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Energy Procedia 17 (2012) 770 – 775

Energy Procedia

2012 International Conference on Future Electrical Power and Energy Systems

# Optimization of Process Parameters for Molecular Distillation Based on NN and GA

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**Abstract**

In order to obtain the optimum craft parameters and improve the product purity and yield,a new optimization design method based on NN and GA is proposed. The neural network is used to build the model of target function, namely, a mapping relationship from craft parameters to purity and yield is established. Taking many craft parameters(feed rate,vacuum, and temperature) as optimal variables, purity and yield as optimization target,the optimization model is build and advance optimizing quality and decrease the number of times of numerical simulation. In this article, the essential oil of schisandra chinensis was produced according to the technology of molecular distillation. The technological parameters were optimized. The process and result prove that this method is effective.



*Keywords-molecular distillation;neural network; genetic algorithm; optimization*

## 1. Introduction

Molecular distillation is a special separation technique, which is widely used in fine chemical, food, medicine & health care and so on. the parameters of feed rate ,vacuum, and temperature directly influence purity and yield of substance by molecular distillation. How to consider these factors so that a very good separation effect can reach has been becoming main considerations in process parameters design of molecular distillation. The process of numerical simulation would be too complex, getting result slowly. The effects of different parameters on the separation result are difficult to study. This paper presents a thorough study of the essential oil of schisandra chinensis, with the purpose to improve optimization efficiency. Taking the process parameters as optimal variables, purity and yield as optimization target, optimization model of parameters is established combined with neural networks algorithm .

## 2. The establishment of optimization model for molecular distillation

 doi:10.1016/j.egypro.2012.02.169

*2.1 Optimal variables determining*

There are many influence factors in molecular distillation. Optimal variables are finally identified, which are temperature, feed rate, wiped film speed, operating pressure, ingredient content and vacuum. There is that ingredient content dealt with as uncontrollable variable, wiped film speed,vacuum and operating pressure as optimal variables,others as optimal variables that need to be optimized. For different materials,the requirements of optimum craft parameters are different. Even it has a good separating efficiency for the differences in the composition of materials, there were differences in processing condition. So, it is needed to accuratly determine parameters depending on the differences of materials or the composition。

*2.2 The determination of the objective function*

The purpose of the molecular distillation is to obtain relatively high yield and purity of the essential oil of schisandra chinensis, which can meet or near the targeted value. The purity is y1 the yield is y2, respectively. The value of goal is T1,T2. The optimizing problems can be showed as formula(1)：

$$\min\{|Y_1(U)-T_1|,|Y_2(U)-T_2|\} \tag{1}$$

*2.3 The determination of the optimization model*

The functions(Y1(U),Y2(U)) between the technology parameters and the yield and purity are very difficult to obtain because of the complicacy of the molecular distillation, which makes that the multiple objective optimization is at a dead end. The mapping relationship from parameters to purity and yield based on neural network takes the place of Y1(U),Y2(U) as the objective function. the final target function called f(U) is obtained by proportion sum with two objective functions. As shown in Figure 1.

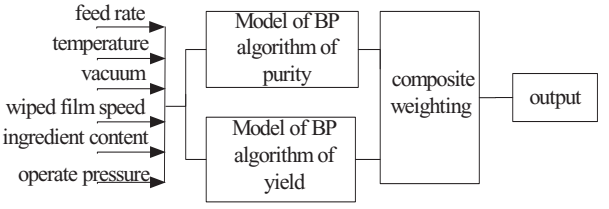


Figure 1. Transform of multi-object function

## 3. Modeling of craft parameters for molecular distillation

Artificial neural network is a kind of algorithm mathematical model model, which imitates animal neural networks, makes distributed parallel information processing. It can realize the capacity of generalization, analogy, dissemination that are similar functions to human brain. BP neural network occupied dominant position in actual engineering at the present time.

Theoretical analysis shows that the three-layer BP network model, which has deviation, at least one hidden layer with S and linear output layer, can approximate any nonlinear continuous functions with any precision. Although the effects of temperature, feed rate on the purity and the yield, there is not definitely functions, a neural network model is established to obtain the mapping relationship between the parameters and the purity and yield by training neural network. Using this model,molecular distillation effect can be gained in different technological parameters rapidly and copiously. The topology of the Neural Network is shown in Figure 2.

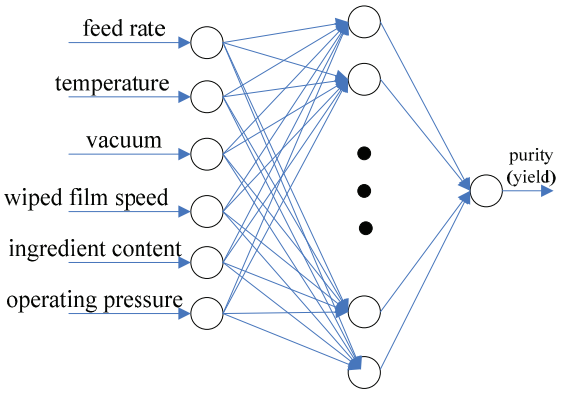


Figure 2. Topology of training neural networks

The BP neural network model is determined by inspection data. The model is accepted if errors do fall within the prescribed limits.Otherwise regulate the parameters of the network or retrain samples. Flow chart is shown in Fig 3.

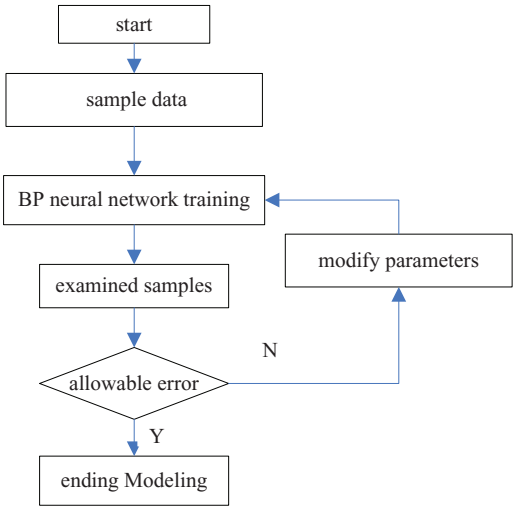


Figure 3. Flow chart of network training

## 4. Method of multi-objective optimization

Artificial neural network has strong capacity of approximation of functions. The mapping relationship between the parameters and the purity and yield can be created with less numerical simulation, which not only insures accuracy but also decrease the number of times of numerical simulation. The objective function value is forecasted with approximation function of BP neural network model,which can realize the real-time solution of adaptive value in the subsequent iterations and decrease the number of numerical simulation. The genetic algorithm as optimization algorithm improves greatly the accuracy and efficiency.

Following is optimal mathematical model:

Optimization variable $U=U(u_1,u_2,u_3\ldots u_6)$

Optimization objective

$$\min\{f(U)\} \tag{2}$$

$$\begin{cases} y_1 = g[v_1 f[w_1[u_1,u_2,u_3,u_4,u_5,u_6]^T - \theta_1] - \gamma_1] \\ y_2 = g[v_2 f[w_2[u_1,u_2,u_3,u_4,u_5,u_6]^T - \theta_2] - \gamma_2] \\ f(U) = W1 * \dfrac{|y_1 - T_1|}{|T_{1\max} - T_{1\min}|} + W2 * \dfrac{|y_2 - T_2|}{|T_{2\max} - T_{2\min}|} \\ T_{1\max} > T_{1\min}, T_{2\max} > T_{2\min}, W1 + W2 = 1 \\ 0.1 \le u_i \le 0.9 \qquad i = 1,2,3,4,5,6 \end{cases} \tag{3}$$

The objective formula is min{$f(U)$}.In Formula 3,$y_1$ and $y_2$ denote respectively purity and yield that are calculated with the neural network model. The $u_1$,$u_2$,$u_3$,$u_4$,$u_5$,$u_6$,denote respectively running efficiency after data normalization. Where,$f[\cdot]$ is asymmetrical function called *S*, $g[\cdot]$ is linear function. $W1$ and $W2$ denote respectively weights of two targets. The $f$(U) is objective functions by proportion sum with purity and yield.

## 5. The solution of optimization target by using the genetic algorithm

### *5.1 The optimization step of genetic algorithm:*

(a) Binary coding and initialization of craft parameters.
(b) Decoding, convert binary number to decimal number.
(c) Selection, the individual that has greater adaptive value is used to mate with probability.
(d) Crossover and mutation, the new generation is formatted by performing operations on mating individual with crossover and mutation.
(e) Repeat step a) to step d), until the criterion of convergence is met.

### *5.2 Review on the optimization results*

Genetic neural network model has wide suitability because the neural network is a black box model and the genetic algorithms seldom limit the objective function.The special place of this design is that introduces neural network to the adaptive function of genetic algorithm. Molecular distillation has a much better effect for BP Net combinating optimizing effect of genetic algorithm; Neural network is a kind of constraint for genetic algorithm. The optimized scope is within practical scope with the simulation of BP.

To compare the optimizing effect of multiple-target optimization optimizing effect under different weights, optimizing experiments of 11 times are carried out with different coefficients of weight respectively based the production data molecular distillation. The weight coefficient of purity is W1, the values of which are 0,0.1,0.2,...,0.9,1.0. The relation between the relative error of optimization value of temperature and the weight coefficient of purity is shown in Figure 4. The relation between the relative error of optimization value of feed rate and the weight coefficient of purity is shown in Figure 5.

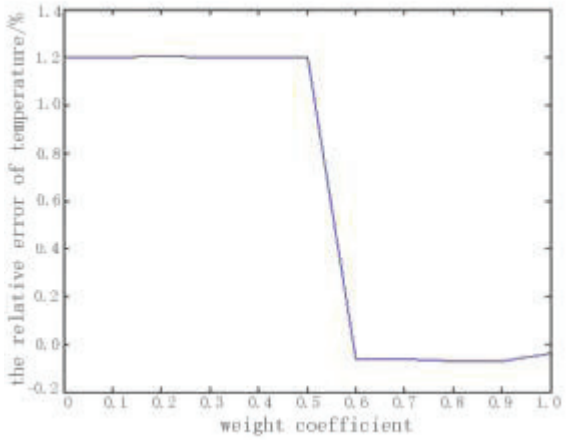


Figure 4. The relative error of optimization value of temperature

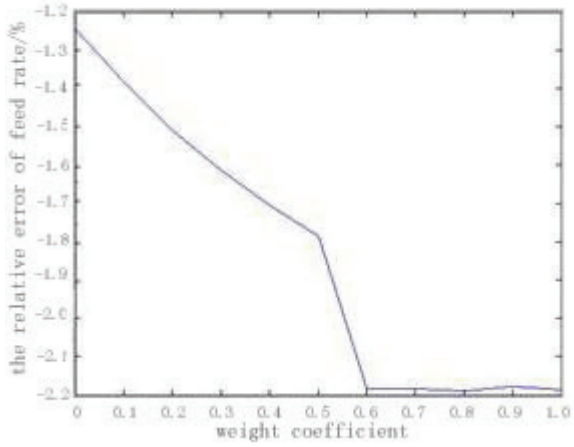


Figure 5. The relative error of optimization value of feed rate

## 6. Conclusion

In this paper, optimization design method based on NN and GA is introduced into the system of molecular distillation and better result has been achieved, so as to provide learning methods for the solution of similar technology and multi-aim optimization problem. According to different requirements of circumstances, selecting a proper network structure and genetic algorithm and constructing exactly target functions could solute the corresponding problems.

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