (Fig. 3). According to the studies made by Radev et.al. [7], Stefanov and Ivanov [8], and Yongli et al. al [6]. It is clear that the stage that has a high reflux rate, like a generous stage, can exchange vapor with liquids extensively, thus maximizing the performance of the dance. However, beyond this level seems to be unproductive, as observed by the marginal decrease of K_{OG}.a as shown in Fig. 3.

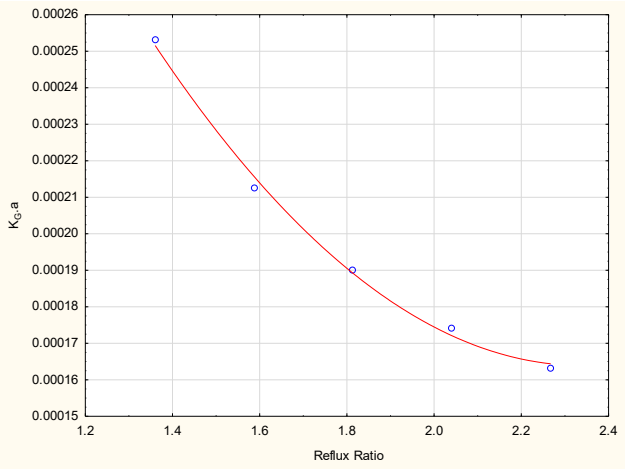

Figure 3. Correlation between mass transfer coefficient and reflux ratio at a constant feed ratio.

Fig. 4 creates another picture as it concentrates on the movement rate of the dance, which is the feed flow rate. In this case, K_{OG}.a is grooved around a moderate feed of 2000 kmole/hr. On top of this optimal pace, the bustling and the hustling become overwhelming, breaking down the harmonious transfer and causing a decrease in K_{OG}.a.

Finally, Fig. 5 introduces the captivating prima ballerina in this dynamic interplay, the benzene concentration. As her presence diminishes or intensifies, the dance falters. K_{OG}.a reaches its peak elegance at a 30% mole fraction of benzene, where the balance between the partners is just right. Deviating from this sweet spot, either to a solo act (low concentration) or a crowded ensemble (high concentration), disrupts the rhythm and leads to a graceful decline in K_{OG}.a.

These interwoven levels, revealed through Figs. 3 to 5, provide invaluable insights into the delicate interplay between operating parameters and K_{OG}.a. By understanding these subtle dances, we can fine-tune our distillation choreography, leading to a performance brimming with efficiency and elegance[20], [21].

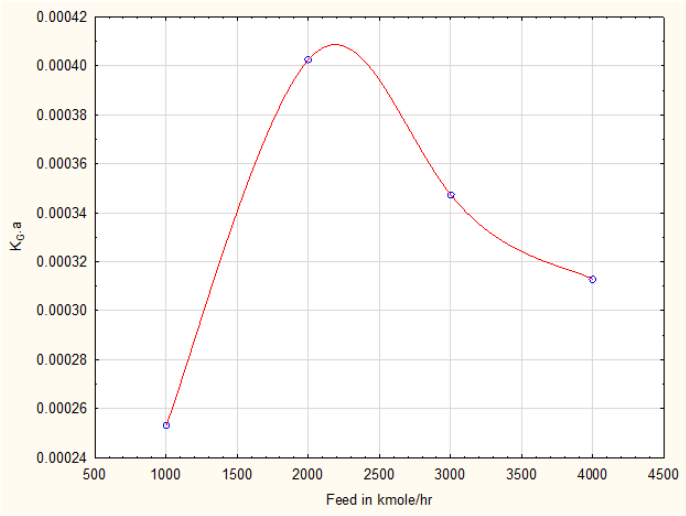

Figure 4. Correlation between the mass transfer coefficient and the feed entering the distillation at a constant reflux ratio.

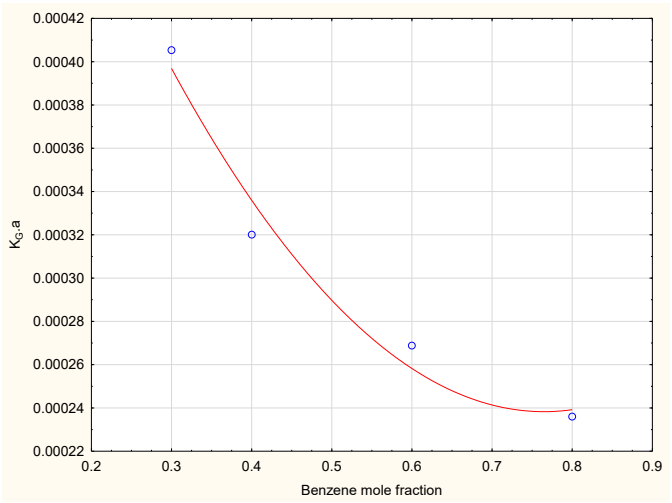

Figure 5. Interdependence between mass transfer coefficient and benzene mole fraction at constant reflux ratio.

3.1 Critical Analysis of Results

3.1.1 Reflux Ratio and $K_{OG}a$

The maximum K_{OG} at a reflux ratio of 1.36 (Fig. 3) agrees with the literature that highlights the equilibrium between the contact between the vapor and liquid and hydrodynamic stability. Hübschmann [22] established that moderate reflux ratios maximize interfacial area in a tray column, whereas excessive reflux causes entrainment, which lowers the efficiency of the mass transfer. This is in line with similar results of Coelho et al. [23] in sieve tray columns, with K_{OG}a peaking at reflux ratios of 1.2-1.5.

Billet and Schultes [24] demonstrated that structured packing is more tolerant of higher reflux ratios (e.g., 2.0-2.5) owing to better liquid distribution, implying system dependency.

The drop of $K_{OG}a$ to below 1.36 (Fig. 3) is probably due to entrainment of liquid, as Domingues et.al. [25] and Zarei et.al. [26] reported the association between flooding tendencies and reflux over-supplies in tray columns.

3.1.2. Feed Flow Rate and $K_{OG}a$

The optimal feed rate of 2000 kmol/hr (Fig. 4) is consistent with the findings of Stichlmair et al. [27], who found a trade-off between premature flooding and enhanced mixing with turbulence. Olujić et al. [28] supported this finding in the case of tray columns by observing that too high a feed rate interferes with the liquid-vapor equilibrium.

Olujić et al. [28] also established that modern structured packings (e.g., Mellapak™) maintain feed rates of 3000 kmol/hr without $K_{OG}a$ losses, highlighting hardware-specific behavior.

3.1.3. Benzene Concentration and $K_{OG}a$

The peak of the $K_{OG}a$ at 30 percent benzene (Fig. 5) is comparable to that of Poling et al. [29], which credited the benefits of benzene in mass transfer to its low viscosity and high diffusivity. Gmehling et al. [30] verified the same tendencies in that case with aromatic systems, where non-ideal interactions stabilize interfacial transfer.

Shiflett and Yokozeki [31] have reported an improved $K_{OG}a$ with >40% benzene in ionic liquid (IL)-mediated systems, whereby ILs are useful in enhancing phase separation.

At low concentrations (<10%), Sternling and Scriven [32] attributed a drop in $K_{OG}a$ to Marangoni instabilities that form chaotic interfacial structures.

3.2. Neural Network Regression

The study applied the Neural Network Toolbox of the STATISTICA software to apply a Multilayer perceptron artificial neural network to simulate the mass transfer coefficient in a tray distillation column. The input layer of the network included three variables: reflux ratio, feed flow rate, and benzene mole fraction. The output layer of the network represented the normalized mass transfer coefficient. The data obtained from the simulation was utilized to train and test the networks. After 1000 iterations, a total of 5 networks were generated.

Table 2 displays the network outcomes obtained during the iteration. It indicates that network number 3, specifically MLP 3:4:1, exhibits the highest training performance with a value of 0.953179. Fig. 6 depicts the structure of the network, whereas Table 3 displays the magnitude of the neurons' weights. Fig. 7 illustrates the correlation between the simulated outcomes and the projected results for the five networks. It is evident that the network labeled MLA 3:4:1 closely aligns with the 45-degree line.

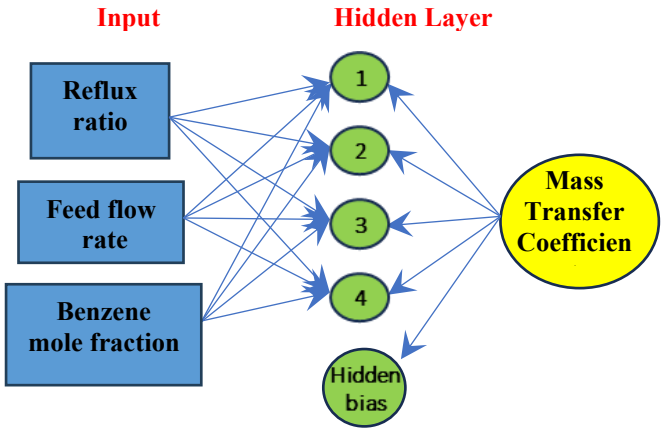

Figure 6. Architecture of the neural network.

Table 2. Neural networks.

	Net Name	Training Performance	Hidden activation	Output activation	Training algorithm
1	MLP 3-9-1	0.836069	Tanh	Logistic	BFGS 4
2	MLP 3-9-1	0.800040	Exponential	Exponential	BFGS 2
3	MLP 3-4-1	0.953179	Exponential	Exponential	BFGS 3
4	MLP 3-6-1	0.825090	Identity	Logistic	BFGS 4
5	MLP 3-10-1	0.830321	Logistic	Logistic	BFGS 2

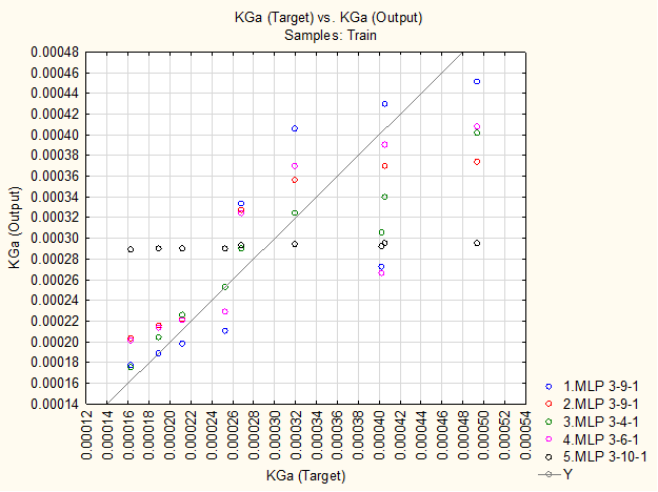

Figure 7. Simulated results versus predicted ones.

Table 3. MLP 3:4:1 weight value.

Connections 3. MLP 3-4-1	Weight values 3.MLP 3-4-1
R -> hidden neuron 1	1.14522
Feed -> hidden neuron 1	-1.32935
bz fraction -> hidden neuron 1	0.42898
R -> hidden neuron 2	0.89596
Feed -> hidden neuron 2	-3.19161
bz fraction -> hidden neuron 2	0.84556
R-> hidden neuron 3	0.12986
Feed -> hidden neuron 3	-2.1121
bz fraction -> hidden neuron 3	0.48058
R-> hidden neuron 4	1.04251
Feed -> hidden neuron 4	-2.10483
bz fraction -> hidden neuron 4	0.6298
input bias -> hidden neuron 1	-0.14529
input bias -> hidden neuron 2	0.03974
input bias -> hidden neuron 3	-0.11294
input bias -> hidden neuron 4	-0.09951
hidden neuron 1 -> KGa	-0.53334
hidden neuron 2 -> KGa	-0.21599
hidden neuron 3 -> KGa	0.35541
hidden neuron 4 -> KGa	-0.43494
hidden bias -> Kga	-0.12968

5. Conclusion

The study's goal of developing a predictive model for calculating the mass transfer coefficient in a tray distillation column was successfully achieved. Reflux ratio, feed flow rate, and benzene mole percentage were used as inputs to train an MLP model using STATISTICA's Neural Network Toolbox. With a training accuracy of 0.953179 and a near match to the 45-degree line, MLP 3:4:1 achieved the best performance among the five networks after 1000 iterations, with strong agreement between simulated and predicted values. These findings show that the ANN may accurately predict the mass transfer coefficient. To increase robustness, future studies might validate the model with experimental data and add variables to compare with other machine-learning techniques.

Acknowledgements

The authors would like to thank Al-Nahrain University (https://nahrainuniv.edu.iq/en), University of Al-Qadisiah (www.qu.edu.iq), Mustansiriyah University (www.uomustansiriyah.edu.iq), the University of Birmingham, UK, and Arden University, UK (https://arden.ac.uk/) for their support in the present work.

Conflict of interest

The authors declare that there are no conflicts of interest regarding the publication of this manuscript.

Author Contribution Statement

Shahad Z. Al-Najjar and Salih A. Rushdi conceived the idea presented in this work and collected the data.

Shahad Z. Al-Najjar, Hayder A. Alhameedi, and Zainab T. Al-Sharify worked on the paper, modeling, and developing the theory and result analysis.

Salih A. Rushdi, Zainab T. Al-Sharify, Helen Onyeaka, and Suzanne Alsamaq designed and carried out the experimental work.

All authors contributed to the final version of the manuscript.

References

[1] Z. Wei, B. Zhang, S. Wu, Q. Chen, and G. Tsatsaronis, "Energy-use analysis and evaluation of distillation systems through avoidable exergy destruction and investment costs," *Energy*, vol. 42, no. 1, pp. 424-433, 2012. doi: https://doi.org/10.1016/j.energy.2012.03.026.

[2] D. Zadravec et al., "Towards a comprehensive approach to optimal control of non-ideal binary batch distillation," *Optimization and Engineering*, vol. 23, no. 4, pp. 2111-2141, 2022. doi: https://doi.org/10.1007/s11081-022-09727-2

[3] C.-Y. Zhao et al., "A comprehensive review on computational studies of falling film hydrodynamics and heat transfer on the horizontal tube and tube bundle," *Applied Thermal Engineering*, vol. 202, p. 117869, 2022. doi: https://doi.org/10.1016/j.applthermaleng.2021.117869.

[4] S. Niazi, J. A. Díaz-López, and A. Nieto-Márquez, "Improvement of energy efficiency and production performance in a heteroazeotropic batch distillation unit: A study on decanter control and feeding strategy," *Separation and Purification Technology*, vol. 357, p. 130132, 2025. doi: https://doi.org/10.1016/j.seppur.2024.130132.

[5] H. Li, et al., "Dynamic real-time energy saving control of pressure-swing distillation based on artificial neural networks," *Chemical Engineering Science*, vol. 282, p. 119271, 2023. doi: https://doi.org/10.1016/j.ces.2023.119271.

[6] S, Yongli, Q Zhao, L Zhang, and B Jiang. "Measurement and correlation of the mass-transfer coefficient for the methyl isobutyl ketone–water–phenol system." *Industrial & Engineering Chemistry Research,* vol 53, no. 9 2014: 3654-3661.https://doi.org/10.1021/ie4036862

[7] D. Radev, D. Georgiev, D. Koleva, and M. Karaivanova, "Comparison of mass transfer coefficients determined by different methods in a distillation column with three trays," *Science & Technologies*, pp. 44-48, 2014. [Online].
Available: https://www.sustz.com/journal/VolumeIV/Number4/Papers/DianRadev1.pdf

[8] Z. Stefanov and Z. Ivanov, "Gas-liquid mass transfer coefficient in sieve tray laboratory column," *Science & Technologies*, vol. 1, no. 4, pp. 34-38, 2011.
[Online].https://www.sustz.com/journal/VolumeI/Number4/Papers/ZhelchoStefanov1.pdf.

[9] P. Pan, et al., "Bubble columns with internals: A review on research methodology and process intensification," *Chemical Engineering and Processing - Process Intensification*, vol. 209, p. 110156, 2025. doi: https://doi.org/10.1016/j.cep.2025.110156.

[10] P. Shahana, A. Jaleel, and N. Priya, "Neural network for identification of heat integrated distillation column," in *2020 International Conference on Futuristic Technologies in Control Systems & Renewable Energy (ICFCR)*, 2020, pp. 1-6. doi: https://doi.org/10.1109/ICFCR50903.2020.9249964.

[11] A. K. Singh, B. Tyagi, and V. Kumar, "First principle modeling and neural network–based empirical modeling with experimental validation of binary distillation column," *Chemical Product and Process Modeling*, vol. 8, no. 1, pp. 53-70, 2013. doi: https://doi.org/10.1515/cppm-2013-0011.

[12] H. Osman and A. Arabi, "Distillation column machine learning model controlled by optimized DMC," in *2022 22nd International Conference on Control, Automation and Systems (ICCAS)*, 2022, pp. 1184-1189. doi: https://doi.org/10.23919/ICCAS55662.2022.10003925.

[13] J. Lee, et al., "Development of the quantitative property–consequence relationship model for prediction of hydrogen leakage and dispersion using response surface method and artificial neural network approaches," *ACS Omega*, vol. 9, no. 39, pp. 40857-40869, 2024. doi: https://doi.org/10.1021/acsomega.4c05841.

[14] N. Elshaboury and M. Marzouk, "Prioritizing water distribution pipelines rehabilitation using machine learning algorithms," *Soft Computing*, vol. 26, no. 11, pp. 5179-5193, 2022. doi: https://doi.org/10.1007/s00500-022-06970-8.

[15] V. Steffen, M. Schmidt de Oliveira, and E. A. da Silva, "A systematic review of the literature on steady-state reactive distillation modeling and simulation: Challenges and opportunities," in *Solvents - Dilute, Dissolve, and Disperse - Insights on Green Solvents and Distillation*, 2024. [Online]. Available: https://www.intechopen.com/chapters/1171550

[16] N. Zhao and J. Lu, "Review of neural network algorithm and its application in temperature control of distillation tower," *Journal of Engineering Research and Reports*, vol. 20, no. 4, pp. 50-61, 2021. doi: https://doi.org/10.9734/jerr/2021/v20i417294.

[17] J. Luo, et al., "Machine learning-based predictive control using on-line model linearization: Application to an experimental electrochemical reactor," *Chemical Engineering Research and Design*, vol. 197, pp. 721-737, 2023. doi: https://doi.org/10.1016/j.cherd.2023.08.017.

[18] B, Affan, W Mulyo U, Sharifah Saon, and Arief Budi Laksono. "Optimization of coagulation process in water treatment plant using artificial intelligence: A systematic literature review and framework." *Journal of Robotics and Control (JRC)* 6, no. 5.2025. 2471-2487. https://doi.org/10.18196/jrc.v6i5.27621

[19] M. Agnese, G Boccardo, and R Pisano. "Enhancing Mass Transfer Coefficient Prediction from Field Emission Scanning Electron Microscope Images Through Convolutional Neural Networks and Data Augmentation Techniques." *Processes* 13, no. 2. 2025. 365. https://doi.org/10.3390/pr13020365

[20] M. M. May-Vázquez, F. I. Gómez-Castro, E. S. Rawlings, V. Rico-Ramírez, and M. A. Rodríguez-Ángeles, "Optimal control of a rate-based modelled batch distillation column: Initialization strategy," *Computers & Chemical Engineering*, vol. 162, p. 107811, 2022. doi: https://doi.org/10.1016/j.compchemeng.2022.107811.

[21] E.-N. Dragoi and Y. Vasseghian, "Modeling of mass transfer in vacuum membrane distillation process for radioactive wastewater treatment using artificial neural networks," *Toxin Reviews*, vol. 40, no. 4, pp. 1526-1535, 2021. doi: https://doi.org/10.1080/15569543.2020.1744659.

[22] H. J. Hübschmann, *Handbook of GC-MS: Fundamentals and Applications*. Hoboken, NJ, USA: John Wiley & Sons, 2025. [Online]. Available: https://www.wiley.com/en-gb/shop/general-chemistry/handbook-of-gc-ms-fundamentals-and-applications-4th-edition-p-9783527354030

[23] T. Coelho, O. Souza, N. Sellin, S. Medeiros, and C. Marangoni, "Analysis of the reflux ratio on the batch distillation of bioethanol obtained from lignocellulosic residue," *Procedia Engineering*, vol. 42, pp. 131-139, 2012. doi: https://doi.org/10.1016/j.proeng.2012.07.403.

[24] R. Billet and M. Schultes, "Prediction of mass transfer columns with dumped and arranged packings: Updated summary of the calculation method of Billet and Schultes," *Chemical Engineering Research and Design*, vol. 77, no. 6, pp. 498-504, 1999. doi: https://doi.org/10.1205/026387699526520.

[25] T. L. Domingues, A. R. Secchi, and T. F. Mendes, "Efficiency evaluation of valve trays with downcomer and dualflow trays of industrial distillation columns," in *Mercosur Congress on Chemical Engineering*, Costa Verde, RJ, Brazil, 2005. [Online]. Available: https://scispace.com/pdf/efficiency-evaluation-of-valve-trays-with-downcomer-and-3dwdyc37ym.pdf.

[26] A. Zarei, S. H. Hosseini, and R. Rahimi, "CFD and experimental studies of liquid weeping in the circular sieve tray columns," *Chemical Engineering Research and Design*, vol. 91, no. 12, pp. 2333-2345, 2013. doi: https://doi.org/10.1016/j.cherd.2013.03.006.

[27] J. G. Stichlmair, H. Klein, and S. Rehfeldt, *Distillation: Principles and Practice*, 2nd ed. Hoboken, NJ, USA: John Wiley & Sons, 2021. [Online]. Available: https://www.wiley.com/en-us/Distillation%3A+Principles+and+Practice%2C+2nd+Edition-p-9781119414667.

[28] Ž. Olujić, A. Seibert, B. Kaibel, H. Jansen, T. Rietfort, and E. Zich, "Performance characteristics of a new high-capacity structured packing," *Chemical Engineering and Processing: Process Intensification*, vol. 42, no. 1, pp. 55-60, 2003. doi: https://doi.org/10.1016/S0255-2701(02)00019-3.

[29] B. E. Poling, J. M. Prausnitz, and J. P. O'Connell, *The Properties of Gases and Liquids*, 5th ed. New York, NY, USA: McGraw-Hill, 2004. [Online]. Available: https://www.mheducation.com/highered/mhp/product/properties-gases-liquids-5e.html?viewOption=student

[30] J. Gmehling, Z. Xue, and T. Mu, "Reply to 'Comments on "Comparison of the a priori COSMO-RS models and group contribution methods: Original UNIFAC, modified UNIFAC (Do), and modified UNIFAC (Do) consortium"'," *Industrial & Engineering Chemistry Research*, vol. 51, no. 41, pp. 13541-13543, 2012. doi: https://doi.org/10.1021/ie3024142

[31] M. B. Shiflett and A. Yokozeki, "Solubilities and diffusivities of carbon dioxide in ionic liquids: [bmim][PF6] and [bmim][BF4]," *Industrial & Engineering Chemistry Research*, vol. 44, no. 12, pp. 4453-4464, 2005. doi: https://doi.org/10.1021/ie058003d.

[32] C. A. Sternling and L. E. Scriven, "Interfacial turbulence: Hydrodynamic instability and the Marangoni effect," *AIChE Journal*, vol. 5, no. 4, pp. 514-523, 1959. doi: https://doi.org/10.1002/aic.690050421.