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A Comprehensive Overview of Microemulsions Innovations Through Artificial Neural Network Approaches

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ABSTRACT

Microemulsions are multifunctional complex colloidal dispersed systems with widely utilized applications in drug delivery systems and chemical engineering. The interwoven relationship within their compositional variables, like surfactants, oil-to-water ratios, and co-surfactant type, leads to highly nonlinear phase behaviors that are difficult to analyze using traditional empirical or mechanistic models. This narrative review mainly focuses on the emerging role of artificial neural networks (ANNs) in optimizing microemulsion systems. Initially, the current study contextualizes the physicochemical factors of microemulsions and identifies their computational bottlenecks in formulation and phase behavior predictions. The review then analyses the relevant neural network structures, including feed forward networks, convolutional neural networks (CNNs), and recurrent neural networks (RNNs), for assessing their applicability to high-dimensional regression and classification and, furthermore, to reduce experimental load in microemulsion research. One of the advancements of using ANN is that it can identify the ideal concentration of excipients for the desirable properties of emulsion. Case studies are addressed wherein neural networks have been tutored on experimental and simulated datasets to estimate the droplet size distribution, construct pseudo-ternary phase diagrams, and identify optimal formulation properties. In addition to that, emphasis is applied to model structural design, feature selection strategies, and model validation techniques. The study also considers the current obstacles, such as paucity of data availability, over-fitting, and the integration of expertise knowledge in the learning models. Looking forward to the next context, this review illustrates that artificial neural network-based approaches provide a scalable and adaptable computational framework for boosting innovation in microemulsion science.

Keywords: Microemulsions, ANN (Artificial Neural Networks), Formulation Optimization, Data-driven models, Phase behavior.

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INTRODUCTION

Artificial neural networks (ANNs) are simulation-programmed models driven by the structures and functions of the human brain. the various studies suggest the technological advancements of ANN, but not the applied applications; hence, this review critically analyzes those advancements and determines how they can be used for the optimization of microemulsions. These models consist of integrated functional units, known as neurons, which are organized in layers that function as shared information [1, 2, 3]. The ANNs are particularly commanding in determining the complex, non-linear relationships among variables, making them suitable for virtual modeling, prediction, and optimization of assignments in numerous scientific fields, including chemistry and materials science. One such area where ANNs have found expanded use cases is in the study of microemulsions [4, 5]. The microemulsion is a thermodynamically unstable system; this type of homogenous liquid mixture consists of water and surfactants, and most of the time it's a combination with co-surfactants. Unlike ordinary emulsions, microemulsions form impulsively and are characterized by their transparency and tiny droplets (typically in the range of 10–100 nm) [6, 7]. They are extensively employed in pharmaceuticals, cosmetics, food processing, and enhanced oil recovery by virtue of their rare physicochemical properties, including low interfacial tension, elevated solubilization capacity, and stability[7, 8]. The preparation of a microemulsion is a challenging process affected by several factors including the type and concentration of surfactant, oil phase, aqueous phase, temperature, and pH being utilized. Experimentally finding all these parameters is time-consuming and costly; hence, computational tools like ANN are frequently used to predict and optimize the microemulsion systems effectively [9].

ANN Modeling and Microemulsion System:

Artificial Neural Networks are specifically very important in modeling the phase behavior or compatibilities studies in microemulsions. The conventional models were heavily relying on empirical and semi-empirical data. However, [10]. Researchers have investigated the Phase behavior using ANN in the case of the Quaternary Microemulsion forming system, including lecithin, isopropyl myristate, and water with different types of co-surfactants varying in their chain length. The structural design of the ANN typically consists of an input layer (representing variable values such as surfactant concentration, soil type, water content, and temperature), two or more hidden layers, and a third layer is the output layer (determines the phase type, particle size, or solubilization efficiency or it analyzes the result) [8] The Programming process needs a well-structured dataset that covers a whole range of formulation conditions or factors in the experiments [11, 12, 13]. The quality or quantity of added input data significantly affects the precision of the ANN experimental model. The validations through techniques like cross-validation are crucial for assuring robust model working capabilities [14].

Basics of Structural and Functional Units of Neural Networks:

Artificial neural networks are composed of three layers of interconnected units, also called as neurons or units. The structural layers network of ANN is given in Figure 1. These layers are composed of the input layer, a hidden layer, and an output layer [15]. Neurons execute a weighted or calculated sum of their inputs and then employ an activation function to generate an output function, each offering input that works differently to the network's learning functionality and responsiveness [16]. ANNs employ a procedure called user instructions, which generally entails supervised learning, to understand the data. The network utilized optimization methods like stochastic gradient descent in conjunction with algorithms or mathematical formulas like back-propagation to modify its weights during training [16]. The main purpose is to minimize the loss function, which further quantifies the discrepancy between the network's predicted and actual outputs. Each recurrent step of training improves the model's ability to map input data to the correct output, which further enables it to generalize to new, unseen data. Overfitting, where a model performs well on training data but poorly on new data, is mitigated using technologies like dropout, regularization, and cross-validation [18].

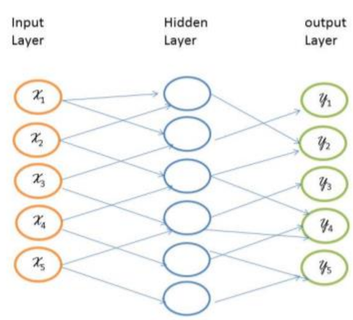

Figure 1: The structural layers of ANN

Classification of Neural Networks: The feed-forward neural networks (FNNs): I

t is the simplest type, in which the data flows from one direction input units to output. These neural networks are impactful for basic classification and regression tasks such as property prediction and finding non-linear relations between variables [7].

Convolutional neural networks (CNNs):

This is used to design image and image sequence analysis. CNNs use convolutional layers to detect the spatial features and are highly effective in visual tasks. and this type of technique is mainly used to study the microstructural properties or units of particles or globules [19].

The recurrent neural networks (RNNs):

In this type of RNN use loops are used that allow the information to survive over time, making them appropriate for sequence data such as text or time series. The vanishing gradient issue that plagues traditional RNNs is addressed by variants such as LSTM (Long Short-Term Memory) and GRU (Gated Recurrent Unit) [20].

The generative adversarial networks (GANs):

This type of neural network is usually employed for picture formation and data augmentation. These networks are the discriminator and the generator, and they further compete with one another to create outputs that may be more realistic than the others [21].

PROPERTIES OF MICROEMULSIONS:

Microemulsions are the clear transparent biphasic liquid dosage form which is generally thermodynamically stable in nature and is made up of oil and water mixture with the help of surfactant [22, 23] and sometimes with a co-surfactant as well. In contrast to traditional emulsions, which exhibit a kinetically and thermodynamically unstable nature, the microemulsions form autonomously driven by the significant reduction in interfacial tension facilitated by the surfactants and cosurfactants activities [24, 25]. Hoar and Schulman first proposed the theory of microemulsion in 1943[26], they found that the microemulsions usually have a droplet size ranging from 10 to 100 nanometers, as a consequence of their nanometer size, they exhibit optically transparency or translucent appearance.

Workflow for the formation of microemulsion with the help of ANN technique:

Various modern pharmaceutical and Nano-technologically oriented companies are swiftly adopting the methodical, economical, and intelligent pathway to formulation creation that the integration of ANN in microemulsion production delivers [27, 28]. The workflow steps are given below:

Problem Definition:

The first goal of the system is to predict the droplet size, stability, or phase behavior of microemulsions. Then to identify the input variables such as surfactant type, oil phase, co-surfactant ratio, temperature, and so on afterward the output variables such as droplet size, zeta potential, and stability index [29, 30].

Data Collection:

The next step is to collect the experimental data from literature work or controlled experimental procedures. In order to ensure diverse and high-quality data the formulator needs to cover a wide formulation data from numerous experiments.

Data Integration:

To Normalize or Standardize the experimental data. Allocate the data into a training set and validate. This step involves the merging of experimental formulation data with calculated physicochemical responses to establish a structured dataset for ANN training.

ANN Model designing:

for the active working of the ANN model, firstly choose the specific type of artificial neural network for most common cases the feed-forward or back-propagation is used. Then examine the number of input units often based on variables, hidden layers/units, and output units. Then further select the activation functions such as ReLU, sigmoid, and so on. There are numerous ANN software tools used for simulation studies and are given in Table 1

Table 1: ANN software tools used for simulation studies

S. No.	Software Tool	Applications in Microemulsion Preparation
1	MATLAB (Neural Network Toolbox)	Training ANN for property prediction
2	Python	ANN for formulation and phase behavior prediction
3	WEKA	Data Mining and ANN Classification
4	NeuroSolutions	Desinging ANN structure for experimental modeling
5	Statistica Neural Networks	Complex modeling in pharmaceutical formulation studies

The Training of ANN:

use the training dataset or loop to construct the model using the backpropagation method or by performing a forward pass, then examine the trained model on unknown data using metrics like accuracy and precision [31].

Validation and Testing:

Validation of ANN Model: Validation of the ANN model is a crucial step in machine learning, in which the training set is validated to avoid overfitting. To validate the ANN model, the system needs to adjust the hyperparameters like, the number of hidden layers or neurons, learning rate, and activation function. After the validation, the model needs to be tested to estimate how the model will perform on real-world data.

Prediction and simulation:

In this step, the trained ANN data set is used to analyze the optimal conditions for microemulsion formulation, and it helps in exploring the formulation design virtually by simulation methods. The typical workflow of ANN in microemulsion studies is given below in Figure 2.

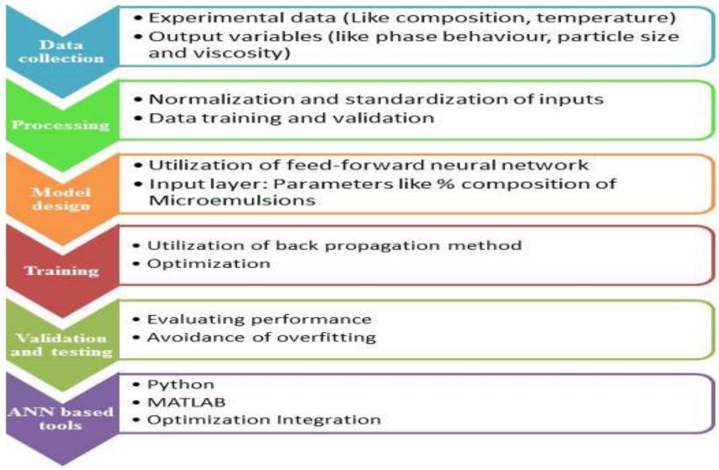

Figure 2: The typical workflow of an ANN in a microemulsion

Artificial Neural Networks and Their Function in Microemulsion Studies:

ANNs are beneficial as prediction, optimization, and designing tools in the field of microemulsion research, in which complex physicochemical interactions control stability, phase behavior, and performance can be easily studied and are given Table 2.

Table 2: Comparison of ANN-based approaches with conventional formulations and modelling method for microemulsions

S. No.	Criterion	Artificial Neural Network (ANN)	Design of Experiments (DoE)	Response Surface Methodology (RSM)	Mechanistic Models
1	Handling non-linearity	efficiently captures non-linear relations	limited to predict	moderate	Variable
2	Performance	Moderate to poor without regularization	good	good	poor
3	Interpretability	Low to Moderate	High	High	High
4	Reduction in Experimental Cost	High	Moderate	Moderate	Low
5	Suitability for early-stage formulation	Moderate	High	High	Low
6	Optimization	High	Moderate	Moderate	Low
7	Chances of Overfitting	High	Low	Low	Not Applicable

Phase Behavior and Stability Prediction:

Estimating phase behavior and stability is one of the most important benefits of artificial neural networks (ANNs) in microemulsion research. Some variables, like the kind of surfactant and co-surfactant, temperature, salinity, oil-water ratio [33, 34,] and concentration of surfactant, influence the phase behavior of a microemulsion system. Phase boundaries and phase inversion locations have been consistently predicted by ANNs trained on data from experiment [33]. This ability to predict saves a great deal of time and money by removing the need for laborious phase diagram development through experimentation. Work [35], for instance, utilized the ANN models to predict Winsor phases in different surfactant-oil-water systems and observed that the model was able to accurately predict the class of microemulsion. In health sectors like pharmaceuticals, where the desired phase is critical to the efficacy of medication delivery, these estimates play a key role in the study [36, 37].

Improving Formulation Parameters:

ANNs are significantly helpful in improving microemulsion formulations[38, 39]. These systems usually need to have their surfactant and co-surfactant ratios with oil and water concentrations, and with other factors meticulously controlled. The formulator may quickly find the best formulations that have the required qualities, such as minimal droplet size, high solubilization capacity, and maximum stability, with the help of ANNs with optimization methods such as genetic algorithms (GAs) [40] utilizing a combination of ANN and GAs to optimize the properties of microemulsion formulations for drug delivery. This worked better than conventional design of experiments (DoE) methods. This type of hybrid system cuts down on the expense of testing and makes it possible to quickly build initial formulations.

Prediction of Droplet Size and Viscosity:

The dimensions and flow resistance of microemulsion droplets are the important factors that impact the medicament delivery [40, 41], elevated oil recovery, and its topical uses. There are many elements that may affect these properties, which makes them suitable for ANN modeling. With the help of ANN models trained on actual experimental data, from previous studies it has been found that droplet sizes can be predicted with a high degree of accuracy. The researchers have explained how ANN models can be utilized to estimate the viscosity of microemulsion systems at wide-ranging shear rates and temperatures [42, 43]. Microemulsions are most of the time utilized in chemical-enhanced oil recovery (CEOR) to facilitate the extraction of oil from porous media. Researchers have employed artificial neural networks (ANNs) to speculate the volume of oil recoverable with the help of surfactant flooding by analyzing the surfactant type, the amount, and the state of the reservoir. These techniques assist petroleum engineers or formulators in selecting optimal formulae or compositions to enhance the likelihood of successful experiments [44]. Developers have developed an artificial neural network structural model to find the optimal salinity and surfactant concentration for microemulsion formulations used for enhanced oil recovery [45]. They found that the current technique is more effective than earlier regression techniques. The combination of artificial neural networks with reservoir modeling platforms is poised to considerably transform enhanced oil recovery strategies [46, 47].

Microemulsion-mediated synthesis of nanoparticles:

Microemulsions establish a controlled environment for the fabrication of nanoparticles with a regular size variation of particles. Artificial Neural Networks (ANNs) have been used to anticipate and optimize the size and morphology of nanoparticles by considering variables such as the quantity of reactants utilized in specific ratios of various phases, and the reaction temperature. This type of predictive model is important in the synthesis of nanomaterials tailored for applications in the electronics and medicinal sectors. From the previous study it has concluded that the utilization of ANN modeling for determining the particle size of silver nanoparticles synthesized in a microemulsion medium, those predictions by that method were quite accurate, enabling improved management of the synthesis properties [48]. This approach is capable of scalable production and replication of nanoparticles.

The Combination of Experimental and Computational Approaches:

Integrating artificial neural networks with other experimental and computational techniques can optimize the accuracy of microemulsion research. Integrating artificial neural networks with molecular dynamics simulatory studies or thermodynamic models promotes the linkage of large-scale predictions to molecule-level workflow. Furthermore, the experiment data obtained from high-throughput screening platforms may be utilized to train artificial neural networks (ANNs), making an interdependent relationship between experimentation and computation that benefits both fields [49]. This research presents that this type of integration is effective when artificial neural network models are trained on chemical constitutional descriptors derived from computational chemistry simulatory studies. This also enables the decision framework of ANN in the microemulsion research, which is given in Table 3.

Table 3: Decision Framework in the Application of ANN Microemulsion Research

S. No.	Decision Criterion	Condition	Modelling Approach Recommended	Rationale
1	Primary Research Objective	Prediction of complex phase behaviour and mechanistic understanding of phase formation	ANN-Hybrid / Mechanistic or thermodynamic models	Efficiently predict the strong nonlinearity and multidimensional interactions
2	Data Set	50 experimental data points	ANN-Hybrid or DoE/RSM models	Conventional data performs better with limited data
3	System Complexity	Multicomponent System	ANN	Handles high-dimensional nonlinear formulation

4	Validation strategy available	External and Internal Validation	ANN	Risk of Optimization performance and overfitting
5	Intended Applications	Pre-formulation screening	ANN/Hybrid Models	Maximizes predictive performance for fine optimization

The case studies on the utilization of artificial neural networks in microemulsion Research:

Microemulsions are thermodynamically stable systems in the combinations of oil, water, surfactant, and co-surfactant, commonly used in medicine delivery in increased oil recovery, and cosmetic products [50]. The previous research has concluded that artificial neural networks (ANNs) have proven to be reliable methods for modeling microemulsions, owing to their capacity to identify non-linear correlations among variables without the need for algorithmic specification [51].

Prediction of Microemulsion Phase Behavior:

multiple investigations have revealed the utility of ANNs they can help in predicting phase behavior. For example, the researchers have crafted a backpropagation ANN model to find microemulsion regions in a water, surfactant, and oil system [52]. This type of model accurately categorized the phase type using different surfactant concentrations, oil types, and temperatures as input units. Likewise, [53] adopted a multilayer perceptron (MLP) to depict the pseudoternary phase diagrams of microemulsions composed of oleic acid and ethanol, which has achieved prediction accuracy above more than 90%.

Solubility Prediction in Drug Delivery:

The dissolvability of hydrophobic drugs in microemulsion carriers is an important parameter for its bioavailability. A study by researcher has analyses the use of artificial neural networks (ANNs) to find drug solubility in water–solvent mixtures [54, 55, 56]. They used 35 experimental datasets and then developed a feedforward backpropagation ANN system with 6-5-1 architectural units. The model depicted a high accuracy, with an overall standard mean percentage deviation (OMPD) of $0.90 \pm 0.65\%$ when trained on complete datasets. Although, the ANN maintained reasonable predictive performance, in comparison to conventional multiple linear regression methods, the ANN approach has given a superior accuracy, highlighting its potential for enhancing drug formulation development.

Optimization of Surfactant and Co-surfactant Ratios:

Optimizing surfactant/co-surfactant ratios is necessary for stable microemulsion formations. From the previous study it has concluded that the ANN-based optimization in which the utilization of the genetic algorithms (GAs) in combination with ANN to determine optimal ratios for formulations targeting oral delivery of curcumin-loaded liposomes has better results than the conventional methods[57]. Their hybrid model successfully narrowed down the best composition with minimal experimental iterations and also helped in improved encapsulation efficiency, consequently reducing time and cost.

Viscosity Prediction and Rheological Analysis:

The ANNs have been used to predict the viscosity, which affects microemulsion efficiency for topical routes and transdermal delivery systems. Some formulators have optimized an ANN system on viscosity data [58, 59] from numerous microemulsions that are most commonly used as a machine learning approach to find the viscosity of microemulsions [60], which is important in enhancing oil recovery processes, by using molecular dynamics simulatory studies. This also facilitates better control over formulation consistency and drug release in the given dosage form.

Stability Studies of Microemulsions:

Predicting the prolonged stability of microemulsions is crucial for commercial applications. The constructed ANN model has trained on stability data over six months, including temperature fluctuations and phase separation events [61]. The model correctly anticipated instability trends, making it a useful tool for formulation scientists in the course of development.

Modeling Release Kinetic:

Investigating the dynamics of drug release from microemulsion carriers is essential to validate its efficacy. The trained ANN model has presented a radial basis function (RBF) ANN to model the in vitro drug release profile of ibuprofen from microemulsion systems [62, 63, 64]. The ANN model gives much better results than conventional models such as Higuchi or Korsmeyer-Peppas and depicts its flexibility in complex kinetic modeling for drug release.

ANN-Based QbD (Quality by Design) in Microemulsions:

The effectiveness of Quality by Design (QbD) is improved by utilizing ANNs. In the recent study, the formulator utilized the ANN models entrenched within a QbD structure to simplify the critical quality attributes (CQAs) of a microemulsion-based gel formulation for topical applications [65, 66]. The ANN productively identified the key input variables that may affect its critical quality attributes, promoting the robust product design.

The current challenges and drawbacks of artificial neural networks in Microemulsions Research:

The ANN gives promising applications for modeling and finding complex behaviors in microemulsion systems because of its resilience and non-linear learning capability. Still, there are several challenges and limitations that restrict its widespread applicability in this field.

Data Dependency and Quality Issues:

One of the major limitations of ANNs is their reliance on quality, broad datasets. The microemulsion systems are innately challenging, comprising interactions between surfactants, co-surfactants, oil, and water phases, which may differ under different conditions [67, 68]. The rareness of comprehensive and standard datasets restricts the ANN's capability to produce reliable results [69]. Additionally, the experimental data in the field of ANN are often rare, unpredictable, and lack the granularity required for its effective model training [70].

Overfitting and Poor Generalization:

Overfitting is a usual error when ANNs are trained on small or uneven datasets [71, 72], which is many times the case in microemulsion research[73, 74]. An ANN trained on a restricted set of formulation parameters may perform well on training data but fail to predict efficiently under unknown conditions or new novel formulations [75]. This type of problem reduces the dependability and strength of ANN models in functional use.

Lack of Physical Interpretability:

The ANN works like a "black box" model, which means that it provides predictions without a clear grasp of the foundational principles[76, 77]. In the case of microemulsion systems, in which mechanistic understanding is important for formulation and optimization, the paucity of interpretability limits the utility of ANN-based predictions [78]. This is generally difficult when trying to understand how surfactant interactions or phase behavior influence its results.

The necessity for specialist consultation in model design:

The efficiency of an ANN is acutely dependent upon the selection of structure, activation functions, and hyper-parameters [79, 80] then in the next step programming a dependable artificial neural network for microemulsion systems frequently necessitates sequential testing and specialized skills, which may not always be approachable in all tests [81]. Insufficient systems may result in underfitting, convergence problems, or erroneous outcomes.

Restricted transferability among Systems:

Owing to the specific thermodynamic and structural characteristics in most of the microemulsion systems, models developed by one dataset might not be applicable to others [82, 83]. This constrains the scalability of ANN models and needs retraining with new datasets for each formulation option, which are both time-consuming and resource-limited [84].

Computational Expense and Training Duration:

Even though some small networks may be trained rapidly, deeper and more accurate models need considerable computer resources. The researchers without any access to high-performance computing applications may face some obstacles in implementing ANN techniques for microemulsion research [85, 86, 87].

Future Prospects of ANN in microemulsion research:

ANN is becoming acknowledged as an effective application in the domain of microemulsion research owing to its capacity to manage intricate, nonlinear interactions among various formulations [89]. The application of microemulsions in pharmaceuticals, cosmetics, petrochemicals, and food science, joined with the incorporation of ANN-based modeling, is expected to be markedly enhanced in designing and optimization processes [90]. An interesting future approach is the utilization of ANN in predicting the phase behavior and microemulsion zones. In the past, the identification of microemulsion zones was done using various experimental techniques which are both time-consuming and resource-intensive [91]. The ANN system is tailored to the specific experimental datasets to predict the phase behavior typically based on input parameters like surfactant concentration, oil-to-water ratio, and ranges to temperature used. This type of model can optimize the formulation process by predicting the most suitable excipient compositions, hence reducing the experimental workload [92]. In a crucial domain is the multi-objective refinement of microemulsion systems. In actual applications, many formulation criteria like the droplet size, viscosity, stability, and drug-loading capacity should be concurrently adjusted. ANN models, when incorporated with optimization methods like genetic algorithms or particle swarm optimization, can encourage the attainment of balanced formulations that fulfill designated performance requirements [93, 94, 95]. This is particularly beneficial in the pharmaceutical or healthcare sector, where bioavailability and formulation stability are pivotal. In the years ahead, ANN is foreseen to be integrated with other machine learning programs and computational methodologies. The combination of ANN models with molecular dynamics simulations or quantum mechanical computational programs may provide an improved understanding of the molecular interactions and structural characteristic properties of microemulsion systems [96, 97]. The combined method would connect macroscopic properties, like as viscosity and conductivity, with microscopic aspects, such as surfactant packing and interfacial behavior, resulting in a more thorough cognition of formulation mechanisms. The actual monitoring and regulation of microemulsion preparation is another fascinating application. ANN can analyze different sets of data from sensors and spectroscopic instruments to identify process variance and provide prompt corrective measures. This type of skill can result in more resilient and uniform production methodologies, by the rules and regulations of the smart manufacturing Industry and healthcare sectors [98, 99, 100]. The precision of ANN predictions is significantly affected by the quality and availability of training data. In the case of microemulsion research, datasets often exhibit constraints in both size and uniformity. On the same side, efforts should concentrate on building open-access databases and defined procedures for data collecting and dissemination. Furthermore, the integration of explainable methodologies might be necessary for enhancing the interpretability and dependability of ANN models, consequently raising their acceptance among formulation scientists.

CONCLUSION:

The opportunities for ANN in microemulsion research are promising and diverse. From dosage form prediction and optimization to actual control and inverse design, ANN is expected to become an important instrument in both academic and industrial fields. With increased data availability and the advancement of complex, predictable models, ANN-driven research will be important in developing the next generation of efficient microemulsion systems. The application of ANN in the formulation development and optimization of microemulsions has emerged as a significant methodology in the domain of pharmaceutical and cosmetic sciences [101, 102,] providing a predictive and efficient source to build stable and effective delivery systems. Microemulsions are intricate systems which, in general, consist of oil, water, surfactants, and co-surfactants, with their properties such as droplet size, stability, viscosity, and drug loading affected by many formulations and processing parameters. Conventional trial-and-error approaches for optimizing these variables are laborious and quite resource-demanding. Conversely, the ANN system provides a data-driven methodology that can simulate non-linear correlations between inputs (such as surfactant concentration, oil type, and temperature) and outputs (including particle size, polydispersity index, and drug release rate) without necessitating a predetermined mathematical model. The use of the ANN model for microemulsion formulation starts with the specification of the problem, in which the aim (e.g., minimizing droplet size, maximizing stability) is established. Subsequently, the data collecting entails aggregating experimental data from either laboratory investigations or from the published literature. The calibration and extent of data substantially influence the model's prediction efficiency. The dataset is then pre-processed, normalized, cleaned, and partitioned into training, validation, and further testing to guarantee an effective model training procedure.

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