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Mathematical and computational modeling of membrane distillation technology: A data-driven review

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ABSTRACT

Membrane distillation (MD) technology is increasingly gaining attention as an environmentally sustainable water treatment method of emerging interest. During last three decades there has been wide efforts to model and improve the performance of this technology. In this study we examine both the mathematical and computational modeling methods used in MD with a data-driven method. To gather the dataset, a broad range of terms related with theoretical modeling of MD were searched in the Scopus database. The collection consists of 526 documents including 116 journals, 14,291 references used by authors, 1252 involved authors and 29.47 % international co-authorship rate. The overall pattern of publications is found to increase over time indicating the enhancing interest on theoretical modeling of MD process. Journal of Membrane Science and Desalination are the top two journals publishing theoretical modeling of MD, with 105 and 100 articles, respectively. Dr. Ghaffour N. contributed with the highest number of articles, 24; and Dr. Khayet M. has the highest articles fractionalized value with 7.08. The dataset was categorized first into mathematical and computational modeling, then into the used mass transport approaches through membrane hydrophobic pores. Recently, in MD field computational modeling has been considered more than mathematical modeling. The combined Knudsen diffusion/ordinary molecular diffusion model is the dominant mass transport approach considered in MD mathematical modeling with 117 articles. On the other hand, computational fluid dynamics is the most used computational method with 114 articles.

1. Introduction

The process of understanding, quantifying, simulating, visualizing, or defining anything (usually a particular part, feature or process) using mathematical equations or other approaches like computer simulations, is known as scientific modeling [1]. Numerous scientific disciplines depend on modeling in one way or another. Scientific modeling helps human to better understand and analyze complex systems, thus it is utilized in a variety of sectors such as science, engineering, economics, and social sciences [2]. One can find in the open literature different scientific modeling approaches like toy models, mathematical (analytical) models, physical (scale) models, numerical models, computational models, conceptual models, mental models, etc.

Various types of models and simulations have been developed in membrane distillation (MD) technology of emerging interest used for water treatment. This non-isothermal separation process can produce distilled water from various sources such as seawater and wastewaters with practically zero liquid discharge to the environment since it can treat high saline solutions up to their saturation including brines and can make use of renewable energies such as solar energy and waste heat [3–6]. The applied driving force is the vapor pressure difference established between the two sides of a porous and hydrophobic membrane (e.g., single hydrophobic layer or multi-layered membrane with at least one hydrophobic layer were used). Therefore, water vapor is transported through dry hydrophobic pores following different mechanisms since different MD configurations have been considered to apply the necessary driving force (i.e., direct contact MD, DCMD; air gap MD, AGMD; vacuum MD, VMD; sweeping gas MD, SGMD, etc.) and different engineered membranes with different pore sizes have been used [7–15]. The main objectives of MD theoretical modeling and simulations is to predict the

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permeate flux of the used membranes and MD configurations, to figure out and understand the mechanism of transport of water vapor through dry membrane pores, to analyze the temperature and concentration polarization effects on the MD performance, to quantify the thermal efficiency in MD systems, to model membrane distribution and/or spacers in modules in order to prevent their wetting and improve their MD performance, to optimize the MD operating parameters in order to reduce energy consumption and increase the MD permeate water production, etc.

1.1. Mathematical modeling in MD

Mathematical modeling using both heat and mass transfer equations, are fundamental in describing and understanding the non-isothermal MD process. The involved equations incorporate complex interactions between the hot feed stream, the membrane, and the cold permeate, depending on the considered MD configuration (DCMD, AGMD, VMD, SGMD, etc.).

In general, the mass transfer of water vapor through the hydrophobic pores of the membrane is written as [16–18]:

$$J = B_m \Delta P_v = B_m \left(P_{fm} - P_{pm}\right) \tag{1}$$

where B_m is the mass transfer coefficient of the membrane, P_{fm} is the partial water vapor pressure at the feed membrane surface and P_{pm} is the partial water vapor pressure at the permeate side of the membrane.

The heat transfer through the membrane is defined as [18–20]:

$$Q_m = h_m \left(T_{fm} - T_{pm}\right) + J\Delta H_v \tag{2}$$

where, Q_m is the membrane heat flux, h_m is the membrane heat transfer coefficient, T_{fm} is the temperature at the feed membrane surface, T_{pm} is the temperature at the permeate membrane surface, J is the total permeate flux and ΔH_v is the latent heat of vaporization.

The amount of heat transferred through the membrane depends mostly on the considered MD configuration and the membrane characteristics [18,20,21]. The thermal efficiency and overall MD performance (i.e. permeate flux and separation factor) are related strongly on the heat transferred throughout the membrane module. The heat transferred by conduction, first term of Eq. (3), is heat lost through the MD process as no mass transfer is associated to this heat. Therefore, membrane modules design plays a pivotal role in achieving successful MD operations.

The Navier–Stokes equations (Eq. (3)) and the energy balance equation (Eq. (4)) are commonly used in MD modeling [19,22–25]. These equations govern the flow behavior of the involved fluids within the membrane module [23,25].

$$\rho\left(\frac{\partial v}{\partial t} + v\nabla v\right) = \nabla\tau + \nabla D \tag{3}$$

where, ρ is the vapor density, v is the vapor velocity vector, t is time, $\nabla\tau$ is the stress tensor representing viscous effects and ∇D is the diffusion tensor representing mass transfer effects.

On the other hand, the energy balance equation (Eq. (4)) accounts for heat transfer mechanisms, including conduction and convection, which are fundamental in characterizing the temperature profiles and heat exchange during MD separation process. The energy balance equation for both the feed and permeate liquids (Eq. (4)) is [26,27]:

$$\rho C_p \vec{v}\nabla T - \nabla\cdot(k\,\nabla T) = 0 \tag{4}$$

where ρ is the feed or permeate liquid density, C_p is its heat capacity at constant pressure, $\vec{v}$ is its velocity vector, T is its absolute temperature and k is its thermal conductivity coefficient.

Inside the membrane, the energy balance equation is written using the following equation (Eq. (5)) [26,27]:

$$\nabla\cdot(k_m \nabla T_m) = 0 \tag{5}$$

where, T_m is the temperature inside the membrane and k_m is the thermal conductivity of the membrane that is calculated based on the membrane porosity (ε), the thermal conductivity of the membrane matrix (k_s) and that of the vapor present inside the membrane pores (k_g).

The mathematical modeling of MD must be done based on assumptions and simplifications depending on the considered MD configuration (direct contact MD, vacuum MD, sweeping gas MD, air gap MD, etc.), membrane type (flat-sheet, hollow-fiber, dual or triple layered, etc.), model applied (e.g. Knudsen diffusion, molecular diffusion, Poisseuille or viscous type models); etc. For instance, in all MD configurations the following assumptions have been made: there is only one flow direction; there is no heat loss from the module; there is no difference in property over the whole length of the membrane (the thickness or permeability of a membrane remain the same in different regions); only vapor phase exists in the membrane pores; there is no convective heat transfer in the pores; at low concentrations the dissolved salt has little effect on the vapor pressure, velocity profile and temperature profile; and the membrane pores are cylindrical and not interconnected; there is no effect of pore size distribution on mass transfer (in mathematical modeling approaches such the Dusty-Gas model through porous media instead of the pore size distribution, the mean pore size is commonly considered) [28–31]. However, ignoring the pore size distribution effect may cause a substantial inaccuracy due to the broad distribution of the pore size of the membranes used in MD since the mass transfer mechanism changes with the pore size compared to the mean free path of the evaporated molecules [20,32]. The disadvantage of applying the Dusty-Gas model is the simultaneous occurrence of Knudsen flow and viscous flow. The contribution of each mass transfer resistance is not necessary the same for both. A more detailed model on this aspect was published for the first time by Essalhi and Khayet [33]. Surface diffusion that refers to matter transport through the membrane matrix (i.e. water transport) is generally ignored in MD, since it is believed that the affinity of water and membrane material, which is hydrophobic or even superhydrophobic, is very low. More details regarding the consideration of mass transport through membrane material in MD together with the membrane pore size distribution instead of the mean pore size can be found in this research study published by Khayet and Matsuura [34], and more detailed MD mathematical modeling reviews can be found elsewhere [17,19,32,35,36].

1.2. Computational modeling in MD

Computational models are approaches that use computers and programming languages to process information faster and more efficiently than humans. They are more complex, reliable, versatile, detailed, and can be tested on many cases. Computers can perform billions of operations per second and handle very large data sets. They can also perform complex operations automatically with programming which make these methods more useful in many systems such as energy, bioscience, geology, mining, and trade for modeling [2,37–42].

Various computational models have been developed for different MD configurations and membrane modules by means of computational fluid dynamics (CFD), response surface methodology (RSM), artificial neural network (ANN), Monte Carlo (MC), molecular dynamics simulations (MDS), machine learning (ML), etc. [43–47].

CFD is the most considered MD computational methodology since it generates predictions of fluid-flow events based on the equations governing fluid motion (i.e. Navier–Stokes equations) and conservation (i.e. conservation of momentum, mass, and energy). With CFD modeling, various modules, membranes and operational parameters design strategies have been carried and, as results, reduced temperature and concentration polarization effects and high thermal efficiencies with high MD performance were possible prior to manufacturing membrane modules and conducting tedious MD experiments. For the MD process, the CFD models can predict the pressure, velocity, temperature, and

concentration distributions throughout the whole membrane modules by solving coupled continuity, energy, momentum, and concentration transport equations [48–50]. Since, CFD modeling is based on standard mass and heat transport theories, in general, the considered assumptions and simplifications in mathematical modeling procedures are also followed in CFD modeling. However, CFD may model not only 2D but also 3D temperature profiles and fluxes of complex modules with distinct spacers and geometric configurations. The final optimal structure or flow dynamics may be obtained numerically. In fact, the majority of CFD applications in MD oversimplified the module geometry or the involved physical phenomena [19,35,36].

Response surface methodology is another approach applied for MD process optimization. RSM approach can model and evaluate a situation in which the response is impacted by several factors, define the quantitative law, and present the contribution of the variables using visual graphics and digital technologies. RSM can minimize the number of experiments while also increasing test precision. More significantly, it can investigate and display the underlying relationships of affecting elements, which is critical for understanding the complicated contamination mechanisms on membrane distillation [51–54]. MD studies employed with RSM has the objectives to optimize water productivity per unit volume of module, permeate flux, water production per unit energy consumption, regeneration performance, near-stable flux, initial flux decline, final foulant thickness, pollutant interactions, etc. For these purposes operational and configurational parameters has been investigated by MD researchers. 3D surface graphs of binary parameters have been sketched for visual verifications. RSM results indicated the interaction effects of the variables had a substantial impact on the objectives and optimum conditions can be determined using this method [44,53–56]. RSM approach is not based on any assumptions but on statistical design of experiments (DoE), in which all MD operating parameters are varied simultaneously allowing the study of the interaction effects between these parameters. The response surface models (i.e. regression models: quadratic models between the responses and the input variables) are obtained based on the collected experimental data depending on the input variables (i.e. operating parameters of MD systems). The response surface models are then tested with analysis of variance (ANOVA) and then used for optimization purposes applying different tools such as canonical analysis, Monte Carlo simulation, etc. [19,57–61].

ANOVA is a statistical tool that allows us to determine the relative relevance of various process factors that impact system performance. The traditional ANOVA method is used to assess if the outcomes of a given data or study are significant and to discard the null hypothesis (which suggests the status quo). The goal of ANOVA in optimization is to group a collection of experimental findings based on a common variable or parameter and an objective function or response. The ANOVA will then reveal how significant the variance in these data is, as well as the link between the system parameters and the system response. The selection of the 95 % confidence interval of the results in the studies has become a standard [62–65]. ANOVA can be used solely, and a complementary technique employed together with other computational modeling techniques in many MD articles. The purpose of using ANOVA in MD varies from determining the statistical significance of the operational parameters to verify the RSM results. The ANOVA applications helped researchers to determine the significance of thickness of the fouling layer on the membrane surface of two different membranes, compiling RSM results and validating the statistical significance of operational factors [53,66–69]. In ANOVA it is assumed that the measurements for all the experimental results have the same population variance. Besides it is assumed that the observations for each input setting are approximately normally distributed. Even though the ANOVA requires these assumptions it is unaffected by minor deviations from equal population variance or a normal distribution. Perhaps it is this versatility of the ANOVA method that makes it one of the most popular modeling methods among MD researchers [70,71].

Monte Carlo method is another type of computational modeling employed in MD. MC methods are computer tools for the (typically approximate) solution of mathematical problems that rely heavily on random sampling. It was initially developed by Stanislaw Ulam, John Von Neumann, and Nicholas Metropolis in the field of physics as part of the Manhattan Project during World War II. MC simulations are used to examine the model's structure and evaluate model uncertainty [72–74]. The MC method has been applied to investigate the penetration of vapor via membrane holes and to analyze heat and mass transport over hydrophobic membranes from various MD configurations such as direct contact or vacuum. The impact of diffusion mechanics was applied in the studies and the results showed very good correlation with experimental data. MC model is widely used in MD modeling because it has the ability to account for the effect of temperature polarization, membrane physical features such as pore interconnectivity, and fluid dynamic [46,75–77]. Besides, MC modeling has more realistic presentation of pore space when compared to other approaches. The drawback of MC method is that it has only validation in Knudsen mechanism [36]. MC modeling approach can theoretically include molecular diffusion through the membrane matrix, when necessary, especially when volatile organic compounds are present in the feed solutions to be treated by MD. It would be important for MD researchers to consider through MC applications the contribution of this type of diffusion to mass transport in order to achieve more accurate results [35].

Another computer modeling used in MD is molecular dynamics simulation (MDS). MDS is an atomic scale computational technique in many scientific areas, which integrates the classical equations of motion for all particles in a system across discrete time intervals. The interaction energies between the atoms and the forces exerted on the atoms play a significant role in the outcomes of MDS. The more accurate and well executed the simulation processes, the more successful the results. This technique enables the observation of microscopic features during the mobility of atoms as well as the determination of the trajectories of atomic motion. It is an effective additional tool for analyzing the outcomes of the experiment [78–81]. Due to the high computing time and spatial scale requirements, MDS have now been widely used in MD to research membrane transport and optimize membrane design, albeit primarily for nanostructures without the involvement of phase change. This method has been utilized to addressing the droplet condensation–evaporation dynamics on fibers, to provide some insight on the oil-surfactant-salt-membrane-water system's intricate relationships, and to model vapor transport through CNT. The MDS approach did a good work to reveal and optimize the vapor transport through membranes, revealing the complex interactions in an MD module and water condensation/evaporation on the surface of fibers [80,82–84]. Although the MDS method has been incorporated in MD modeling, it has not avoided some assumptions and simplifications. Some studies have adopted approaches such as choosing to use a simple mathematical equation, reducing to a single type of molecule instead of using air (which is composed of different molecules), and downscaling to increase computational speed, modifying some parameters to adjust the specified research [80,85]. Moreover, MDS in general is confined to systems with length scales of nanometers and time spans of nanoseconds [86]. However, despite these limitations, MDS which was first started to be used in the late 1950s [87], remains one of the highly preferred methods by MD researchers.

Machine learning (ML), a subset of artificial intelligence, tries to predict an outcome by extracting patterns from massive data sets, typically in the structure of an algorithm and the ML techniques are now widely used and have gained ground in many fields. The general workflow of machine learning [88] can be seen in Fig. 1. Supervised, unsupervised, and reinforcement learning are the three main categories of ML. The most popular type of ML is supervised learning, where the model is developed using labeled data (input) that has been annotated with tags that correspond to the desired outputs. Unsupervised learning trains models to find recurring patterns in the input dataset using

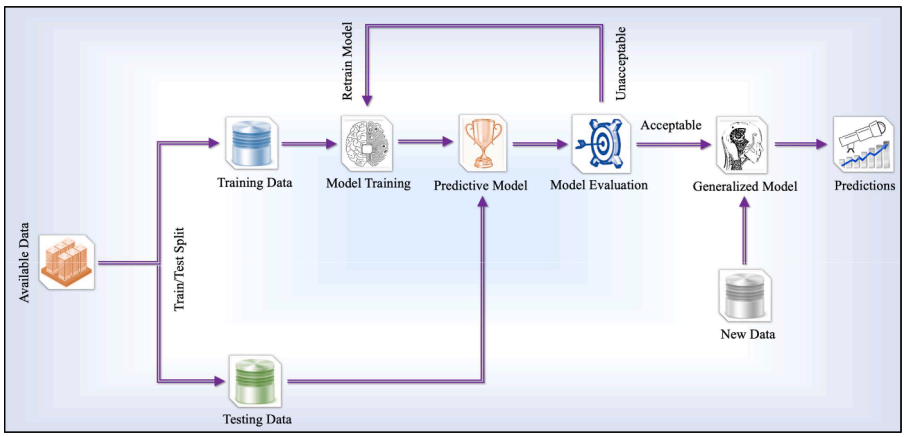

Fig. 1. Basic flow chart of machine learning.

unlabeled data. With only input data and the objective of optimizing the cumulative reward, the reinforcement learning algorithm learns behavior through trial and error [89–95]. Artificial Neural Network, which is suited to discovering challenging correlations and patterns across datasets, has grown as a strong tool in the field of ML. This popularity can be due to ANN's ability to interpret complicated patterns [96]. The use of machine learning in MD is recognizable. The use of machine learning in MD domain can assist to identify the key elements, identifying the impacts of operating parameters on membrane fouling, performance, etc. in MD configurations such as sweeping gas, direct contact, air gap and vacuum. The results of the studies show how important the use of machine learning in the MD domain is and that ML can be very useful in understating the dynamics of MD processes [45,47, 97–99]. ML has started to surpass other computational methods in versatility and computational power. ML also offers better performance, less coding, less human intervention, and more general solutions. For example, RSM can draw a 3D response surface by performing multiple response analysis to study not only the effects of the input variables on the response but their interaction effects. While this requires multiple response analysis, ML approaches (tree-based, linear, sample-based, support vector machines) can be used to estimate the relative contribution of all input variables affecting the system to the output variable in just a single analysis. ML can apply a multidimensional regression and does not need to have a complex physical analysis of an MD system. In general, to date ML is the most efficient method for optimization. Although ML techniques are considered to be state of the art modeling methods, it should be noted that, the size of the data set, the accuracy of the data, the type of data, the division of the data (training/test/validation sets) and the pre-processing of the data are important factors affecting the accuracy of the application [36,100].

Accurate modeling with mathematical and/or computational approaches enables MD researchers to evaluate the overall MD system performance, predict permeate fluxes, and optimize operating conditions to ensure sustainable and efficient MD processes for addressing global water scarcity challenges [24].

This paper is a data-driven review that addresses recent research statistics of mathematical and computational modeling of MD. Unlike traditional review, a data-driven review, also known as data mining, has a clearly stated purpose and a specified search approach with inclusion and exclusion criteria. A data-driven review is objective, balanced and impartial, and determines the emphasis and scope of the interested domain [101,102]. This data-driven review employs data analysis, data mining and bibliometrics. Due to the large number of publications in MD modeling, a data-driven review is a needed to provide a critical evaluation of the publications. The analysis of this research reveals the development and trends of mathematical and computational modeling of MD over time, as well as the methods used by researchers. There isn't a one ideal modeling strategy that works well in every situation, MD configuration or MD application; but depending on the modeling goals, there ought to be a best strategy to follow. The work carried out by researchers to fully understand the dynamics of MD and to develop more efficient systems continues unabated. Despite the ongoing intensive efforts in both the scientific community and industry, the modeling approaches applied to understand the dynamics of the MD method have not reached the ultimate goal, which is to make MD a worldwide leading and industrial separation process. This research provides a comprehensive assessment of the current state of knowledge with a coherent synthesis and classification of MD modeling approaches, which systematically identifies gaps to be overcome for the improvement of this technology. In general, modeling processes are based on assumptions and simplifications, because a holistic approach to model a system requires funding, manpower, know-how, computational power, etc. One of the impacts of the results of this data driven review is to reveal important information such as leading scientists, approaches, resources in the MD modeling domain and to encourage collaborations to enable holistic modeling of MD. The findings also allow membrane researchers to track which modeling approaches are used more, which are trending, modeling efforts on membrane configurations, and modeling gaps that need to be filled in the literature.

2. Methodology

In order to collect all MD articles a search was carried out in the Scopus database on 13.07.2023 using a broad spectrum of keywords. The main reason for selecting Scopus database for the present study are that it covers many major publishing organizations, meets the requirements of indexing, and has more content than other databases [103]. Our search criteria were as follows: "a membrane distillation term" AND "a modeling term". In this case AND is an operator. Membrane distillation terms used are: membrane distillation, MD, transmembrane distillation, pervaporation, capillary distillation, membrane pervaporation, thermopervaporation, direct contact membrane distillation, DCMD, air gap membrane distillation, AGMD, sweeping gas membrane distillation, SGMD, sweep gas membrane distillation, membrane air stripping, MAS, vacuum membrane distillation, VMD, vacuum enhanced membrane distillation, VEMD, permeate gap membrane distillation, PGMD, liquid gap membrane distillation, LGMD, water gap membrane distillation, WGMD, conductive gap membrane distillation, CGMD, material gap membrane distillation, MGMD, thermostatic sweeping gas membrane distillation and TSGMD. Modeling terms used are: Knudsen, molecular diffusion, transition, free molecular flow, viscous, Poiseuille, ordinary molecular diffusion, numerical model, convective transport, convective, convection, diffusive transport, diffusive, diffusion, Navier–Stokes, surface diffusion, energy balance

equation, Darcy, Knudsen–viscous, theoretical modeling, mathematical modeling, computational modeling, data-driven modeling, modeling, dusty gas model, Stefan–Maxwell, Stefan diffusion, mathematical modeling, numerical simulation, simulation, Brownian, Nusselt number, computational fluid dynamics, CFD, response surface methodology, RSM, Monte Carlo, machine learning, ML, neural network, artificial neural network, ANN, deep learning, supervised learning, unsupervised learning, reinforcement learning, analysis of variance, ANOVA, and molecular dynamics simulation, MDS. Additional refinement criteria were also applied to improve the processability of the collection. These are, document type: article, publication stage: final, source type: journal, language: English. After the data set was obtained, it was manually reviewed, and irrelevant data was deleted. After carrying out all filtering operations the collection contained 526 articles.

Manual and software-based approaches were used to uncover the hidden and significant statistical values in the MD collection. Some figures were created with Flourish online studio (https://flourish.studio). R programming language was the main source for the data analysis. In R, Biblioshiny (Bibliometrix) and ComplexUpset libraries were utilized. Massimo Aria and Corrado Cuccurullo created Biblioshiny, a program that offers the full complement of tools required for scientific stats workflow to carry out a thorough bibliometric analysis [104]. ComplexUpset library is a very useful tool for visualization of intersecting sets with its additional features [105]. The methods followed in the calculations are as follows [106,107];

The average citations per document (*ACD*) value of the dataset was calculated as:

$$ACD = \frac{TC}{ND} \tag{6}$$

where *TC* is the total number of citations of the documents, and *ND* is the total number of documents. The co-authors per document (*cAD*) of the dataset was determined with the following equation:

$$cAD = \frac{AA}{ND} \tag{7}$$

where *AA* is the authors appearances. For this index, the number of authors in each article is averaged. Besides repeated author names are taken into consideration.

The international co-authorship (*IcA*) value of the dataset can be computed as in Eq. (8):

$$IcA = \frac{MCP}{ND}\ x\ 100 \tag{8}$$

where *MCP* is the multiple country publications.

The times cited per year (*TCY*) value of a document is calculated as:

$$TCY = \frac{TC_n}{DA_n} \tag{9}$$

where TC_n is the total number of citations of the document *n* and DA_n is the age of the document *n*. DA_n is determined as $(Y_f - Y_n)$ in which Y_f is the year of the collected dataset, Y_n is the publication year of the document *n*.

The normalized average citations (*NAC*) of a collection can be determined with Eq. (10):

$$NAC = \frac{\sum_1^n TCY}{ND} \tag{10}$$

The articles fractionalized (*AF*) value of an author can be computed as follows:

$$AF = \sum_{i=1}^{m} \frac{1}{N_{cad}} \tag{11}$$

where *m* is the number of co – authored documents of an author and N_{cad} is the number of co – authors in the corresponding document.

3. Results and discussions

The main statistical details of the 526 documents in the collection are given in Table 1.

The dataset covers 37 years of modeling efforts carried out on MD separation process. It started with the first article published on mathematical modeling of MD entitled "Heat and mass transfer in membrane distillation" published by Schofield et al. in 1987 [108]. In this study experimental research was conducted to establish and validate equations for heat and mass transport in MD. The temperature polarization phenomenon was presented and demonstrated for the first time for a better understanding experimental result. Combining Knudsen and molecular diffusion was a reasonable approach to describe vapor transport through dry and hydrophobic membrane pores [108].

A total of 116 sources (i.e., journals) were registered in the collected dataset indicating that the MD application area is extremely wide and diversified. This also suggests that the MD modeling field is multidisciplinary, or it includes a wide variety of branches. The average number of citations per document is 34.73, which is a proof of a dynamic research area with a considerable influence on following research studies. The documents in this topic are well-founded and supported by prior literature, and the publications are extensive and thorough, as attested by the 14,291 references. With 1252 involved authors in MD modeling, the field clearly has a sizable and vibrant research community. It was found only12 single-authored documents, indicating that teams or groups of researchers, rather than lone researchers, conduct research on MD modeling. The average number of co-authors per document is 4.07, showing that the research studies in this area was generally performed by teams or groups of researchers. This could also suggest that the study in this area is diverse or interdisciplinary and that the researchers' backgrounds and expertise are quite wide. The reasonably good number of international co-authorships, 29.47 %, confirmed the considerable amount of international cooperation and exchange of knowledge in this field of research. The gradual increasing trend of the annual publications on MD modeling studies can be seen in Fig. 2.

Fig. 2 shows that the interests on theoretical modeling of MD, both on mathematical and computational modeling, is expanding worldwide and drawing more attention of MD researchers. Only during the last year, 2022, it was collected 54 publications, which is the highest number throughout the whole dataset timespan. Note that 2023 covers only a 6-month period, but the trend of publications clearly shows that by the end of 2023, the number of articles involving mathematical and computational modeling may exceed the number of articles published in 2022. Some years, 1989, 1992 and 1995 appear without any publication, while during the last decade, 2013–2023, a total of 382 articles have been published with and an average of 38.2 publications per year. This indicates that 72.6 % of all articles in the dataset were published during the last decade. This might be attributed partly to the progress of computational approaches and software. In a recent published article [103], it is reported that the number of publications in the whole MD domain experienced a significant increase, especially since 2012. The positive breakthroughs in the mathematical and computational modeling of MD are seen also during the same period. Therefore, it is

Table 1
Main information about the collection.

Timespan	1987:2023
Sources (Journals)	116
Average citations per document	34.73
References	14,291
Authors	1252
Single-authored documents	12
Co-Authors per document	4.07
International co-Authorships (%)	29.47

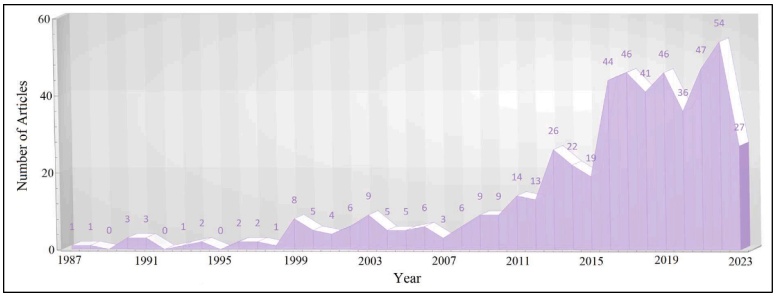

Fig. 2. Yearly published MD modeling articles.

obvious that there is a correlation between MD publications and MD modeling studies. The obtained data also reveals some notable peaks or fluctuations in the number of publications over various years. This can be due to various reasons such as the variation in received funds, policies, technologies and materials advances, organized conferences and congresses, collaborations, etc.

Journals that publish a large number of articles on a given topic can be called core journals. Fig. 3 shows the top 10 journals where MD modeling research studies have been published.

The top two journals in the dataset, with 105 and 100 articles each, are Journal of Membrane Science and Desalination, respectively. These two journals are identified as the most outstanding and suitable for communication of this subject with ~39 % of published articles in the dataset since both the heat and mass transport are carried out through porous membranes and desalination is the most appropriate application of MD technology. Desalination and Water Treatment, the third journal in the collection, published 54 articles. Although there are 116 journals publishing articles on MD modeling, most publications are concentrated in the above mentioned three specific journals.

The page count and cited by values of the published articles were visualized with box plot integrated into beeswarm plot. The results can be seen in Fig. 4. Note that 76 articles did not have the page count information when retrieved from the source.

The page count values range from 1 to 69 with a mean of 10.4 and a median of 10. The most frequent value is 10, which occurs 45 times. The page count figure is skewed to the right, which means that while some numbers are significantly higher than the average, most values are at low page count. The obtained data in this study can be compared to those published [109], on the whole MD literature to figure out both the global and local subjects in MD, although there is a difference of about 6 months in terms of annual coverage. The average page count value of the articles in the entire MD domain was found to be 11.10, which means that theoretical modeling articles is shorter than the average page count of MD articles. A regular MD article is between 8 and 12 pages, which is equal to that in MD modeling. Besides, the median values are the same for both. The cited by values range from 0 to 592, with a mean of 32.6 and a median of 17. The most frequent value is 0, which occurs 37 times indicating that these articles have not received citations yet. However, the average publication year of these articles is ~2022. Since these articles were published recently, it is obvious that it is early to receive citations. Similar to the page count, the cited by plot is also highly skewed to the left (i.e., most articles are clustered at low citation value, while a few articles are cited much higher than others). Again, if we compare the cited by values of this dataset with the results reported elsewhere [109] the mean value of times cited found when analyzing the whole MD domain is 32.76, which is very close to that found in the present MD modeling collection (i.e., 32.6). Besides, the median value of the whole MD dataset is 16, which is lower than that of this MD modeling collection (i.e., 17).

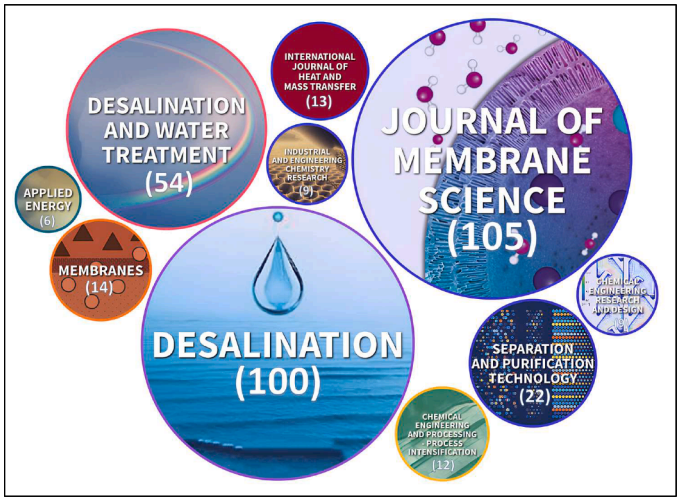

Fig. 3. Top 10 journals considered for MD modeling publications.

Knowing the top authors in an area may help the readers to keep up with new findings and advancements, locate trustworthy sources of knowledge and inspiration, and uncover fresh angles and ideas. The top 10 authors of MD modeling research studies based on the number of publications are listed in Fig. 5.

From Fig. 5 it can be seen Dr. Ghaffour N. contributed with the highest number of articles (24). This means that he is the most productive and active author in MD theoretical modeling research field. Dr. Khayet M. comes second with 19 published articles and Dr. Zhang J. ranks the third with 14 published articles. Fractionalized articles are a method of quantifying each author's contribution to a publication by splitting credit evenly among all coauthors of the same publication. When evaluating the productivity or influence of various authors or organizations, the value of fractionalized articles is important for preventing any possible double-counting of publications [110]. Considering the calculated fractionalized values, the highest (7.08) belongs to Dr. Khayet M. and this result reflects that he often publishes with less co-authors than the other researchers that appear within the top 10 authors.

Citations analysis is an effective way of identifying a research work's origins and impacts. it may show the significance and relevance of a certain article within its field of research. It was claimed that the top features of a highly cited articles is summarized as, a title of 7–13 words that includes some common terms, an article with more than 33,600 characters, including references (about 5600 words), six authors or more, and at least six figures and two tables [111,112]. Fig. 6 shows the top 10 articles based on their total citations.

As it is indicated in Fig. 6, Journal of Membrane Science published 9 of the top 10 articles. The journal Desalination published only 1 article among the top 10. The most cited article in the dataset with 592 citations is the first published paper by Schofield et al. [108] in 1987 on modeling of MD entitled "Heat and mass transfer in membrane distillation". Although this is the most cited article, considering the publication year of the articles, the most cited one on an annual basis is Qtaishat et al.

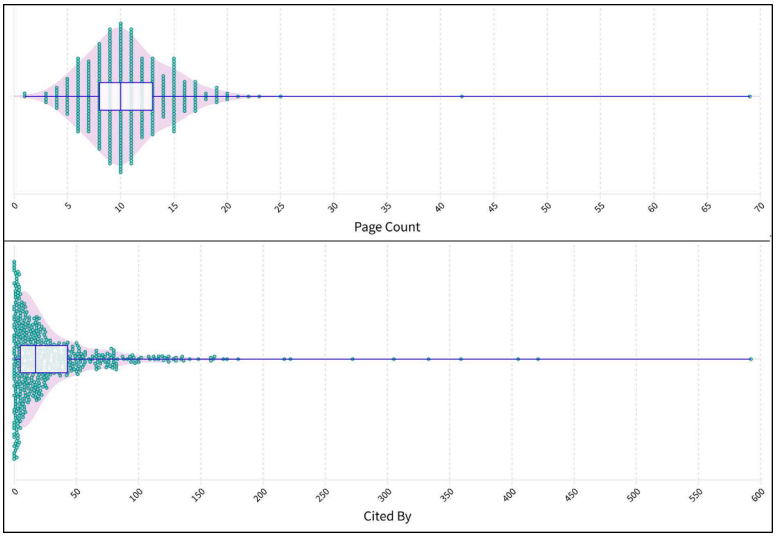

Fig. 4. Box plot integrated besswarm graph of page count and cited by values of the MD modeling collection.

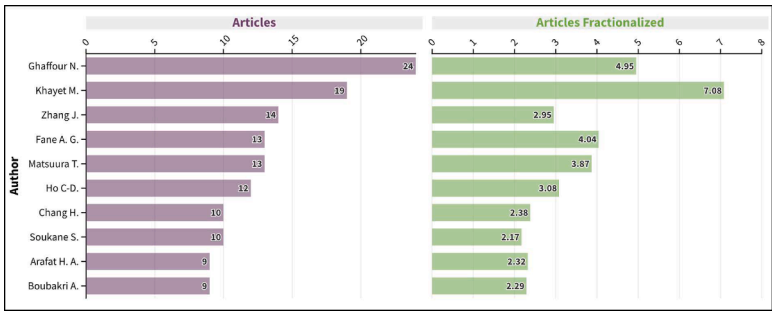

Fig. 5. Top 10 authors based on the published number of articles.

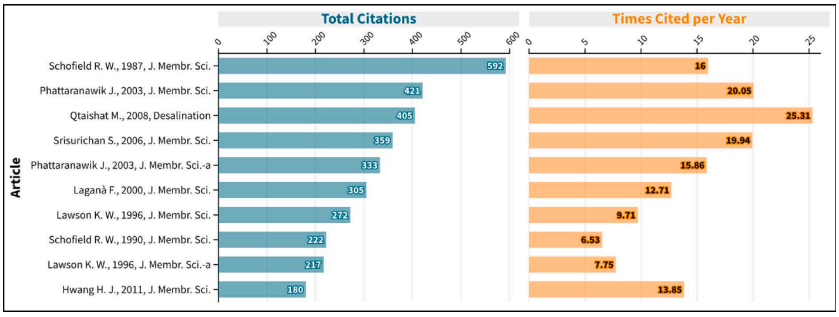

Fig. 6. Top 10 articles based on their total citations.

[113] entitled "Heat and Mass Transfer Analysis in Direct Contact Membrane Distillation", with a value of 25.31 citations/year. This indicates that if the trend continues this way, Qtaishat M.'s article will become the most cited one in the near future. In this study a complete and comprehensive research on heat and mass transfer in DCMD. It was found that mass transfer influenced the heat transfer flux in the feed thermal boundary layer, across the membrane, and through the permeate thermal boundary layer. To analyze the experimental results of the thermal boundary layers' heat transfer coefficients, membrane/liquid interface temperatures, temperature polarization coefficient, membrane mass transfer coefficient, and evaporation efficiency, a mathematical model was developed and numerically computed. It was claimed that the mass transfer contributed significantly to the total heat transfer only in the membrane area, whereas it was insignificant in both the feed and permeate boundary layers. The membrane conductive heat transfer coefficient was determined utilizing a trial-and-error technique in tandem with the solution of the proposed model equations [113].

As stated in the Introduction section, MD separation process is classified into four main variants based on the way the permeate is collected (DCMD, SGMD, AGMD, VMD) [8]. The advantages and drawbacks of these configurations were reviewed elsewhere [7]. Briefly the advantages and disadvantages of these MD configurations can be summarized as follows:

- DCMD – *Advantage:* reasonably high flux, simple design and operation. *Disadvantage:* low non-volatile rejection, high conductive heat loss.

- SGMD – *Advantage:* high flux, low conductive heat loss. *Disadvantage:* high costs, necessity for large condenser.
- AGMD – *Advantage:* low heat loss, high non-volatile compounds rejection, low membrane wetting. *Disadvantage:* relatively low permeate flux, high mass transfer resistance.
- VMD – *Advantage:* high flux, negligible heat loss. *Disadvantage:* high risk of membrane wetting [7].

MD researchers are still looking for the appropriate designs of the MD configurations through the improvement of engineered membranes and modules. The majority of the proposed designs suffer from the low thermal efficiency, low permeate flux, membrane wetting and fouling among others as well as scale-up difficulties. Recent configurations such as vacuumed air gap membrane distillation (VAGMED), sub-atmospheric AGMD, conductive gap or material gap membrane distillation (CGMD or MGMD), permeate gap, liquid gap or water gap membrane distillation (PGMD, LGMD or WGMD), flashed-feed-VMD, vacuum-enhanced membrane distillation (VEMD) and vacuum multi-effect membrane distillation (V-MEMD) are all hybrid MD configurations trying to enhance their MD performance [114]. In this research we investigated the mathematical and computational modeling of different MD configurations using an upset plot. When representing the intersections of numerous sets, which is difficult to perform using conventional techniques, an upset plot is very helpful [103]. The resulting upset plot is shown in Fig. 7.

As can be seen in Fig. 7, the most modeled configuration is DCMD. This is expected since DCMD is the most considered configuration from experimental standpoint and the DCMD set-ups exhibit a relatively more simple operation provided that both water evaporation and condensation are carried out at both sides of the membranes pores [115]. In total 197 articles deal with DCMD theoretical modeling. Among these articles, 187 were devoted only to DCMD, while 5 also included AGMD (i.e. DCMD and AGMD) [48,116–119], 3 incorporated VMD (i.e. DCMD and VMD) [120–122], and 1 article also involved LGMD (i.e. DCMD and LGMD) [123]. It was found that one article included the 3 configurations, DCMD, AGMD and VMD [124]. It can be seen in Fig. 7 that VMD is the second configuration most modeled with a total of 97 articles. VMD was mentioned 3 times in the same article with DCMD [120–122], 2 times with AGMD [125,126] and 1 time together with both DCMD and AGMD [124]. The least modeled configurations were found to be the hybrid TSGMD and MGMD with one time each [127,128]. This is attributed partly to the fact that these two MD variants are generally least considered in MD. TSGMD is a hybrid configuration combining both AGMD and SGMD as the inert gas that flows through the permeate side of the membrane is cold down by a cooling surface increasing therefore the driving force through the membrane module length and improving the permeate flux as consequence [129]. The third MD configuration that has been mathematically and/or computationally modeled is AGMD with a total of 76 articles. Among the main MD variants, few theoretical models were developed for SGMD (10 articles). In general, this configuration also received very few experimental attentions since inert gases are involved to carry out the produced water vapor and condensation takes place outside the membrane modules. The most striking point in Fig. 7 is that there are very little attempts have been made to model TSGMD and MGMD processes, and even there is a lack of comparison of MGMD with other MD configurations. Fig. 7 also indicates the years of the published MD studies. From the annual distribution of MD configuration-based publications, the light green color (≥2017) is by far the most dominant in most columns. This confirms that most of the developed MD theoretical models have been conducted during last 6 years. The fact that only the mathematical and computational modeling of LGMD, and LGMD together with DCMD articles were published since 2017, is also an indication of the importance attributed to LGMD and the need to understand its links with the main configurations. Both SGMD and MGMD are not very popular among MD scientists. Therefore, mathematical, and computational modeling of these configurations have not been studied much. The most important conclusion to be drawn from Fig. 7 is that a general theoretical model valid for the four MD main configurations has not yet been developed.

After the overview of the whole dataset, the mathematical and computational modeling articles were categorized, and the obtained number of articles were found to be 285 and 241, respectively. Fig. 8 shows the number of articles published each year for each theoretical modeling methodology.

As can be seen in Fig. 8, mathematical modeling of MD has been considered since 1987 [108], whereas computational MD modeling started much later, in 2004, with the publication of the first article by Imdakm and Matsuura entitled “A Monte Carlo simulation model for membrane distillation processes: Direct contact (MD)” [46]. Since then, computational modeling has attracted a lot of attention in MD research

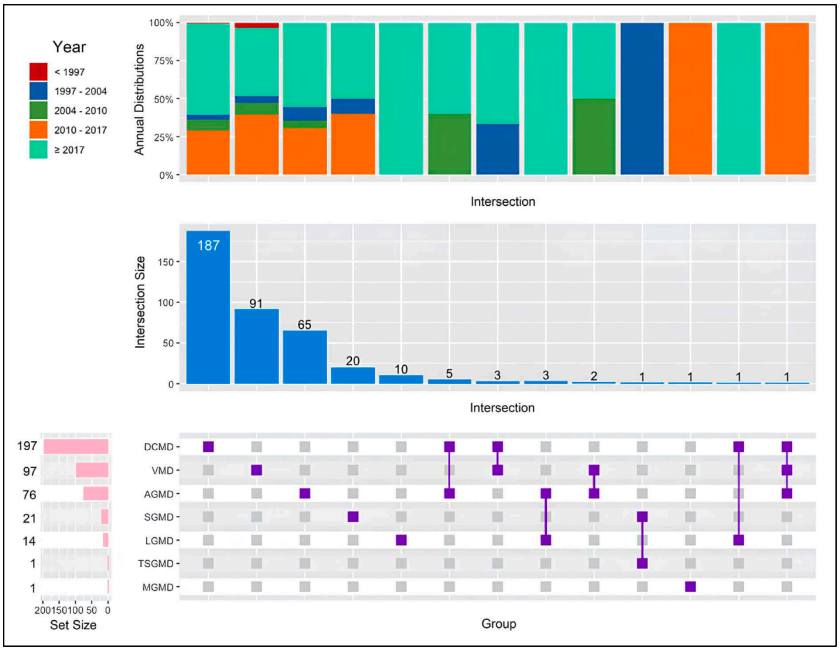

Fig. 7. Upset plot of modeling of different MD configurations.

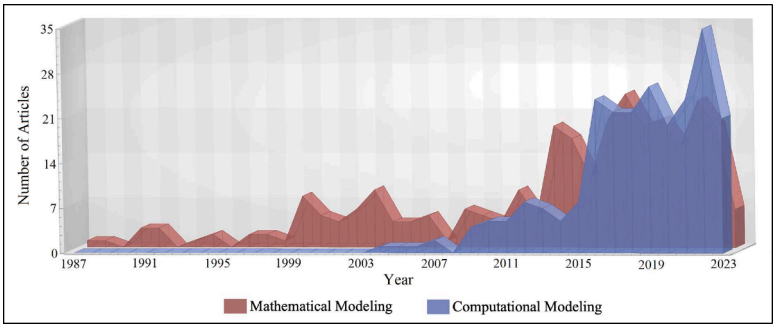

Fig. 8. Yearly publications of the mathematical and computational MD modeling approaches.

field. For instance, during last 8 years the number of published articles focused on computational MD modeling surpasses those developed considering mathematical MD modeling. Besides, the average age of the published articles using computational models, 4.40, is much lower than that of the articles focused on mathematical models, 9.87. This result is understandable because the generation and accessibility of large volumes of data together with the incredible advance of computer technologies (i.e., huge increase in CPU and GPU based computational power). The number of mathematical modeling articles published in 2017 is 24, whereas that of computational modeling articles published in 2022 is 35. However, the question is: what are the average number of citations? While the computational modeling articles has an average of 34.83 citations, the mathematical modeling articles has an average of 44.39 citations. This result may be misleading because the articles devoted to mathematical modeling started to be published earlier (from 1987 onwards) than those of computational modeling. Therefore, it is normal for the mathematical modeling articles to receive more citations than the computational modeling. It would be more explanatory to examine the normalized average citations (NAC) values. The NAC of the mathematical modeling collection is 4.50 whereas that of the computational modeling collection is higher, 7.05. This indicates that the computational approaches are more popular within the MD researchers than the mathematical models. The Journal of Membrane Science is ahead of Desalination in publishing articles containing mathematical methods with 75 and 58 published articles, respectively. However, the opposite occurs for the publication of computational modeling articles, finding that Desalination is ahead of Journal of Membrane Science with 42 and 30 published articles, respectively.

A general classification of both mathematical and computational modeling methods has been conducted to further elaborate the analysis of the collected MD modeling dataset. The results are illustrated in Fig. 9.

As can be observed in Fig. 9, mathematical modeling approaches can be categorized into 10 distinct groups. The most prevalent approach is the utilization of the combined Knudsen diffusion/ordinary molecular diffusion model (or Bosanquet equation [33]) for water vapor transport through porous and hydrophobic pores in MD, with a total of 117 published articles. Depending on the MD configuration, the applied mean temperature and the pore size of the used membrane, Knudsen diffusion flow model, molecular diffusion model (i.e., Brownian diffusion model) and viscous or Poiseuille flow model or the combination between them have been considered [17,20]. The Knudsen diffusion model is used to model mass transfer processes through membrane pores whose size is smaller than the mean free path of water vapor molecules, describing the resistance imposed by the membrane structure in absence of air. Its combination with the diffusive ordinary molecular model in presence of air (e.g. in DCMD configuration) or with the viscous model for large membrane pores and when a hydrostatic pressure difference is applied between the feed and permeate (e.g. VMD configuration) describe the mass transport of membranes subjected to different conditions.

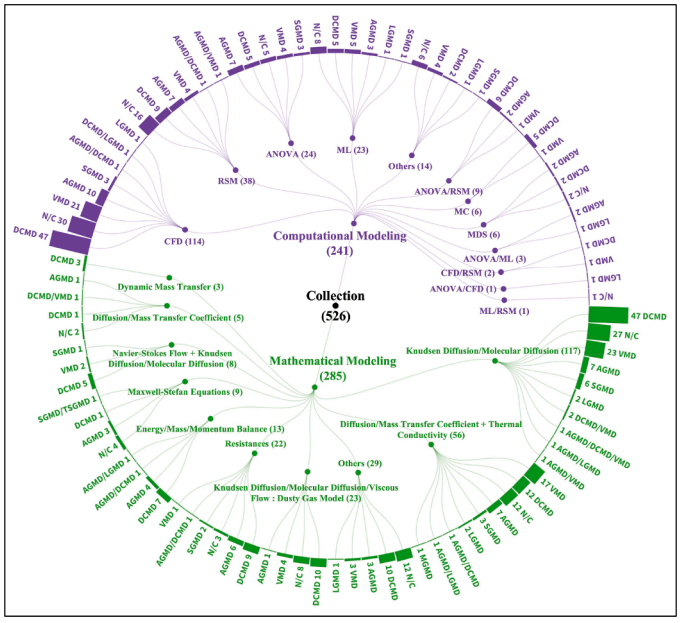

Fig. 9. Categorization of mathematical and computational modeling approaches (N/C denotes none categorized MD configuration).

While a significant portion of model development has been concentrated in the domain of mass transfer relevant to MD processes, thermal process modeling had also been subject to meticulous scrutiny. Other categories encompassed convective heat transfer, mass transfer coefficient/diffusion + static thermal conductivity and Brownian motion, heat transfer, heat transfer: dynamic model, heat transfer: Fourier's law, Maxwell–Stefan equations, Dusty Gas Model (i.e. general model based on kinetic theory of gases through porous media). These categories merged the development of both mass and heat transfer models. Once again, the DCMD configuration emerged as the most studied by all models, except within the category of mass transfer coefficient/diffusion + thermal conductivity, where the VMD configuration ranked first with 17 publications. These two configurations, DCMD and VMD along with AGMD, encompassed ~91 % of the investigated MD modeling literature, marking them as configurations of paramount interest to MD researchers.

Among the categorization of computational models used in MD, CFD is dominantly ahead of other techniques with a total of 114 published articles. Almost all configurations, especially DCMD that has been considered in 47 articles, have been analyzed by means of CFD modeling [130–132]. Response surface methodology (RSM) is the second most preferred approach in computational modeling contributing with a total of 38 articles [133–135]. Interestingly SGMD configuration has not been evaluated yet by MD researchers. The ANOVA approach was also considered in the optimization of MD separation process mainly

together with RSM modeling [136–138]. Recently, Machine Learning (ML), the hot topic of the present century, has been applied in MD process. Very limited number of studies, 23 published articles, have performed MD simulation using ML [139–141]. ML is a fast-expanding approach that it will continue to play an increasingly crucial role in science and technology in the future including in MD research field. Therefore, it is important for the future of MD that membranologists already start applying different applications of ML (classification, clustering, object detection, natural language processing, forecasting, etc.) in their research domains. Others class include proportional–integral control algorithm, multi-component simulation, CHEMCAD simulation, Aspen Custom Modeler simulation, Engineering Equation Solver simulation, etc. It is obvious that more inclusion of such neglected methods in the literature would be helpful in understanding and clarifying some unsolved issues in MD technology. It was also found that Monte Carlo simulation was used for DCMD and VMD and not for other configurations [75,76,142] Likewise molecular dynamics simulation approach was only applied in 2 configurations, DCMD and AGMD [80,83,143,144]. It is seen in Fig. 9 that there are articles where more than one computational modeling was applied, and process dynamics were explored. Multiple computational modeling approaches such as ANOVA/ML, CFD/RSM, ANOVA/CFD, ML/RSM have been applied in a limited number of cases for some of the basic configurations [145–148]. It is important to further investigate the application of such comparative or complementary computational modeling, since very little studies have been done on these topics. More accurate and reliable results may be obtained in the MD field. As a future perspective, all modeling approaches in the literature can be used to evaluate the thermal energy cost and electricity cost depending on the operating conditions. However, MD modeling processes need to be a reference for the industrial use of MD with a holistic approach, taking into account the costs arising from investment, maintenance and pre-treatment [19].

4. Conclusions

MD is gaining popularity as an environmentally and economically sustainable method for water treatment especially for desalination. There has been an increasing effort in theoretical modeling MD to understand mass and energy transfer and to improve the process's performance. This study uses a data-driven approach to investigate the mathematical and computational modeling of MD to reveal the state of the literature. On July 13, 2023, 526 documents dealing with theoretical MD modeling were found in the Scopus database. The dataset consists of 37 (1987–2023) years of modeling effort. 116 different journals have been involved in the publication of these documents. The collection includes 1252 authors, and 29.47 % international collaboration demonstrated that the field is quite broad and influential.

The overall pattern of publication has been observed to increase over time especially after 2012. The top two journals publishing MD modeling are Journal of Membrane Science and Desalination, with 105 and 100 articles, respectively. Dr. Ghaffour N. has published most articles (24) and Dr. Khayet M. has the highest article fractionalized value (7.08). Journal of Membrane Science published 9 of the top 10 articles. Schofield et al.'s publication [108] received the highest number of citations (592). With 25.31 citations per year, Qtaishat et al.'s study [113] is the most cited article on an annual basis. In total, 197 articles deal with DCMD modeling. VMD was discovered to be the second most modeled configuration, with a total of 97 articles. According to the upset plot, most of the theoretical modeling efforts have been conducted recently after the year 2017.

It was observed that computational modeling efforts have attracted more attention than mathematical modeling during last 8 years. When the end-leaves (approaches used in mathematical and computational modeling) were examined, it was found that in mathematical modeling the combined Knudsen diffusion/ordinary molecular diffusion model is the most considered (117 articles) being the DCMD configuration the most considered (47 articles). It is obvious that the dynamic mass transfer and diffusion/mass transfer coefficient approaches have been somewhat overlooked in mathematical modeling of MD. In computational MD modeling, it was observed that CFD is the most considered technique in almost all configurations, especially DCMD. RSM is the second most preferred approach, but SGMD configuration has not been evaluated yet with RSM. MC simulation and MDS are only applied for some MD configurations (DCMD, AGMD, VMD). Multiple computational modeling approaches (ANOVA/ML, CFD/RSM, ANOVA/CFD, ML/RSM) are used in a limited number of cases for some of the basic MD configurations, but their benefits and challenges should be discussed further. MD is a separation process of emerging interest with applications in various environmental fields (treatment of brines, industrial wastewaters, use of waste heat and renewable energies, production of pure water for hydrogen production, etc.). Continued research and development in MD modeling to better understand the mass transfer, the effects of different operating parameters, the different membrane structures, the temperature and concentration polarization phenomena, etc. on the MD performance (i.e. permeate flux and rejection factor), thermal efficiency, fouling and scaling among others, will improve the potential of MD as a leading sustainable and effective water treatment solution, especially for the separation on non-volatile solutes from water such as in desalination.

CRediT authorship contribution statement

Ersin Aytaç: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Jorge Contreras-Martínez:** Formal analysis, Investigation, Methodology, Resources, Validation, Visualization, Writing – original draft, Writing – review & editing. **Mohamed Khayet:** Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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References

[1] K. Börner, A. Scharnhorst, Visual conceptualizations and models of science, J. Informetr. 3 (2009) 161–172, https://doi.org/10.1016/j.joi.2009.03.008.
[2] R. Melnik, Universality of mathematical models in understanding nature, society, and man-made world, in: Mathematical and Computational Modeling, 2015, pp. 1–16.
[3] M. Boukhriss, M. Timoumi, H.B. Bacha, Experimental of membrane distillation unit coupled with a DCMD using solar energy, Solar Comp. 7 (2023) 100055, https://doi.org/10.1016/j.solcom.2023.100055.
[4] S. Memon, H.-S. Lee, W.-S. Kim, Y.-D. Kim, Parametric investigation of modular configuration of multi-stage direct contact membrane distillation powered by waste heat of wind turbine, Desalination 533 (2022) 115770, https://doi.org/10.1016/j.desal.2022.115770.
[5] T.O. Obidara, M.A. Azeem, D.U. Lawal, M.A. Alfaraj, M.A. Abdulhamid, T. N. Baroud, Novel hexa-fluorinated intrinsically porous polyimide membranes for

the desalination of high saline water by air-gap membrane distillation, Desalination 566 (2023) 116948, https://doi.org/10.1016/j.desal.2023.116948.
[6] H.B. Madalosso, R.d.S. Silva, R.A.F. Machado, C. Marangoni, Superhydrophobic PA membrane for robust anti-wetting membrane distillation to water reclamation from textile wastewater, J. Water Process Eng. 49 (2022) 103162, https://doi.org/10.1016/j.jwpe.2022.103162.
[7] S. Parani, O.S. Oluwafemi, Membrane distillation: recent configurations, membrane surface engineering, and applications, Membranes 11 (2021) 934, https://doi.org/10.3390/membranes11120934.
[8] V.R. Moreira, J.V. Raad, J.X. Lazarini, L.V.S. Santos, M.C.S. Amaral, Recent progress in membrane distillation configurations powered by renewable energy sources and waste heat, J. Water Process Eng. 53 (2023) 103816, https://doi.org/10.1016/j.jwpe.2023.103816.
[9] L. García-Fernández, M. Khayet, M.C. García-Payo, 11 - Membranes used in membrane distillation: preparation and characterization, in: A. Basile, A. Figoli, M. Khayet (Eds.), Pervaporation, Vapour Permeation and Membrane Distillation, Woodhead Publishing, Oxford, 2015, pp. 317–359.
[10] H. Chamani, J. Woloszyn, T. Matsuura, D. Rana, C.Q. Lan, Pore wetting in membrane distillation: a comprehensive review, Prog. Mater. Sci. 122 (2021) 100843, https://doi.org/10.1016/j.pmatsci.2021.100843.
[11] S.M. Alawad, A.E. Khalifa, M.A. Abido, M.A. Antar, Differential evolution optimization of water gap membrane distillation process for water desalination, Sep. Purif. Technol. 270 (2021) 118765, https://doi.org/10.1016/j.seppur.2021.118765.
[12] S.M. Alawad, A.E. Khalifa, Analysis of water gap membrane distillation process for water desalination, Desalination 470 (2019) 114088, https://doi.org/10.1016/j.desal.2019.114088.
[13] S.M Alawad, D.U. Lawal, A.E. Khalifa, I.H. Aljundi, M.A. Antar, T.N. Baroud, M.A. M. Eltoum, Optimization and design analysis of multistage water gap membrane distillation for cost-effective desalination, Desalination 566 (2023) 116894, https://doi.org/10.1016/j.desal.2023.116894.
[14] A. Hafiz Al Hariri, A.E. Khalifa, S.M. Alawad, Techno-economic analysis of solar-powered membrane distillation system with circulated permeate gap, Solar Energy 267 (2024) 112243, https://doi.org/10.1016/j.solener.112243.
[15] X. Li, M.C. Garcia-Payo, M. Khayet, M. Wang, X. Wang, Superhydrophobic polysulfone/polydimethylsiloxne electrospun nanofibrous membranes for water desalination by direct contact membrane distillation, J. Membr. Sci. 542 (2017) 308–319, https://doi.org/10.1016/j.memsci.2017.08.011.
[16] E. Drioli, A. Ali, F. Macedonio, membrane distillationMembrane distillation: recent developments and perspectives, Desalination, 356, (2015), 56-84, 10.1016/j.desal.2014.10.028.
[17] M. Khayet, Membranes and theoretical modeling of membrane distillation: a review, Adv. Coll. Int. Sci. 164 (2011) 56–88, https://doi.org/10.1016/j.cis.2010.09.005.
[18] S.O. Olatunji, L.M. Camacho, Heat and mass transport in modeling membrane distillation configurations: a review, Front. Energy Res. 6 (2018) 130, https://doi.org/10.3389/fenrg.2018.00130.
[19] Y. Dong, X. Dai, L. Zhao, L. Gao, Z. Xie, J. Zhang, Review of transport phenomena and popular modelling approaches in membrane distillation, Membranes 11 (2021) 122, https://doi.org/10.3390/membranes11020122.
[20] M. Khayet, M.K. Souhaimi, T. Matsuura. Membrane Distillation: Principles and Applications, Elsevier, 2011.
[21] M. Essalhi, M. Khayet. Fundamentals of membrane distillation, Pervaporation, Vapour Permeation and Membrane Distillation, Elsevier, 2015, pp. 277–316.
[22] K. Charfi, M. Khayet, M.J. Safi, Numerical simulation and experimental studies on heat and mass transfer using sweeping gas membrane distillation, Desalination 259 (2010) 84–96, https://doi.org/10.1016/j.desal.2010.04.028.
[23] F. Eleiwi, N. Ghaffour, A.S. Alsaadi, L. Francis, T.M. Laleg-Kirati, Dynamic modeling and experimental validation for direct contact membrane distillation (DCMD) process, Desalination 384 (2016) 1–11, https://doi.org/10.1016/j.desal.2016.01.004.
[24] M.M.A. Shirazi, A. Kargari, A.F. Ismail, T. Matsuura, Computational fluid dynamic (CFD) opportunities applied to the membrane distillation process: state-of-the-art and perspectives, Desalination 377 (2016) 73–90, https://doi.org/10.1016/j.desal.2015.09.010.
[25] J. Zhang, M. Duke, M. Hoang, Z. Xie, A. Groth, C. Tun, S. Gray, Modelling of vacuum membrane distillation, J. Membr. Sci. 434 (2013) 1–9, https://doi.org/10.1016/j.memsci.2013.01.048.
[26] M. Bhattacharya, S.K. Dutta, J. Sikder, M.K. Mandal, Computational and experimental study of chromium (VI) removal in direct contact membrane distillation, J. Membr. Sci. 450 (2014) 447–456, https://doi.org/10.1016/j.memsci.2013.09.037.
[27] M. Hasanizadeh, P. Jafari, B. Farshighazani, M.K. Moraveji, CFD simulation of heat and mass transport for water transfer through hydrophilic membrane in direct-contact membrane distillation process, Desalin. Water Treat. 57 (2016) 18109–18119, https://doi.org/10.1080/19443994.2015.1094675.
[28] C. Fernández-Pineda, M.A. Izquierdo-Gil, M.C. García-Payo, Gas permeation and direct contact membrane distillation experiments and their analysis using different models, J. Membr. Sci. 198 (2002) 33–49, https://doi.org/10.1016/S0376-7388(01)00605-6.
[29] M. Khayet, J.I. Mengual, Effect of salt concentration during the treatment of humic acid solutions by membrane distillation, Desalination 168 (2004) 373–381, https://doi.org/10.1016/j.desal.2004.07.023.
[30] S. Srisurichan, R. Jiraratananon, A.G. Fane, Mass transfer mechanisms and transport resistances in direct contact membrane distillation process, J. Membr. Sci. 277 (2006) 186–194, https://doi.org/10.1016/j.memsci.2005.10.028.
[31] M. Khayet, M.P. Godino, J.I. Mengual, Study of Asymmetric polarization in direct contact membrane distillation, Sep. Sci. Technol. 39 (2005) 125–147, https://doi.org/10.1081/SS-120027405.T.
[32] J. Schnittger, J.R. McCutcheon, T. Hoyer, M. Weyd, I. Voigt, A. Lerch, Modified ceramic membranes for the treatment of highly saline mixtures utilized in vacuum membrane distillation, Desalination 567 (2023) 116943, https://doi.org/10.1016/j.desal.2023.116943.
[33] M. Essalhi, M. Khayet, Self-sustained webs of polyvinylidene fluoride electrospun nanofibers at different electrospinning times: 2. Theoretical analysis, polarization effects and thermal efficiency, J. Membr. Sci. 433 (2013) 180–191, https://doi.org/10.1016/j.memsci.2013.01.024.
[34] M. Khayet, T. Matsuura, Pervaporation and vacuum membrane distillation processes: modeling and experiments, AIChE J 50 (2004) 1697–1712, https://doi.org/10.1002/aic.10161.
[35] I. Hitsov, T. Maere, K. De Sitter, C. Dotremont, I. Nopens, Modelling approaches in membrane distillation: a critical review, Sep. Purif. Technol. 142 (2015) 48–64, https://doi.org/10.1016/j.seppur.2014.12.026.
[36] Y. Zhu, H. Chang, Z. Yan, C. Liu, Y. Liang, F. Qu, H. Liang, R.D. Vidic, Review of ammonia recovery and removal from wastewater using hydrophobic membrane distillation and membrane contactor, Sep. Purif. Technol. 328 (2024) 125094, https://doi.org/10.1016/j.seppur.2023.125094.
[37] A.M. Quarteroni, Mathematical models in science and engineering, Not. Am. Mat. Soc. 56 (2009) 10–19, https://doi.org/10.1002/9781118207239.
[38] S.S. Fetsov, N.A. Lutsenko, A novel computational model and OpenFOAM solver for simulating thermal energy storages based on granular phase change materials: advantages and applicability, J. Energy Storage 65 (2023) 107294, https://doi.org/10.1016/j.est.2023.107294.
[39] J.T. Haselman, J.W. Nichols, K.Z. Mattingly, M.W. Hornung, S.J. Degitz, A biologically based computational model for the hypothalamic-pituitary-thyroid (HPT) axis in Xenopus laevis larvae, Math. Biosciences 362 (2023) 109021, https://doi.org/10.1016/j.mbs.2023.109021.
[40] Y. Liu, S. Sun, C. Lin, High-precision computational modeling of soil-rock mixtures considering realistic shape of rock blocks, Eng. Geol. 323 (2023) 107236, https://doi.org/10.1016/j.enggeo.2023.107236.
[41] S. Gharehdash, B.-A. Sainsbury, S. Shelyag, M. Barzegar, An integrated field scale computational model for hydraulic conductivity of high energy explosive driven fracturing, Int. J. Rock Mech. Mining Sci. 165 (2023) 105368, https://doi.org/10.1016/j.ijrmms.2023.105368.
[42] E. Aytaç, Forecasting Turkey's hazelnut export quantities with Facebook's prophet algorithm and box-cox transformation, ADCAIJ-Adv. Distrib. Comp. Art. Intell. J. 10 (2021) 33–47, https://doi.org/10.14201/ADCAIJ20211013347.
[43] J. Qi, J. Lv, Z. Li, W. Bian, J. Li, S. Liu, A numerical simulation of membrane distillation treatment of mine drainage by computational fluid dynamics, Water (Basel) 12 (2020) 3403, https://doi.org/10.3390/w12123403.
[44] D. Cheng, W. Gong, N. Li, Response surface modeling and optimization of direct contact membrane distillation for water desalination, Desalination 394 (2016) 108–122, https://doi.org/10.1016/j.desal.2016.04.029.
[45] S. Mittal, A. Gupta, S. Srivastava, M. Jain, Artificial neural network based modeling of the vacuum membrane distillation process: effects of operating parameters on membrane fouling, Chem. Eng. Process. - Process Intensif. 164 (2021) 108403, https://doi.org/10.1016/j.cep.2021.108403.
[46] A.O. Imdakm, T. Matsuura, A Monte Carlo simulation model for membrane distillation processes: direct contact (MD), J. Membr. Sci. 237 (2004) 51–59, https://doi.org/10.1016/j.memsci.2004.03.005.
[47] J. Ma, H. Xu, A. Wang, A. Wang, L. Gao, M. Ding, Machine learning-guided underlying decisive factors of high-performance membrane distillation system: membrane properties, operation conditions and solution composition, Sep. Purif. Technol. 327 (2023) 124964, https://doi.org/10.1016/j.seppur.2023.124964.
[48] A. Yadav, C.P. Singh, R.V. Patel, A. Kumar, P.K. Labhasetwar, Investigations on the effect of spacer in direct contact and air gap membrane distillation using computational fluid dynamics, Colloids Surf. A: Phys. Eng. Asp. 654 (2022) 130111, https://doi.org/10.1016/j.colsurfa.2022.130111.
[49] A. Ansari, F.M. Galogahi, G. Millar, F. Helfer, D.V. Thiel, S. Soukane, N. Ghaffour, Computational fluid dynamics modelling of air-gap membrane distillation: spacer-filled and solar-assisted modules, Desalination 546 (2023) 116207, https://doi.org/10.1016/j.desal.2022.116207.
[50] H.H. Hu, Chapter 10 - computational fluid dynamics, in: P.K. Kundu, I.M. Cohen, D.R. Dowling (Eds.), Fluid Mechanics (Fifth Edition), Academic Press, Boston, 2012, pp. 421–472.
[51] A.S. Thomareis, G. Dimitreli, Chapter 12 - techniques usedfor processed cheese characterization, in: M. El-Bakry, B.M. Mehta(Eds.), Processed Cheese Science and Technology, Woodhead Publishing,(2022) , pp. 295-349,.
[52] M. Nassiri Mahallati, Chapter 9 - advances in modeling saffron growth and development at different scales, in: A. Koocheki, M. Khajeh-Hosseini (Eds.), Saffron, Woodhead Publishing, 2020, pp. 139–167.
[53] H. Deng, X. Yang, R. Tian, J. Hu, B. Zhang, F. Cui, G. Guo, Modeling and optimization of solar thermal-photovoltaic vacuum membrane distillation system by response surface methodology, Solar Energy 195 (2020) 230–238, https://doi.org/10.1016/j.solener.2019.11.006.
[54] X. Yan, G. Wang, C. Ma, J. Li, S. Cheng, C. Yang, L. Chen, Effects of pollutants in alkali/surfactant/polymer (ASP) flooding oilfield wastewater on membrane fouling in direct contact membrane distillation by response surface methodology, Chemosphere 282 (2021) 131130, https://doi.org/10.1016/j.chemosphere.2021.131130.
[55] F. Ricceri, B. Blankert, N. Ghaffour, J.S. Vrouwenvelder, A. Tiraferri, L. Fortunato, Unraveling the role of feed temperature and cross-flow velocity on organic

fouling in membrane distillation using response surface methodology, Desalination 540 (2022) 115971, https://doi.org/10.1016/j.desal.2022.115971.
[56] J. Liu, H. Ren, F.I. Hai, A.K. Albdoor, Z. Ma, Direct contact membrane distillation for liquid desiccant regeneration and fresh water production: experimental investigation, response surface modeling and optimization, Appl. Therm. Eng. 184 (2021) 116293, https://doi.org/10.1016/j.applthermaleng.2020.116293.
[57] C. Cojocaru, M. Khayet, Sweeping gas membrane distillation of sucrose aqueous solutions: response surface modeling and optimization, Sep. Purif. Technol. 81 (2011) 12–24, https://doi.org/10.1016/j.seppur.2011.06.031.
[58] M. Khayet, M. Essalhi, C. Armenta-Déu, C. Cojocaru, N. Hilal, Optimization of solar-powered reverse osmosis desalination pilot plant using response surface methodology, Desalination 261 (2010) 284–292, https://doi.org/10.1016/j.desal.2010.04.010.
[59] C. Cojocaru, M. Khayet, G. Zakrzewska-Trznadel, A. Jaworska, Modeling and multi-response optimization of pervaporation of organic aqueous solutions using desirability function approach, J. Hazard. Mater. 167 (2009) 52–63, https://doi.org/10.1016/j.jhazmat.2008.12.078.
[60] M. Essalhi, M. Khayet, C. Cojocaru, M.C. Garcia-Payo, P. Arribas, Response surface modeling and optimization of electrospun nanofiber membranes, Open Nanoscience J 7 (2013) 8–17, https://doi.org/10.2174/1874140101307010008.
[61] M. Khayet, J.A. Sanmartino, M. Essalhi, M.C. García-Payo, N. Hilal, Modeling and optimization of a solar forward osmosis pilot plant by response surface methodology, Solar Energy 137 (2016) 290–302, https://doi.org/10.1016/j.solener.2016.07.046.
[62] W.-H. Chen, M. Carrera Uribe, E.E. Kwon, K.-Y.A. Lin, Y.-K. Park, L. Ding, L. H. Saw, A comprehensive review of thermoelectric generation optimization by statistical approach: Taguchi method, analysis of variance (ANOVA), and response surface methodology (RSM), Renew. Sust. Energy Rev. 169 (2022) 112917, https://doi.org/10.1016/j.rser.2022.112917.
[63] S. Sinharay, An overview of statistics in education, in: P. Peterson, E. Baker, B. McGaw (Eds.), International Encyclopedia of Education, Third Edition, Elsevier, Oxford, 2010, pp. 1–11.
[64] A.S. Reddy, S. Kalla, Z.V.P. Murthy, Nano-particles enhanced hydrophobic membranes: high-performance study for dye wastewater treatment using membrane distillation, J. Water Process Eng. 46 (2022) 102610, https://doi.org/10.1016/j.jwpe.2022.102610.
[65] G. Campagna, A. Signore, Basic statistics for nuclear medicine and radiology, in: A. Signore (Ed.), Nuclear Medicine and Molecular Imaging, Elsevier, Oxford, 2022, pp. 622–630.
[66] W. Ma, R. Han, L. Zhu, L. Jiang, W. Zhang, H. Zhang, L. Chen, Efficient recovery of ammonia from digestate by membrane distillation: nano-FeOOH re-entry structure modification, anti-fouling, and anti-wetting performance, Sep. Purif. Technol. 323 (2023) 124414, https://doi.org/10.1016/j.seppur.2023.124414.
[67] K. Ali, A.A. Alwan, S. Bahayan, E. Alhseinat, M.I. Hassan Ali, A numerical analysis of the electromagnetic field effect on direct contact membrane distillation performance, Energy Convers, Manag 292 (2023) 117328, https://doi.org/10.1016/j.enconman.2023.117328.
[68] S.R. Sawant, S. Kalla, Z.V.P. Murthy, Enhanced properties of the PVDF membrane with carboxylated MWCNT and sodium alginate for membrane distillation, J. Environ. Chem. Eng. 11 (2023) 109259, https://doi.org/10.1016/j.jece.2022.109259.
[69] G. Gopi, M. Vasanthkumar, G. Arthanareeswaran, A.F. Ismail, Y.L. Thuyavan, P. S. Goh, T. Matsuura, Performance, energy and economic investigation of airgap membrane distillation system: an experimental and numerical investigation, Desalination 551 (2023) 116400, https://doi.org/10.1016/j.desal.2023.116400.
[70] R. DeLoach, Analysis of variance in the modern design of experiments. 48th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition, 2010.
[71] D.J. Navarro. Learning Statistics with R: A tutorial for psychology students and other beginners, LibreTexts, Wales, 2018.
[72] A.M. Johansen, Markov chain Monte Carlo, in: P. Peterson, E. Baker, B. McGaw (Eds.), International Encyclopedia of Education, Third Edition, Elsevier, Oxford, 2010, pp. 245–252.
[73] G. Romeo, Chapter 14 - essential Monte Carlo analysis, in: G. Romeo (Ed.), Elements of Numerical Mathematical Economics with Excel, Academic Press, 2020, pp. 763–795.
[74] I. Hitsov, L. Eykens, K.D. Sitter, C. Dotremont, L. Pinoy, B.V.d. Bruggen, I. Nopens, Calibration and analysis of a direct contact membrane distillation model using Monte Carlo filtering, J. Membr. Sci. 515 (2016) 63–78, https://doi.org/10.1016/j.memsci.2016.05.041.
[75] M. Khayet, A.O. Imdakm, T. Matsuura, Monte Carlo simulation and experimental heat and mass transfer in direct contact membrane distillation, Int. J. Heat Mass Trans. 53 (2010) 1249–1259, https://doi.org/10.1016/j.ijheatmasstransfer.2009.12.043.
[76] A.O. Imdakm, M. Khayet, T. Matsuura, A Monte Carlo simulation model for vacuum membrane distillation process, J. Membr. Sci. 306 (2007) 341–348, https://doi.org/10.1016/j.memsci.2007.09.021.
[77] A.O. Imdakm, T. Matsuura, Simulation of heat and mass transfer in direct contact membrane distillation (MD): the effect of membrane physical properties, J. Membr. Sci. 262 (2005) 117–128, https://doi.org/10.1016/j.memsci.2005.05.026.
[78] A. Laaksonen, Y. Tu, Chapter 1 - Methods of incorporating quantum mechanical calculations into molecular dynamics simulations, in: P.B. Balbuena, J. M. Seminario (Eds.), Theoretical and Computational Chemistry, Elsevier, 1999, pp. 1–29.
[79] R. Trobec, F. Merzel, D. Janežič, Computational complexity of split symplectic MD integration method, in: E.H. D'Hollander, F.J. Peters, G.R. Joubert, U. Trottenberg, R. Völpel (Eds.), Advances in Parallel Computing, 1998, pp. 541–548.
[80] S. Raza, J. He, H.V. Tafreshi, J. Liu, Molecular dynamics simulation of steady-state droplet condensation on a fiber in direct contact membrane distillation settings, J. Mol. Liq. 368 (2022) 120736, https://doi.org/10.1016/j.molliq.2022.120736.
[81] Q. Wang, X. Yang, L.-Z. Zhang, Development, testing, and molecular dynamics simulation of a membrane that resists fouling by gel pollutants for humidification–dehumidification–type seawater desalination, Desalination 561 (2023) 116686, https://doi.org/10.1016/j.desal.2023.116686.
[82] S. Velioğlu, L. Han, J.W. Chew, Understanding membrane pore-wetting in the membrane distillation of oil emulsions via molecular dynamics simulations, J. Membr. Sci. 551 (2018) 76–84, https://doi.org/10.1016/j.memsci.2018.01.027.
[83] E. Norouzi, C. Park, Water distillation performance of carbon nanotube membrane: non-equilibrium molecular dynamics simulation, Desalination 479 (2020) 114299, https://doi.org/10.1016/j.desal.2019.114299.
[84] W. Zhang, S. Yu, R. Ning, P. Li, X. Ji, Y.Xu, Treatment of high-salinity brine containing dissolved organic matters by vacuum membrane distillation: a fouling mitigation approach via microbubble aeration, J. Environ. Manag., Toronto Metropolitan University Open Access Publishing, Yalova, 342, (2023) 118142, 10.1016/j.jenvman.2023.118142.
[85] C.-Y. Zhu, Y.-H. Ding, Y.-B. Wu, L. Gong, Molecular dynamics study of membrane distillation process through nanopores, J. Mol. Liquids 394 (2024) 123694, https://doi.org/10.1016/j.molliq.2023.123694.
[86] E.R. Smith, P. Theodorakis, Multiscale simulation of fluids: coupling molecular and continuum, Phys. Chem. Chem. Phys. (2023), https://doi.org/10.1039/D3CP03579D.
[87] S.A. Hollingsworth, R.O. Dror, Molecular dynamics simulation for all, Neuron 99 (2018) 1129–1143, https://doi.org/10.1016/j.neuron.2018.08.011.
[88] E. Aytaç, M. Khayet. Machine learning applications on membrane distillation, 14th International Conference on Thermal Engineering: Theory and Application, Toronto Metropolitan University Open Access Publishing, Yalova, Türkiye, 2023.
[89] R. Bonetto, V. Latzko, Chapter 8 - machine learning, in: F.H.P. Fitzek, F. Granelli, P. Seeling (Eds.), Computing in Communication Networks, Academic Press, 2020, pp. 135–167.
[90] E. Aytaç, Unsupervised learning approach in defining the similarity of catchments: hydrological response unit based k-means clustering, a demonstration on Western Black Sea Region of Turkey, Int. Soil Water Cons. Res. 8 (2020) 321–331, https://doi.org/10.1016/j.iswcr.2020.05.002.
[91] E. Aytaç, Havzaların Benzerliklerini Tanımlamada Alternatif Bir Yaklaşım, hiyerarşik Kümeleme Yöntemi Uygulaması, Afyon Kocatepe Üni. Fen Müh, Bil. Dergisi 21 (2021) 958–970, https://doi.org/10.35414/akufemubid.870649.
[92] E. Aytaç, Exploring electrocoagulation through data analysis and text mining perspectives, Environ. Eng. Manag. J. 21 (2022) 671–685.
[93] E. Aytaç, Modeling future impacts on land cover of rapid expansion of hazelnut orchards: a case study on Samsun, Turkey, Eur. J. Sustain. Dev. Res. 6 (2022) em0193, https://doi.org/10.21601/ejosdr/12167.
[94] J. Komuro, D. Kusumoto, H. Hashimoto, S. Yuasa, Machine learning in cardiology: clinical application and basic research, J. Cardiol. 82 (2023) 128–133, https://doi.org/10.1016/j.jjcc.2023.04.020.
[95] H. Wang, T. Fu, Y. Du, W. Gao, K. Huang, Z. Liu, P. Chandak, S. Liu, P. Van Katwyk, A. Deac, A. Anandkumar, K. Bergen, C.P. Gomes, S. Ho, P. Kohli, J. Lasenby, J. Leskovec, T.-Y. Liu, A. Manrai, D. Marks, B. Ramsundar, L. Song, J. Sun, J. Tang, P. Veličković, M. Welling, L. Zhang, C.W. Coley, Y. Bengio, M. Zitnik, Scientific discovery in the age of artificial intelligence, Nature 620 (2023) 47–60, https://doi.org/10.1038/s41586-023-06221-2.
[96] A. Benhadjira, M.I. Sayyed, O. Bentouila, K.E. Aiadi, Artificial neural network approach for calculating mass attenuation coefficient of different glass systems, Nuclear Eng. Technol. (2023), https://doi.org/10.1016/j.net.2023.09.013.
[97] M. Shirzadi, Z. Li, T. Yoshioka, H. Matsuyama, T. Fukasawa, K. Fukui, T. Ishigami, Performance analysis and optimization of sweep gas membrane distillation module using high-resolution computational model and machine learning, Chem. Eng. J. 473 (2023) 145078, https://doi.org/10.1016/j.cej.2023.145078.
[98] P. Behnam, A. Shafieian, M. Zargar, M. Khiadani, Development of machine learning and stepwise mechanistic models for performance prediction of direct contact membrane distillation module- a comparative study, Chem. Eng. Process. - Process Intensif. 173 (2022) 108857, https://doi.org/10.1016/j.cep.2022.108857.
[99] C. Yang, Neural networks for predicting air gap membrane distillation performance, J. Indian Chem. Soc. 100 (2023) 100921, https://doi.org/10.1016/j.jics.2023.100921.
[100] O.I. Abiodun, A. Jantan, A.E. Omolara, K.V. Dada, N.A. Mohamed, H. Arshad, State-of-the-art in artificial neural network applications: a survey, Heliyon 4 (2018) e00938, https://doi.org/10.1016/j.heliyon.2018.e00938.
[101] M.W. Gaultois, T.D. Sparks, C.K.H. Borg, R. Seshadri, W.D. Bonificio, D.R. Clarke, Data-driven review of thermoelectric materials: performance and resource considerations, Chem. Mater. 25 (2013) 2911–2920, https://doi.org/10.1021/cm400893e.
[102] W. Karugahe, A. Jones, Data driven review of commonalities and differences in gender and self-reported victimisation in Ugandan urban sample and Western published literature, Aggress, Violent Behav. 58 (2021) 101550, https://doi.org/10.1016/j.avb.2021.101550.

[103] E. Aytaç, M. Khayet, A deep dive into membrane distillation literature with data analysis, bibliometric methods, and machine learning, Desalination 553 (2023) 116482, https://doi.org/10.1016/j.desal.2023.116482.
[104] M. Aria, C. Cuccurullo, Bibliometrix: an R-tool for comprehensive science mapping analysis, J. Informetr. 11 (2017) 959–975, https://doi.org/10.1016/j.joi.2017.08.007.
[105] M. Krassowski, ComplexUpset. https://github.com/krassowski/complex-upset, 2022 (accessed July 30, 2023).
[106] M. Khayet, E. Aytaç, T. Matsuura, Bibliometric and sentiment analysis with machine learning on the scientific contribution of Professor Srinivasa Sourirajan, Desalination 543 (2022) 116095, https://doi.org/10.1016/j.desal.2022.116095.
[107] E. Aytaç, A. Fombona-Pascual, J.J. Lado, E.G. Quismondo, J. Palma, M. Khayet, Faradaic deionization technology: insights from bibliometric, data mining and machine learning approaches, Desalination (2023) 116715, https://doi.org/10.1016/j.desal.2023.116715.
[108] R.W. Schofield, A.G. Fane, C.J.D. Fell, Heat and mass transfer in membrane distillation, J. Membr. Sci. 33 (1987) 299–313, https://doi.org/10.1016/S0376-7388(00)80287-2.
[109] E. Aytaç, M. Khayet, A topic modeling approach to discover the global and local subjects in membrane distillation separation process, Separations 10 (2023) 482.
[110] J. Demaine, Fractionalization of research impact reveals global trends in university collaboration, Scientometrics 127 (2022) 2235–2247, https://doi.org/10.1007/s11192-021-04246-w.
[111] M. Elgendi, 5 features of a highly cited article. https://www.nature.com/nature-index/news/five-features-highly-cited-scientific-article, 2019 (accessed August 11, 2023).
[112] M. Elgendi, Characteristics of a highly cited article: a machine learning perspective, IEEE Access 7 (2019) 87977–87986, https://doi.org/10.1109/ACCESS.2019.2925965.
[113] M. Qtaishat, T. Matsuura, B. Kruczek, M. Khayet, Heat and mass transfer analysis in direct contact membrane distillation, Desalination 219 (2008) 272–292, https://doi.org/10.1016/j.desal.2007.05.019.
[114] L. Francis, F.E. Ahmed, N. Hilal, Advances in membrane distillation module configurations, Membranes 12 (2022) 81, https://doi.org/10.3390/membranes12010081.
[115] R. Ullah, M. Khraisheh, R.J. Esteves, J.T. McLeskey, M. AlGhouti, M. Gad-el-Hak, H. Vahedi Tafreshi, Energy efficiency of direct contact membrane distillation, Desalination 433 (2018) 56–67, https://doi.org/10.1016/j.desal.2018.01.025.
[116] A.M. Alklaibi, N. Lior, Heat and mass transfer resistance analysis of membrane distillation, J. Membr. Sci. 282 (2006) 362–369, https://doi.org/10.1016/j.memsci.2006.05.040.
[117] H. Chang, J.-S. Liau, C.-D. Ho, W.-H. Wang, Simulation of membrane distillation modules for desalination by developing user's model on Aspen Plus platform, Desalination 249 (2009) 380–387, https://doi.org/10.1016/j.desal.2008.11.026.
[118] I. Hitsov, K. De Sitter, C. Dotremont, P. Cauwenberg, I. Nopens, Full-scale validated air gap membrane distillation (AGMD) model without calibration parameters, J. Membr. Sci. 533 (2017) 309–320, https://doi.org/10.1016/j.memsci.2017.04.002.
[119] A. Ansari, F.M. Galogahi, D.V. Thiel, F. Helfer, G. Millar, S. Soukane, N. Ghaffour, Downstream variations of air-gap membrane distillation and comparative study with direct contact membrane distillation: a modelling approach, Desalination 526 (2022) 115539, https://doi.org/10.1016/j.desal.2021.115539.
[120] J. Phattaranawik, R. Jiraratananon, A.G. Fane, Effect of pore size distribution and air flux on mass transport in direct contact membrane distillation, J. Membr. Sci. 215 (2003) 75–85, https://doi.org/10.1016/S0376-7388(02)00603-8.
[121] A.S. Kim, H.-S. Lee, D.-S. Moon, H.-J. Kim, Self-adjusting, combined diffusion in direct contact and vacuum membrane distillation, J. Membr. Sci. 543 (2017) 255–268, https://doi.org/10.1016/j.memsci.2017.08.059.
[122] D. Brogioli, N.Y. Yip, Energy efficiency analysis of membrane distillation for thermally regenerative salinity gradient power technologies, Desalination 531 (2022) 115694, https://doi.org/10.1016/j.desal.2022.115694.
[123] J. Amigo, R. Urtubia, F. Suárez, Exploring the interactions between hydrodynamics and fouling in membrane distillation systems – a multiscale approach using CFD, Desalination 444 (2018) 63–74, https://doi.org/10.1016/j.desal.2018.07.009.
[124] J. Koo, S. Lee, J.-S. Choi, T.-M. Hwang, Theoretical analysis of different membrane distillation modules, Des. Water Treat. 54 (2015) 862–870, https://doi.org/10.1080/19443994.2014.927801.
[125] C.M. Guijt, G.W. Meindersma, T. Reith, A.B.d. Haan, Air gap membrane distillation: 2. Model validation and hollow fibre module performance analysis, Sep. Purif. Technol. 43 (2005) 245–255, https://doi.org/10.1016/j.seppur.2004.09.016.
[126] J.A. Andrés-Mañas, I. Requena, A. Ruiz-Aguirre, G. Zaragoza, Performance modelling and optimization of three vacuum-enhanced membrane distillation modules for upscaled solar seawater desalination, Sep. Purif. Technol. 287 (2022) 120396, https://doi.org/10.1016/j.seppur.2021.120396.
[127] L. Francis, N. Ghaffour, A.A. Alsaadi, G.L. Amy, Material gap membrane distillation: a new design for water vapor flux enhancement, J. Membr. Sci. 448 (2013) 240–247, https://doi.org/10.1016/j.memsci.2013.08.013.
[128] C.A. Rivier, M.C. García-Payo, I.W. Marison, U. von Stockar, Separation of binary mixtures by thermostatic sweeping gas membrane distillation: I. Theory and simulations, J. Membr. Sci. 201 (2002) 1–16, https://doi.org/10.1016/S0376-7388(01)00648-2.
[129] M.C. García-Payo, C.A. Rivier, I.W. Marison, U. von Stockar, Separation of binary mixtures by thermostatic sweeping gas membrane distillation: II. Experimental results with aqueous formic acid solutions, J. Membr. Sci. 198 (2002) 197–210, https://doi.org/10.1016/S0376-7388(01)00649-4.
[130] H. Yu, X. Yang, R. Wang, A.G. Fane, Analysis of heat and mass transfer by CFD for performance enhancement in direct contact membrane distillation, J. Membr. Sci. 405-406 (2012) 38–47, https://doi.org/10.1016/j.memsci.2012.02.035.
[131] X. Yang, H. Yu, R. Wang, A.G. Fane, Analysis of the effect of turbulence promoters in hollow fiber membrane distillation modules by computational fluid dynamic (CFD) simulations, J. Membr. Sci. 415-416 (2012) 758–769, https://doi.org/10.1016/j.memsci.2012.05.067.
[132] H. Hayer, O. Bakhtiari, T. Mohammadi, Simulation of momentum, heat and mass transfer in direct contact membrane distillation: a computational fluid dynamics approach, J. Ind. Eng. Chem. 21 (2015) 1379–1382, https://doi.org/10.1016/j.jiec.2014.06.009.
[133] A.E. Khalifa, D.U. Lawal, Application of response surface and Taguchi optimization techniques to air gap membrane distillation for water desalination—a comparative study, Desalin. Water Treat. 57 (2016) 28513–28530, https://doi.org/10.1080/19443994.2016.1189850.
[134] M. Khayet, C. Cojocaru, C. García-Payo, Application of response surface methodology and experimental design in direct contact membrane distillation, Ind. Eng. Chem. Res. 46 (2007) 5673–5685, https://doi.org/10.1021/ie070446p.
[135] S. Fadhil, Q.F. Alsalhy, H.F. Makki, R. Ruby-Figueroa, T. Marino, A. Criscuoli, F. Macedonio, L. Giorno, E. Drioli, A. Figoli, Seawater desalination using PVDF-HFP membrane in DCMD process: assessment of operating condition by response surface method, Chem. Eng. Commun. 206 (2019) 237–246, https://doi.org/10.1080/00986445.2018.1483349.
[136] T. Mohammadi, P. Kazemi, M. Peydayesh, Optimization of vacuum membrane distillation parameters for water desalination using Box–Behnken design, Des. Water Treat. 56 (2015) 2306–2315, https://doi.org/10.1080/19443994.2014.961173.
[137] J. Li, S. Xu, M. Hassan, J. Shao, L.-F. Ren, Y. He, Effective modeling and optimization of PVDF–PTFE electrospinning parameters and membrane distillation process by response surface methodology, J. Appl. Polym. Sci. 136 (2019) 47125, https://doi.org/10.1002/app.47125.
[138] S.T. Bouguecha, A. Boubakri, S.E. Aly, M.H. Al-Beirutty, M.M. Hamdi, Optimization of permeate flux produced by solar energy driven membrane distillation process using central composite design approach, Water. Sci. Technol. 74 (2016) 87–98, https://doi.org/10.2166/wst.2016.126.
[139] S.S. Ray, R.K. Verma, A. Singh, S. Myung, Y.-I. Park, I.-C. Kim, H.K. Lee, Y.-N. Kwon, Exploration of time series model for predictive evaluation of long-term performance of membrane distillation desalination, Process Saf. Environ. Prot. 160 (2022) 1–12, https://doi.org/10.1016/j.psep.2022.01.058.
[140] A. Qamar, S. Kerdi, N. Amin, X. Zhang, J. Vrouwenvelder, N. Ghaffour, A deep neural networks framework for in-situ biofilm thickness detection and hydrodynamics tracing for filtration systems, Sep. Purif. Technol. 301 (2022) 121959, https://doi.org/10.1016/j.seppur.2022.121959.
[141] F.A. Almehmadi, A. Najib, E. Ali, H. Al-Ansary, J. Orfi, Sustainable approach of generating water and energy: techno-economic analysis of a hybrid solar photoactive thermal system coupled with direct contact membrane distillation for water purification and electricity generation, Appl. Sci. 12 (2022) 9137, https://doi.org/10.3390/app12189137.
[142] D. Perdue, L. Chen, L. Schaefer, Exergetic relationship between the thermal properties of direct contact membrane distillation, J. Heat Transf. 142 (2020), https://doi.org/10.1115/1.4045748.
[143] H. Chang, G.-B. Wang, Y.-H. Chen, C.-C. Li, C.-L. Chang, Modeling and optimization of a solar driven membrane distillation desalination system, Renew. Energy 35 (2010) 2714–2722, https://doi.org/10.1016/j.renene.2010.04.020.
[144] M.R.S. Kebria, A. Rahimpour, G. Bakeri, R. Abedini, Experimental and theoretical investigation of thin ZIF-8/chitosan coated layer on air gap membrane distillation performance of PVDF membrane, Desalination 450 (2019) 21–32, https://doi.org/10.1016/j.desal.2018.10.023.
[145] P. Yazgan-Birgi, M.I. Hassan Ali, J. Swaminathan, J.H. Lienhard, H.A. Arafat, Computational fluid dynamics modeling for performance assessment of permeate gap membrane distillation, J. Membr. Sci. 568 (2018) 55–66, https://doi.org/10.1016/j.memsci.2018.09.061.
[146] M. Khayet, C. Cojocaru, Artificial neural network modeling and optimization of desalination by air gap membrane distillation, Sep. Purif. Technol. 86 (2012) 171–182, https://doi.org/10.1016/j.seppur.2011.11.001.
[147] S. Zare, A. Kargari, CFD simulation and optimization of an energy-efficient direct contact membrane distillation (DCMD) desalination system, Chem. Eng. Res. Des. 188 (2022) 655–667, https://doi.org/10.1016/j.cherd.2022.10.001.
[148] A. Boubakri, S. Elgharbi, I. Dhaouadi, D. Mansour, S. Al-Tahar Bouguecha, Optimization and prediction of lead removal from aqueous solution using FO–MD hybrid process: statistical and artificial intelligence analysis, J. Environ. Manag. 337 (2023) 117731, https://doi.org/10.1016/j.jenvman.2023.117731.