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Overview of soft intelligent computing technique for supercritical fluid extraction

Sitinoor Adeib Idris[1], Masturah Markom[2]
[1]Faculty of Chemical Engineering, Universiti Teknologi MARA, Malaysia
[1,2]Departement of Chemical and Process Engineering, Universiti Kebangsaan Malaysia, Malaysia

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ABSTRACT

Optimization of Supercritical Fluid Extraction process with mathematical modeling is essential for industrial applications. The response surface methodology (RSM) has been proven to be a useful and effective statistical method for studying the relationships between measured responses and independent factors. Recently there are growing interest in applying smart system or artificial technique to model and simulate a chemical process and also to predict, compute, classify and optimize as well as for process control. This system works by generalizing the experimental result and the process behavior and finally predict and estimate the problem. This smart system is a major assistance in the development of process from laboratory to pilot or industrial. The main advantage of intelligent systems is that the predictions can be performed easily, fast, and accurate way, which physical models unable to do. This paper shares several works that have been utilizing intelligent systems for modeling and simulating the supercritical fluid extraction process.

Corresponding Author:

Sitinoor Adeib Idris,
Faculty of Chemical Engineering,
Universiti Teknologi MARA,
40450, Shah Alam, Selangor, Malaysia.
Email: adeib@salam.uitm.edu.my

1. INTRODUCTION

Traditional computational approaches and methods could only model and analyze simple systems. Complex systems such as in machining, biology, medicine and similar fields often remained unsolvable to conventional mathematical and analytical methods. Assumptions and simplification of mathematical model are sometimes not reliable and many conventional mathematical models have been both challenging and impractical. Soft computing however, deals with imprecision, uncertainty, partial truth and approximation to achieve tractability, robustness and more importantly low solution cost. Figure 1 shows the available components of soft computing. There are five types which are neural networks, fuzzy systems, evolutionary computation, ideas about probabilities and swarm intelligence. This study is will focus on an overview of previous research applying some of the components such as neural networks, fuzzy systems, genetic algorithm and its hybrid in supercritical fluid extraction process.

Conventional techniques are largely based on formal logical systems and rely heavily on computer-aided numerical analysis. Soft computing techniques are intended to complement each other. Hard computing schemes strive for accurateness and full truth whereas soft computing techniques exploit the given tolerance of imprecision, partial truth, and uncertainty for a particular problem or data. In overall, soft computing technique is similar and imitating the genetic processes more closely than the traditional technique. It applies the ability to learn, observe and memorize in a situation of full of factors and important data.

Whereas, hybrid intelligence systems deal with the integration of two or more of the technologies. The combined use of technologies has resulted in effective problem solving in comparison with each technology used individually and exclusively. As illustrated in Figure 2, each of these technologies individually and in combination can be employed to solve problems. For example, when neural network combines with fuzzy systems, a neuro-fuzzy hybrid will develop and when neural network and evolutionary algorithm combines, a neuro-evolutionary will be developed.

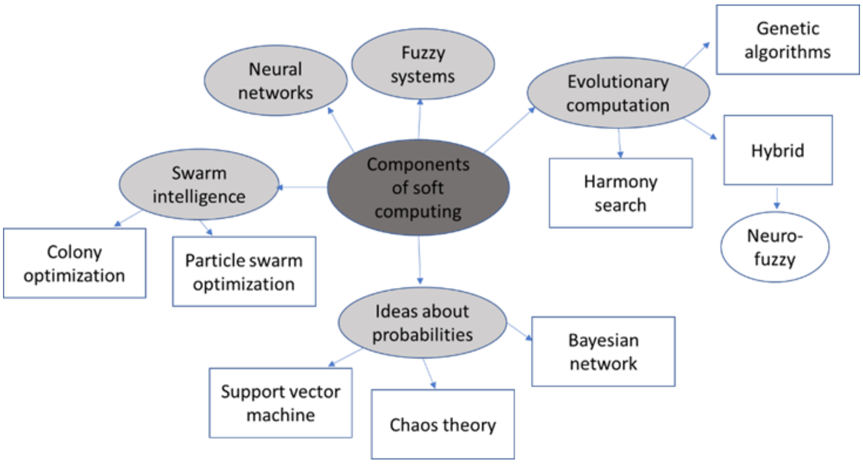

Figure 1. Components of soft computing [1]

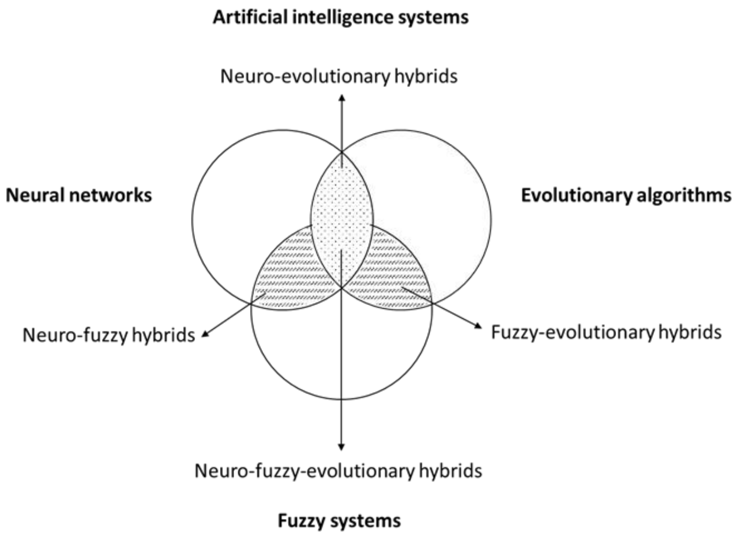

Figure 2. Integration of neural networks, fuzzy systems and evolutionary algorithm technologies by [2]

2. PREVIOUS STUDY APPLYING SOFT INTELLIGENT COMPUTING TECHNIQUE

In order to develop a reliable model to represent the data, neural network have been applied to several supercritical fluid extraction processes in predicting yield of extraction [1-6] and solubility predictions [7-9]. Besides that, fuzzy systems also has been applied to determine the extractant quantities at desired temperatures and pressures [10].

There are several studies using a hybrid model combining ANN and FIS which is called as ANFIS to predict solubility [11] and mass of extract [12, 13]. Another type of hybrid is by combining ANN with a conventional mathematical model [14]. This type of hybrid was mainly to solve the black box issues of not understanding the process of SFE. By ANN-Mathematical model hybrid, one can solve the issue [15].

Some studies even compare the results of application of ANN and ANFIS in order to identify the best system that can represent the data and reliable for optimization process [16-19].

Genetic algorithm also one of the promising tools in optimization of SFE [20-24]. It has been applied in determining constants in mathematical model in order to minimize error between model results and experimental data [25]. It can also be used in generating the non-linear binary interaction parameter of the conventional mathematical model such as in Peng–Robinson equation [26].

3. ARTIFICIAL NEURAL NETWORK (ANN) AND ADAPTIVE NEURO-FUZZY INFERENCE SYSTEM (ANFIS)

Adaptive Neuro-Fuzzy Inference System (ANFIS) is considered as one type of hybrid model for optimization process since it combines the Artificial Neural Network (ANN) and Fuzzy Inference System (FIS) system. Table 1 describes the advantages and disadvantages applying ANN model independently.

Table 1. Advantages and limitations of ANN-based models [27]

Advantages	Limitations
Easy for correlation of data although absent of suitable function	Hard to interpret and analyze the output
The model can easily be developed and took less time to be developed compared to other models	The training of the data might take much time, even days
No theoretical knowledge of process and literature parameters needed to develop the model	A large set of experimental data needed covering wide operating conditions needed because of he training of an ANN used the experimental data
It can handle noise, incomplete and inconsistent data whenever the over-fitting is avoided	The architecture depends on the variation of conditions when trained and cannot be predicted

The ‘black-box’ nature of ANN models and unsatisfactory extrapolation by ANN models have led to the development of hybrid neural network models which combine ANNs with simple models. These are expected to perform better than ANNs in process identification tasks, since generalization and extrapolation are confined only to the uncertain parts of the process while the basic model is always consistent with first principles [28].

In a study on quercetin extraction from *Rosa damascene* Mill an experiment was conducted using a modified supercritical CO_2 with ethanol as co-solvent [19]. The recovery of extraction was predicted using Adaptive neuro-fuzzy inference system (ANFIS) and Artificial neural network (ANN). The variables were translated into coded value of -2, -1, 0, +1 and +2. Table 2 shows the coded variables for this process. The coded variables are usually applied when RSM, ANN and ANFIS is going to be used as tools for optimization process.

Table 2. Uncoded and coded levels of independent variables used in the RSM, ANN and ANFIS

Coded variables	Temperature, T (°C)	Pressure, P (MPa)	Dynamic time, t (min)	Flow rate of CO_2, Q (ml/min)
-2	35	10	40	0.3
-1	40	15	60	0.6
0	45	20	80	0.9
+1	50	25	100	1.2
+2	55	30	120	1.5

Generally, ANFIS architecture consists of 5 layers as shown in Figure 3. The architecture of ANFIS in Figure 3 maps the inputs through input membership functions (MF) and fuzzy rules. Similarly, output mapping is done through output membership functions along with its fuzzy rules. The number of membership function assigned to each input variable is chosen by trial and error. Figure 3 shows the general architecture of ANFIS for SFE system.

The hybrid of a neural network and fuzzy logic in ANFIS makes it have both, low-level learning and computational power of neural network and advantages of high-level human like thinking of fuzzy systems. Therefore, this neuro-fuzzy model able to overcome their individual disadvantages and can complement each other [29].

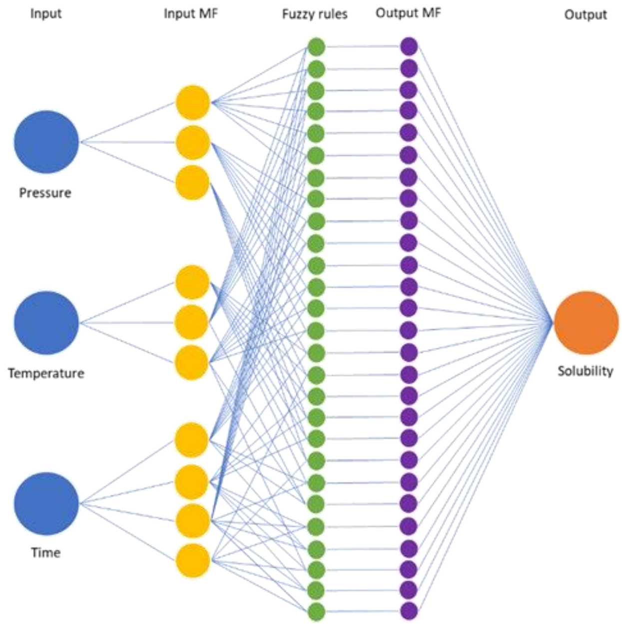

Figure 3. ANFIS architecture

4. MATHEMATICAL MODEL-NEURAL NETWORK HYBRID

Hybrid models can also be combining both physical laws and observed measurements and including all available knowledge of the process. This model can be arranged in series or in parallel. In the series approach, heuristic model estimates unmeasured process parameters of mathematical modeling such that the first principle constrains are satisfied. In the parallel approach, the hybrid model prediction is combination of the outputs of the mathematical and initial heuristic models thus residuals between the process and the mathematical model is compensated [27]. This type of hybrid can solve the black box issues of neural network where the knowledge of the process is lacking. When combining both, the model will become more reliable and can represents the data well.

A parallel hybrid model was developed by researchers from Iran [13] for prediction of Epigallocatechin gallate (EGCG) recovery of supercritical extraction which combines conventional mathematical modeling based on the differential mass balance in the solid and mobile phases with ANFIS (Figure 4). Using analytical model in this structure, the accuracy of ANFIS would be increased in non-training domains. Additionally, ANFIS solves the problem of unknown analytical parameters. In other words, the hybrid model could simulate the extraction system with having any arbitrary value of adjustable parameters of mathematical modeling [27].

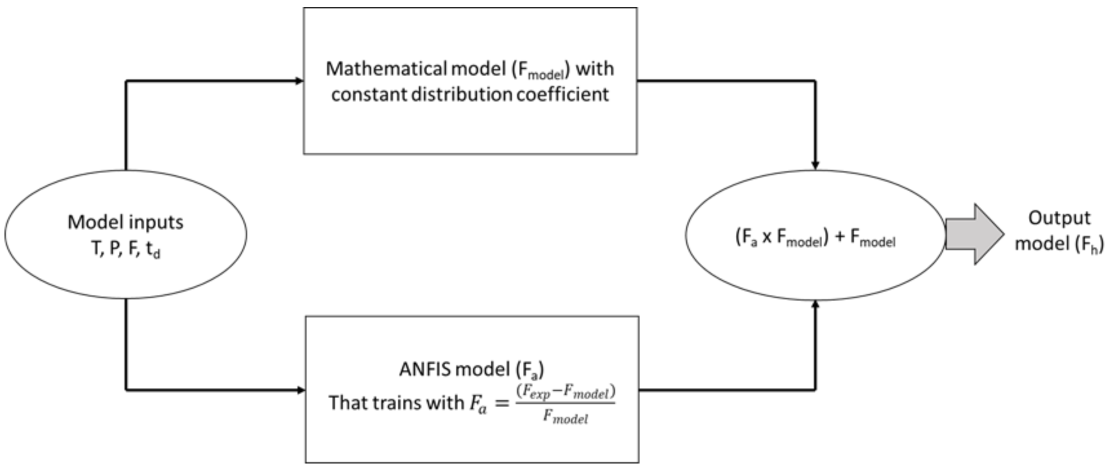

Figure 4. Parallel combination of mathematical model and ANFIS network in a hybrid structure by [15]

In 2003, a group of researchers from Canada proposed a hybrid model of Radial Basis Function-Peng Robinson (RBF-PR) model. The hybrid model was developed by first developing a simple RBF model. A simple RBF model consist of three inputs of T, p and other factors with one output which is yield rate. This model has no knowledge on the whole process. To overcome the black box problem of the RBF model, the model is correlated with the Peng-Robinson equation becomes a hybrid RBF-PR model (Figure 5). In the Peng-Robinson equation of state, there is unknown interaction parameter k_{12}, for a binary mixture, whereby the predicted solubility is sensitive. The k_{12} can be obtained from the physical property data for the mixture, but it requires trial and error process for obtaining it. Besides, the parameters were all temperature dependent which does not really fit the data compared to pressure. The proposed hybrid model by [30] can compensate the black box problem. It can fit the experiment data very well and also keep the physical meaning of the whole SFE process. The detailed description on previous research applying ANFIS and the hybrid of it for yield and solubility prediction is shown in Table 3.

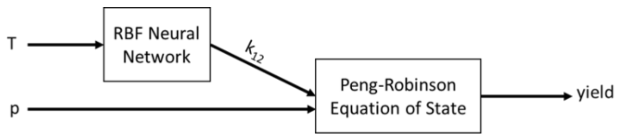

Figure 5. Schematic diagram of the proposed hybrid model by [31]

Table 3. Compilation of research applying hybrid model-ANFIS tools for predicting yield and solubility for SFE

Model	Sample	Extract	Purpose	Remarks	References
ANFIS	Solid compound	-	Estimation of solubility	The input parameters: critical pressure, acentric factor, critical temperature and molar volume as well as the operating temperature and pressure The output parameter: solubility	[13]
ANFIS	*Pimpinella anisum L.* seed	Seed oil	Prediction mass of extract	The input parameters: pressure, solvent mass flow rate, and extraction time The output parameter: mass of extract Within 369 observations, 277 observations were used to train the network, and the remaining 92 observations were kept for further testing the developed network	[14]
ANFIS	*Glycyrrhiza glabra L.*	Glycyrrhizic acid (GA)	Modeling the recovery of extraction	Independent variables: dynamic time (t), pressure (P), temperature (T) and flow rate of SCCO2 (Q). Dependent variable: Recovery of GA	[19]
ANFIS	Pomegranate	Seed oil	Simulation of oil yield	Comparing the data obtained between ANN and ANFIS model	[20]
ANFIS	Rosa damascene Mill	Quercetin	Modeling the recovery of extraction	Independent variables: dynamic time (t), pressure (P), temperature (T) and flow rate of SCCO2 (Q). Dependent variable: Recovery Comparing the data obtained between ANFIS and RSM Refer Table 2	[21]
RBF-PR hybrid	Benzoic acid	-	Modeling the yield	Input parameters: Temperature, pressure and one other factors Output parameter: yield rate Mathematical model: Peng-Robinson model Refer Figure 5	[31]
Mathematical model-ANFIS hybrid	Green tea	Epigallocatechin gallate (EGCG)	Modeling the recovery of extraction	Input parameters: dynamic time, pressure, temperature and flow rate of SC-CO2 Output parameter: model output Mathematical model: differential mass balance in the solid and mobile phases model Refer Figure 4	[15]

5. GENETIC ALGORITHM (GA)

Genetic algorithms are a class of optimization programs that can handle complicated problems. They consist of a random-search method, that made efficient by using explorative search. The method resembles evolutionary development in nature, using “mutation” and “mating”. In contrast to expert systems no heuristic knowledge is applied other than the ultimate goal [32].

In 2016, a group of researchers in Iran did an optimization of essential oil extraction from *Launaea acanthodes Boiss* using genetic algorithm [33]. In their study, they applied the hybrid ANN-GA methodology whereby, ANN model was used as the fitness function, which measures the quality of individuals in the population. The model was then used to obtain the optimal operation conditions, such as pressure, temperature, flow rate, and co solvent besides determining the maximum extraction yield of essential oil from *L. acanthodes*. The general procedure to apply GA for most system was as shown in Figure 6. Table 4 has the description of previous application of GA in SFE for various materials.

Figure 6. Genetic algorithm procedure for optimization process

Table 4. Genetic algorithm application for optimization in SFE

Sample	Extract	Purpose	Remarks	References
Launaea acanthodes Boiss	Essential oil	Optimization of extraction yield	ANN model was used as the fitness function, which measures the quality of individuals in the population	[33]
Soybean meal	Isoflavone	Optimization of profitability	The objective function of this study is profitability which is more comprehensive than the cumulative isoflavone production rate	[24]
Green tea	Epigallocatechin gallate	Optimization of extraction recovery	The fitness function for this study is extraction recovery	[25]
Macela flowers (*Achyrocline satureioides*)	Bioactive compound	Determination of constant	Adjustable parameters, K, a, and b, were determined by criteria that the sum of the squares of the difference between the experimental extraction yield and the predicted extraction yield by the model should be minimized	[28]
Solid compounds	-	Optimization of the radius of influence of FIS	The Genetic Algorithm (GA), which is an optimization algorithm, was implemented to measure the optimum value of radius of influence of FIS parameter	[13]
Ferulaga angulate	-	Optimization of yield	The ANN model coupled with genetic algorithm (GA) was used to generate the optimal value	[34]
Benzoic acid	-	Dynamic optimization of process	A dynamic optimization model for supercritical fluid extraction is proposed by combining a transformation based genetic algorithm and the Peng-Robinson equation of state	[35]

6. CONCLUSION

Overall, the application of smart system or artificial technique to model and simulate a chemical process has been done in SFE process together with RSM method. Smart system models generalize the experimental result and present process behavior and finally predict and estimate problem. The model can be applied individually or by combining two or more models called as hybrid to achieve the best estimation and prediction data. The appropriate model is beneficial in the development of new products by saving experimental time and cost. However, research and study on dynamic process for SFE using artificial technique is lacking and the area is recommended for further research.

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BIOGRAPHIES OF AUTHORS

Sitinoor Adeib Idris received her bachelor's and master's degrees in chemical engineering from Universiti Teknologi MARA (UiTM), Shah Alam, Selangor, Malaysia. She is a PhD student at the Department of Chemical Engineering and Process, Faculty of Engineering and Built Environment, at Universiti Kebangsaan Malaysia (UKM), Bangi, Selangor, Malaysia. Her research is in the field of supercritical fluid extraction.

Masturah Markom is an associate professor of Chemical Engineering at the Department of Chemical Engineering and Process, UKM. She received her PhD in 2007 and master's degrees in chemical engineering from Universiti Malaya (UM) in 1998. Her research interest are separation technology and supercritical fluid extraction.