Inverse Model to Determine the Optimal Number of Drops of RDC Column Using Fuzzy Approach

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Abstract: - Inverse modeling is natural in many real world application including industrial chemical engineering problems. This paper describes the process of determines optimal input and output of number of drops in various stage of rotating disc contactor column using fuzzy model. An algorithm of the fuzzy model is developed to simulate the above process.

Key-Words: - Liquid-Liquid Extraction, RDC Column, Drop Distribution, Inverse Model, Fuzzy Environment, Fuzzy Algorithm.

1 Introduction

Liquid-Liquid Extraction is a process of separating components of a liquid using other liquid. The process of liquid-liquid extraction is commonly used in chemical, biochemical, biotechnology and Industry.

Many types of devices have been used over the years in solvent extraction processes, but the Rotating Disk Contactor (RDC) is the most widely adopted since it was developed by the Royal Dutch/Shell Group in the middle of the last century.

The geometrical properties of RDC column consists of a series of stages separated by equally spaced horizontal stators [1, 2] (see Fig.1 [9]).The RDC column has several advantages such as simplicity in construction, high throughput and low power consumption [2]. The mathematical modeling of RDC column is usually concern with the drops distribution and drops diffusion. Both forward model and inverse model are used to predict the distribution of drops, we can describe the forward model in general as a process in obtaining values of outputs of drops distribution by using input of average drop diameter. The output obtained in the forward model is used in the inverse model to determine the value of the input parameters for a desired value of the output parameters [3].



The basic principles of fuzzy modelling were laid by Zadeh [4] in 1973. There are three principles in developing a fuzzy model, the use of linguistic variables in place of or in addition to numerical variables, the characterization of simple relation between variables by conditional fuzzy statements and the characterization of complex relation by fuzzy algorithms. These principles from the basic of two methods used for fuzzy modelling, namely the direct approach and system identification. In the first method, the system in first described linguistically using term from natural language and then translates into the formal structure of a fuzzy system. The second method is developed from structure identification to the parameters identification.

2 Drop size distribution

This section discusses the procedure of the Expected Value Method (EVM) to determine drop size distribution [5]. The drop size distribution is later used as an input value to our fuzzy model. The Expected value method depends on four steps which are the bulk breaking process, the determination of number of drops broken, number of daughters produced from broken drops and number of daughter in each class.

The detailed procedure is given below

2.1. General

We define the stage of RDC column as collection of classes between stators and rotators. Shown in Fig.2



Fig.2 Stages and Classes

Tables 1 and 2 show the geometrical properties of RDC column and physical properties of system used.

Table 1: The Geometrical Properties of RDC Column

Geometrical properties of RDC							
Number of stages	23						
Height of compartment(m)	0.076						
Diameter of rotor disk (m)	0.1015						
Diameter of column (m)	0.1520						
Diameter of stator ring(m)	0.1110						
Rotor speed (rev/s)	4.2						

Table 2: Physical Properties of the System Used.

Physical properties of the system (cumene/isobutyric acid /water)						
Continuous Phase: isobutyric acid in water						
Dispersed Phase: isobutyric acid in cumene						
Viscosity of continuous phase (kg / ms)	0.100E-2					
Viscosity of dispersed phase (kg / ms)	0.710E-3					
Density of continuous phase (kg / m^3)	0.100E+4					
Density of dispersed phase (kg / m^3)	0.862E+3					
Interfacial tension (mN/m)	31.7					

The initial drop size will be used the basis for the calculation of the classes size [5]. If the initial drop diameters is d_0 , and the required number of classes is N_{cl} , then the size of the class j, c_j which will hold drops of class j with diameters between $d_{E,j}$ and $d_{E,j+1}$ is

$$c_{j} = d_{E,j+1} - d_{E,j} \tag{1}$$

Where $j = 1, ..., N_{cl}$ and $d_{E,j} = \frac{d_0}{N_{cl}} \times (j-1), j = 1, ..., N_{cl}$ (2)

In many mass transfer and flow processes it is

desirable to work only with average diameters instead of the complete drop size distribution (Mugele and Evans [1951]). Since the volume of a drop is important in the calculation of the mass transfer performance, the average diameter is obtained by averaging the volume of the drops, rather than taking the arithmetic average diameter. Assuming that the drops are randomly produced and the diameter of the drops are uniformly distributed in each class, the volume average diameter $d_{av,j}$ of drops in class j, whose diameter ranges from $d_{E,j}$ to $d_{E,j+1}$, $j = 1, ..., N_{cl}$ can be written as

$$d_{av,j} = \left[\frac{1}{4} \left(d_{E,j} + d_{E,j+1}\right) \left(d_{E,j}^{2} + d_{E,j+1}^{2}\right)\right]^{\frac{1}{3}}$$
(3)

Then the critical drop size d_{cr} is obtained by

$$\frac{d_{cr}}{D_r} = 0.685W e_{D,w}^{-1.2} \operatorname{Re}_{D,w}^{0.7}$$
(4)

Where

$$We_{D,w} = \frac{\rho_c \omega^2 D_r^3}{\gamma} \tag{5}$$

$$Re_{D,w} = \frac{\rho_c \omega D_r^2}{\mu_c} \tag{6}$$

Equations (5) and (6) are disc angular Weber number and a Reynolds number respectively.

And found correlation for critical drop size and rotor speed [6], suitable for their wide ranges of experimental data in different size column (152,300,600 mm):

Equivalent to:

$$\omega_{cr} = 0.802 \frac{\gamma^{0.7}}{\rho_c^{0.3} \mu_c^{0.4} d^{0.59} D_r^{0.71}}$$
(7)

Where $\omega = 2\pi N$ the angular rotor speed and ω_{cr} denote the critical angular rotor speed appropriate to drop size *d*.

To obtain the probability of breakage for classes with average drop size larger than the critical drop size. Cauwenberg [7] used a modified angular Weber number in equations (8) and (9) for laminar $(\operatorname{Re}_{D,\omega} < 10^5)$ and turbulent $(\operatorname{Re}_{D,\omega} \ge 10^5)$ respectively :

$$P = \frac{0.258We_{D,\omega,m}^{1.16}}{1 + 0.258We_{D,\omega,m}^{1.16}}$$
(8)

$$P = \frac{0.00312We_{D,\omega,m}^{1.01}}{1 + 0.00312We_{D,\omega,m}^{1.01}}$$
(9)

Where

$$We_{D,\omega,m} = \frac{\rho_c^{0.5} \mu_c^{0.5} \left(\omega^{1.5} - \omega_{cr}^{1.5}\right) D_r d}{\gamma} \quad (10)$$

for (laminar)

$$We_{D,\omega,m} = \frac{\rho_c^{0.8} \mu_c^{0.2} \left(\omega^{1.8} - \omega_{cr}^{1.8}\right) D_r^{1.6} d}{\gamma}$$
(11)

for (turbulent)

2.2. Simulation result

In this section we can describe Expected Value Method process, as two parts the first for first stage is called Bulk Breaking Process see Fig.3 and the second part for all stage also using BBP for all classes of previous stage to get new stage.

In the simulation of drops break-up using this method, the bulk breaking process will be applied to the swarm of drops from the moment the swarm of drops enters the column. As the swarm of N drops hits the first rotor disc, since the diameters of all drops entering from the distributer are larger than the critical drop size d_{cr} , they will undergo all the steps of the bulk breaking process, which produces number of daughter drops in the classes of the first stage.

After obtaining the drops in each classes of the first stage, the bulk breaking process is used again on the swarm of drops in each class. Assuming that the average diameter of drops in some of the classes of the first stage is greater than the critical drop size d_{cr} , then as the swarm of daughter drops in each class of the first stage hit the second rotor disc, only those drops in a class with average diameter greater than the

critical drop size will undergo the bulk breaking process, which produces is turn number of daughter drops in the classes of the second stage. The drops in the class with average diameter less than critical drops size will just move to next stage without breaking.

In general, the number of daughter drops in the classes of the ith stage can be obtained by applying the bulk breaking process, class by class to the swarm of drops in the (i-1)th stage.





Fig.3 Bulk Breaking Process

After use all equations and using Expected value Method we get the simulation of distribution of Number of drops for all stages, we can show in Table 3 the number of drop distribution in each class of stage 1 and also in table 4 shows the number of drops of each class of stage 5.

 Table 3: Drop Distribution (Stage1)

Class	1	2	3	4	5	6	7	8	9	10
No. of drops	1	7	20	38	60	84	107	121	117	768

Table 4: Drop Distribution (Stage5)

Class	1	2	3	4	5	6	7	8	9	10
No. of drops	6	38	96	172	247	299	310	275	204	267

3 Fuzzy Flow Chart

This flow chart introduce by Ahmed [8] to describe input and output process using fuzzy approach. The three steps processes are Fuzzification, Fuzzy environment and Defuzzification.



Fig.4 Fuzzy Flow Chart

3.1. Fuzzification

Variables involved in an engineering design are usually referred to as parameters which are classified as input, output and performance parameters. In our problem the input parameters are the geometrical configuration and physical properties, and the input number of drops. The geometrical configurations are the diameters of rotor disc, the column, the rotor speed etc. Meanwhile the physical properties are the viscosity and the density of the continuous and dispersed phase etc. The output parameters are the number of drops. In this model, we assume that the input parameters of the geometrical configurations and physical properties are fixed for certain values. These values are taken from experimental data (see Tables 1 and 2). The performance parameter is also assumed to be fixed. The actual input parameters of the model are the input number of drops. On the other hand the output parameters are the output number of drops.

3.2. Fuzzy Environment

The fuzzified input parameters from fuzzification phase are then used to determine the induced output parameters. This process can be done by assuming that all the fuzzy sets (taken from the previous phase), F_{Pi} , express preferences of all input parameters $p_i \in P_i$ with $P_i \subset R^+$ to be determined, normalized and convex, P is a closed interval positive real number.

In this phase, the input, output and performance parameter must be determined. We should also be able to specify the model or function (Expected Value Method) used which map the input parameters to the output parameters.

3.3. Defuzzification

In this phase the optimal combination of the input parameters will be determined. First we must determine the $\alpha - cut$ for F_{Pi} of the corresponding f^* . After this value has been determined, all 4 combinations of the endpoints of the intervals representing $\alpha = f^* - cut$ must be generated. These four combinations of inputs values are actually the possible solutions of the problem.

In the fuzzy flow chart, the process of input and output based on algorithm done by Maan(2005), the number of drops in stage 5 (classes 5 and 6) is obtained using input value of number of drops in stage 1 (classes 5 and 6). The optimal number of drops and errors are also shown.

4 Fuzzy Algorithm

Step 1: input parameters with domain and output parameters with domain.

Step 2: select appropriate value of $\alpha - cut$ such that $\alpha_1, \alpha_2, ..., \alpha_k \in (0, 1]$.

Step 3: for each P_i (input parameters) determine the end points of all $\alpha_k - cut$, F_{P_i} (i = 1, 2).

Step 4: for each Q_i (output parameters) determine the end points of all $\alpha_k - cut$, for preferred output parameters F_{OP} (i = 1, 2).

Step 5: generate all 2^m combinations of all endpoints of intervals representing $\alpha_k - cut$. Each combination is an m-tuple (in this problem m=2).

Step 6: determine r_j (using EVM) for all combination from step 5, $j = 1, 2, ..., 2^m$.

Step 7: for each $\alpha - cut$, determine the induced output parameters, F_{ind} by taking the min value and max value of each element of i, let

$$F_{ind} = \left[\min r_j \wedge \max r_j\right]$$

for all $j = 1, 2$

Step 8: set $F_{QP} \wedge F_{ind}$ and find the fuzzy number of $f^* = \sup(F_{QP} \wedge F_{ind})$.

Step 9: find the α -*cut* of F_{Pi} for corresponding value of f^* .

Step 10: repeat steps 5 and 6 for $\alpha = f^*$ and denote the corresponding output parameters as r_{j}^* for each $j \in [1, 2, ..., 2^m]$.

Step 11: determine the optimal combination of input parameters and stop.

Now applied fuzzy algorithm on stage 1 (classes 5 and 6) and stage 5 (classes 5 and 6) to show the effect.

Table 5: Preferred Input Value

Input parameters	Domain	Suggested value		
Class 5	[45 75]	60		
Class 6	[62 106]	84		

Table 6: Preferred Output Value

output parameters	Domain	Suggested value
Class 5	[185 309]	247
Class 6	[221 377]	299

These values in tables 5 and 6 are now ready to be fuzzified by the triangular membership function. Figures 4 and 5 show the triangular fuzzy number of the preference input and output parameters respectively. The two limits of domain will have fuzzy value of zeroes whereas the suggested value will be assigned a fuzzy value equal to one.



Fig.5 Triangular Fuzzy Number of Input Parameters.



Fig.6 Triangular Fuzzy Number of Output Parameters.

Now using suitable $\alpha - cut$ as 0, 0.2, 0.4, 0.6, 0.8 and 1. all the input and output parameters obtained from Figures 4 and 5, for example take $\alpha = 0.2$, then the $\alpha = 0.2 - cut$ for preferred input is

$$A_{\alpha=0.2} = \left\{ p_i \in P_i \, | \, \mu_A(p_i) \ge 0.2 \right\}$$

If i=1, and $\alpha = 0.2 - cut$ is

$$A_{\alpha=0.2} = \left\{ p_1 \in P_1 \mid \mu_A(p_1) \ge 0.2 \right\}$$

= $\left[45 + 0.2(60 - 45), 75 - 0.2(75 - 60) \right]$
= $[48, 72]$

The same procedure is used to calculate the $\alpha - cut$ for each values are the listed in tables 7 and 8.

The next step is to generate all the possible combinations of the endpoints of the interval representing each $\alpha - cut$ for the input parameters. We have 4 combination of 2-tuple for each $\alpha - cut$. Shown in table 9.

Input parameters	$\alpha - cut$ values							
	0.2	0.4	0.6	0.8	1			
Class 4	[48.0 72.0]	[51.0 69.0]	[54.0 66.0]	[57.0 63.0]	[60.0 60.0]			
Class 5	[66.4 101.6]	[70.8 97.2]	[75.2 92.8]	[79.6 88.4]	[84.0 84.0]			

Table 7: $\alpha - cut$ Values for Input Parameters

Table 8: $\alpha - cut$ Values for Output Parameters

Output parameters	$\alpha - cut$ values						
	0.2	0.4	0.6	0.8	1		
Class 4	[197.4 296.6]	[209.8 284.2]	[222.2 271.8]	[234.6 259.4]	[247.0 247.0]		
Class 5	[236.6 361.4]	[252.2 345.8]	[267.8 330.2]	[283.4 314.6]	[299.0 299.0]		

Table 9: the Combination for Each α – *cuts* Values Parameter

Combination of input (class 4 & class5)	$\alpha - cut$ values						
	0.2	0.4	0.6	0.8	1		
1 st combination	(48.0 66.4)	(51.0 70.8)	(54.0 75.2)	(57.0 79.6)	(60.0 84.0)		
2 nd combination	(48.0 101.6)	(51.0 97.2)	(54.0 92.8)	(57.0 88.4)	(60.0 84.0)		
3 rd combination	(72.0 66.4)	(69.0 70.8)	(66.0 75.2)	(63.0 79.6)	(60.0 84.0)		
4 th combination	(72.0 101.6)	(69.0 97.2)	(66.0 92.8)	(63.0 88.4)	(60.0 84.0)		

Now using EVM to get the output parameters, show in Table 10

Table 10: the Output of Each Combination of Each α – *cuts*

Combination of input (class 4 & class5)	$\alpha - cut$ values					
	0.2	0.4	0.6	0.8	1	
	Class4 class5	Class4 class5	Class4 class5	Class4 class5	Class4 class5	
1 st combination	68.4 107.6	69.4 108.6	70.4 109.6	70.4 110.6	71.4 111.6	
2 nd combination	68.4 114.6	69.4 113.6	70.4 112.6	70.4 111.6	71.4 111.6	
3 rd combination	74.4 107.6	73.4 108.6	73.4 109.6	72.4 110.6	71.4 111.6	
4 th combination	74.4 114.6	73.4 113.6	73.4 112.6	72.4 111.6	71.4 111.6	

After that find the induced output parameters F_{ind} . The induced output parameters can be obtained by taking the minimum and maximum value (endpoints of interval) for each element of output parameters. As an example, in Table 10, the output of number of drops is equal to 68.4 and 74.4(class 4) for each input combination of $\alpha = 0.2$ in this procedure take the minimum value is 68.4 and maximum value of 74.4. This indicates that $\alpha = 0.2$ -cut for the first induced output parameter is [68.4, 74.4]. The same process is repeated for different values of alpha to obtain the corresponding $\alpha - cut$.

Now we can show the intersection between induced and preferred output in Figures 6 and 7



Fig.7 Intersection between Induced and Preferred Output for Class 5.



Fig.8 Intersection between Induced and Preferred Output for Class 6.

The intersection point z= 0.999 and z=997 respectively. These f^* – values are then processed in the defuzzification phase. In this phase, defuzzification is carried out to get the

best possible combination of the input parameters in order to produce the output parameters which are close to the desired output value. Each of the four combinations of the endpoints of the interval is determined and these values are then used to calculate the output parameters. All the data are given in Tables 11 and 12.

Table 11: Input Combination with Fuzzy Value z = 0.999.

Combination of input	Input value		
1 st combination	(59.985	83.978)	
2 nd combination	(59.985	84.022)	
3 rd combination	(60.015	83.978)	
4 th combination	(60.015	84.022)	

Table	12:	Input	Combination	with	Fuzzy	Value	z =
0.997.		-					

Combination of input	Input valu	e
1 st combination	(59.955	83.934)
2 nd combination	(59.955	84.066)
3 rd combination	(60.045	83.934)
4 th combination	(60.045	84.066)

For the four combinations of the input parameters given in Tables 11 and 12 we have to choose only one combination which can provide the optimal solution.

Also to output

Table 13: Output Combination with Fuzzy Value z = 0.999.

Combination of output	output value	e
1 st combination	(246.983	298.922)
2 nd combination	(246.983	299.078)
3 rd combination	(247.062	298.922)
4 th combination	(247.062	299.078)

Table 14: Output Combination with Fuzzy Value z = 0.997.

Combination of output	output value	
1 st combination	(246.814	298.766)
2 nd combination	(246.814	299.234)
3 rd combination	(247.186	298.766)
4 th combination	(247.186	299.234)

For the four combinations of the output parameters given in Tables 13 and 14 we have to choose only one combination which can provide the optimal solution.

Table 15: Optimized Input Parameters (Stage 1)

Input parameters	Calculate input value	Preferred value	Error(%)
Class 5	59.985	60	0.025
Class 6	83.978	84	0.026

 Table 16:
 Optimized Output Parameters (Stage 5)

Output parameters	Calculate output value	Preferred value	Error(%)
Class 5	247.062	247	0.025
Class 6	299.078	299	0.026

The values of the input parameters for desired values of the output parameters are successfully determined. The values are shown in Tables 15 and 16. The input values differ from the preferred values with an error of 0.025% and 0.026% respectively. The percentage error for each of the output parameters of the system are 0.025% and 0.026% respectively.

5 Conclusions

This work describes the inverse model identify the number of drops of each class. The optimal number of drops depends on the result obtained by the Expected Value Method. An effective fuzzy algorithm gives error between induced value and preferred value less than 1%.

Nomenclature:

D _r	R otor diam eter
d ₀	initial drop diam eters
d _{E,j}	D rop size L im it for each drop size class.
d _{c,r}	Critical drop size
$d_{av,j}$	average diam eter
We _{D,m}	M odified disc W eber num ber
We _{D,ω}	disc angular W eber num ber
We _{D,ω,m}	M odified disc angular W eber num ber
R e _{D,w}	Reynolds number
γ	Interfacial tension
μ _c	Continuous phase viscosity
ρ _c	Continuous phase density
ω	Angular velocity
ω _{cr}	Critical angular rotor velocity

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