Genetic Algorithm Approach in Prediction of Mass Transfer and Axial Dispersion Coefficients of Rotating Disc Liquid-Liquid Extraction Contactors
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Abstract:

The liquid-liquid extraction process is well-known for its complexity and often entails intensive modeling and computational efforts to simulate its dynamic behavior. This paper presents a new application of Genetic Algorithm to predict the modeling parameters of a chemical pilot plant: a rotating disc liquid-liquid extraction contactor. In this process the droplet behavior of the dispersed phase has a strong influence on the mass transfer performance of the column. Mass transfer mechanism inside the drops of the dispersed phase was modeled by Handlos and Baron circulating drop model with considering the effect of forward mixing. Using the Genetic Algorithm method and the NAG software (Numerical Analysis Group) the mass transfer and axial dispersion coefficients in the continuous phase in these columns were optimized. In order to achieve RDC column parameters a least-square function of differences between the simulated and experimental concentration profiles (SSD) and %95 confidence limit in plug flow number of transfer unit prediction were considered. Minus %95 confidence limit and sum of square deviations for the GA method justified it as a successful method for optimization of mass transfer and axial dispersion coefficients of Liquid-liquid extraction columns.
Keywords: Liquid-Liquid Extraction, Rotating Disc Contactor, Genetic Algorithm

1. Introduction

There have been numerous attempts to obtain values of mass transfer parameters required to apply extraction column models, based on either differential contact with axial dispersion or stage wise contact with backflow. The normal approach has been to determine first the axial dispersion or backflow coefficients from tracer response experiments in the absence of mass transfer. Next, mass transfer experiments could be performed to obtain values of mass transfer coefficients, assuming that previously measured tracer response results may be used to predict axial dispersion or backflow coefficients. The approaches, and the available results, have been adequately summarized [1, 2 and 3]. Tracer response results [4-7], and occasional attempts [8, 9] to use mass transfer results to generate mass transfer coefficients, were reported.
The simultaneous determination of axial dispersion (or backflow) and mass transfer coefficients from solute concentration profiles should give more reliable results than the two-step method outlined above, provided that the model itself is satisfactory. This approach has received much attention over the years with numerous publications devoted to sampling techniques, summarized by Bonnet and Jeffreys [10], and to the method of application of the theory, including analyses of errors [11-14]. But there have been very few results reported [10, 15, 16 and 17] and no comparison of results obtained by the different approaches.

In this work the selected apparatus is a countercurrent extraction column of the rotating disc contactor type [18]. Here the dispersed phase was modeled by the forward mixing model [19, 20 and 21], which assumes as the basis a variation of sizes of drops traveling in the forward direction with different drop velocities and residence times. The continuous phase was modeled by plug flow with axial dispersion, also for drop side; to determine the mass transfer coefficients the Handles-Baron [22] turbulent circulating drop model was used. Cruz-Pinto [21], Al-Husseini[23], Ismail [24] and Young [25] confirmed that the Handles-Baron drop model was the most accurate model for predicting column results. An optimization method, GA, is applied to obtain the values of the continuous phase mass transfer, K_c and axial dispersion, E_c coefficients which most accurately predict measured continuous phase concentration profiles. This method, Genetic Algorithm approach, was used to achieve the minimized difference between the simulated and experimental concentration profiles. Here desired parameters are those that create the lowest sum of squared differences between the simulated and experimental concentration profiles. A simple global scheme of the procedure to predict the continuous phase mass and axial dispersion coefficients has been shown in figure (1).

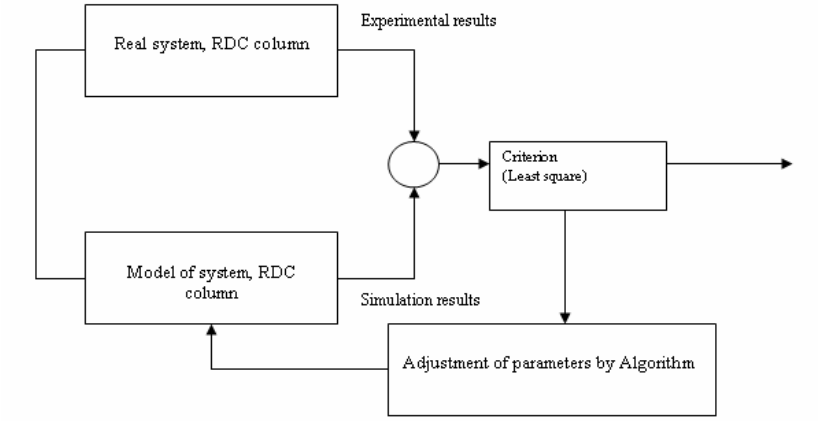

Fig (1): Global scheme of GA model

An introduction to real-coded Genetic Algorithm (GA), which is used in this paper, was presented first. Then the dispersed and continuous phases models of the RDC column were described and finally, the proposed method was applied to identify the parameters of RDC column.

2. Real-coded Genetic Algorithms

A Genetic Algorithm [26] (GA) is a computational model that emulates biological evolutionary theories to solve optimization problems. A GA comprises a group of individual elements (population). A set of biologically inspired operators is defined over the population itself. According to evolutionary theories only the most suitable individuals in a population are likely to survive and generate offspring for transmitting their biological heredity to new generations.

In computing terms, a GA maps a problem to a set of strings (chromosomes). Each string represents a potential solution of problem to be solved. The string can be constituted with orderly alignment of binary or real-coded variables of system. The fitness function, defined in GA method, attributes a fitness value to each string of population upon which GA manipulates the most promising strings to search for improved solutions.
Although many applications of GAs use classical GA with binary codification of system variables, there is an increasing interest in the employment of real-coded GAs for optimization problems with continuous variables. Generally, the real-coded GAs offer the advantage to be better adapted to the numerical optimization problems with continuous variables, to accelerate research process and to give very easily a hybrid method with other classical methods. However, the real-coded GAs needs to develop special GA,s operators in function of application . A GA operates typically through a simple cycle of four stages:

1. Creation of a population of string;
2. Evaluation of each string;
3. Selection of best string;
4. Genetic manipulation to create the new population of string.

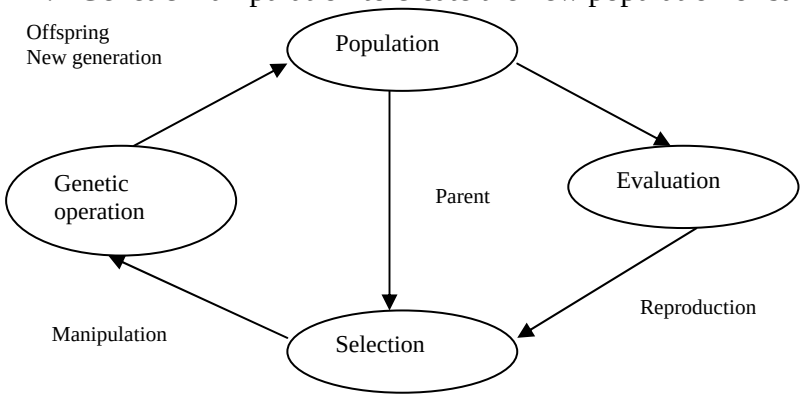

Fig 2: Genetic Algorithm cycle

Figure (2) shows these four stages using the biologically inspired GA terminology. In each cycle a new generation of possible solutions for a given problem is produced.
At the first stage, an initial population of potential solutions is randomly created as a starting point for the search process. Each individual of the population (chromosome) is created by alignment of system variables. In the next stage, the performance or fitness of each individual of the population is evaluated, with respect to the constraints imposed by the problem. Based on each individual's fitness, a selection mechanism chooses mates for the genetic manipulation process. The selection policy is ultimately responsible for assuring survival of the best fitted individuals. The combined evaluation and selection process is called reproduction.
There are several solutions to choose the selection policy (such as proportional selection, etc.). In this paper, the selection by arrangement method is employed in order to take in consideration the diversity of individuals in the population. This method consists of arrangement of individuals by decreasing the order of their fitness value and attributes a probability of selection ρ_j to each individual as a function of its row «j» [27]:

$$\rho_j = \left\lfloor \varphi - \left(r_j - 1\right)\left(2\varphi - 2\right)/\left(n-1\right)\right\rfloor / n \quad (1)$$

Where: ρ_j : Probability of selection of j^{th} row; n: Population size;

φ : Pressure of selection and $\varphi \in [1,2]$; r_j : Row of j^{th} individual.

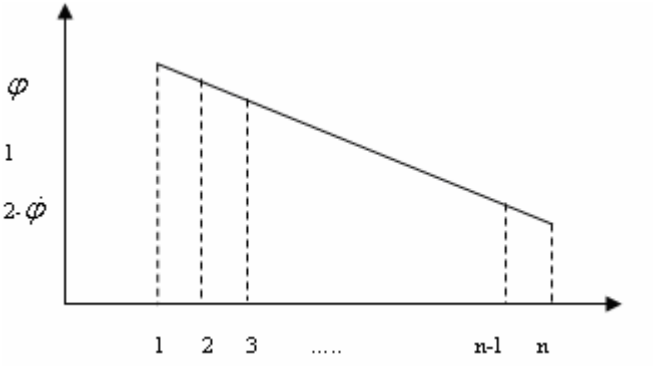

Fig3: Selection by arrangement method

Figure (3) shows the average number of offspring versus the row of individuals. In this figure, the pressure of selection φ represents the average number of offspring of the best individual and therefore the worst one will have necessary (2-φ) offspring.

The manipulation process employs genetic operators to produce a new population of individuals (offspring) by manipulating the genetic information, called «genes», possessed by members (parents) of the current population. It comprises two operators, namely Crossover and Mutation.

Crossover operator is responsible for recombining the genetic material of a population. The Crossover operator takes two parents-individuals with a probability ρ_c and swaps a part of their genetic information to produce new offspring-individuals.

In this paper an effective completely continued crossover is used. Let A (t) and B (t) be two individuals to be crossed, which are consisted of system of variables $a_1, a_2, ..., a_m$ (genes) to be optimized:

$$A\,(t) = [a_1, a_2, ..., a_m] \quad (2)$$

$$B\,(t) = [b_1, b_2, ..., b_m] \quad (3)$$

Then, the two offsprings A (t+1) and B (t+1) are produced as linear combination of their parents:

$$A(t+1) = \left[\rho_1 a_1 + (1-\rho_1) b_1, ..., \rho_m a_m + (1-\rho_m) b_m\right] \quad (4)$$

$$B(t+1) = \left[\rho_1 b_1 + (1-\rho_1) a_1, ..., \rho_m b_m + (1-\rho_m) a_m\right] \quad (5)$$

Where $\rho_1, \rho_2, ..., \rho_m \in [0,1]$ are random values (uniform probability distribution).

The mutation operator comes into action because the recombination process alone can not avoid the loss of a part of search area, which could lead to local optimum, and also is not capable to explore search space sections not represented in the population.

In real-coded GA, the mutation operator alters the parameters of selected individuals by a random change in predefined domains.
Let A (t) be the individual subjected to the mutation operator. Each gene represents a parameter of system and m is the number of parameters to be optimized. Each gene is going to undergo an important modification during the first generations. Gradually, the rate of alteration will be decreased as long as the research progressively continues. For the t^{th} generation, two numbers (p) and (r) are randomly taken into consideration:

$p^+ = +1$ positive alteration
$p^- = -1$ negative alteration (6)
$r \in [0,1]$ uniform distribution

(p^+) and (p^-) are randomly selected with equal probability, r is selected following a uniform distribution which determines indirectly the amplitude of alteration. Then, the mutated parameter is given by [26]:

$$a_k' = a_k + (a_{k\max} - a_k).(1 - r^{(1-\frac{t}{T})^5}) \quad \text{if} \quad p=+1$$
$$a_k' = a_k - (a_k - a_{k\min}).(1 - r^{(1-\frac{t}{T})^5}) \quad \text{if} \quad p=-1 \qquad (7)$$

$k \in [1, m]$

Where $a_{k\min}$ and $a_{k\max}$ stand for lower and upper bound values of a_k parameter respectively and T is the generation index at which the mutation amplitude is canceled. Figure (4) shows the distribution of mutation amplitude for different generations as function of random number «r».

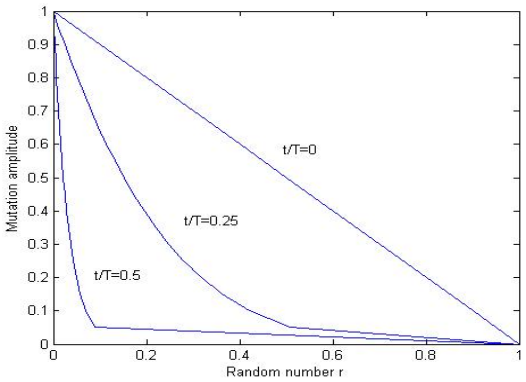

Fig5: The distribution of mutation amplitude for different generations

Finally, the offspring produced by the genetic manipulation process originates the next population to be evaluated. GAs can either replace a whole population (generation approach) or a part of their loss-fitted members. It can be interesting to keep intact the best fitted individual during the passage of a generation to the next. The creation- evaluation-manipulation cycle is repeated until a satisfactory solution to the problem is found [28, 29, and 30].

3. Experimental Apparatus

The data used in this paper were obtained from two contactors whose dimensions are given in Table (1). The columns were essentially the same as those used by Al-Husseini [24] and by Ismail [25], whose results with toluene-acetone-water system have been published. In all of the experiments the organic phase was dispersed to avoid large scale coalescence on the columns internals. Low (<10%) solute concentrations were used, with transfer from the continuous aqueous to dispersed organic phase [18]. More details about the experimental operating conditions are given elsewhere [18].
Systems used and their physical properties are summarized in Table (2).

Table 1: Experimental Equipments

column	small	large
Diameter, cm	7.62	21.9
Height, cm	73.6	151
Disc diameter, cm	4	11
Stator diameter ,cm	4.5	13.2
Stage height , cm	2.5	7.2
No. of stages	27	20
Cross-sectional area $\left(cm^2\right)$	42	352

Table 2: physical properties of the systems (at $25^{\circ}C$)

Physical property	Toluene-acetone-water	Butanol-succinic acid-water
$\rho_c\ (gcm^{-3})$	1	0.993
$\rho_D (gcm^{-3})$	0.86	0.835
$\mu_C\ (gcm^{-1}s^{-1})$	9.2(10^-6)exp(2063/T)	6.72(10^-7)exp(2924/T)
$\mu_D\ (gcm^{-1}s^{-1})$	1.6(10^-4)exp(1050/T)	2.07(10^-6)exp(2843/T)
$\delta (gs^{-2})$	32	1.4
m	Log(1/m)=-2.1056+659/(t+273)	1.497-0.0183t+0.0003t^2

Note: tem in $^{\circ}C$, Tem in k

4. The Mathematical Model

The overall objective of the design of a liquid-liquid extraction column is to combine a model of the mass transfer with a model of the phase flow behavior in order to accurately predict the required column dimensions or other parameters.
The current model has the following main assumptions:

- Constant, uniform physical properties in each phase.
- One solute transferring between the two phases.
- Low solute concentration in both phases.
- Constant distribution coefficient.
- Dispersed phase is represented by small and spherical droplets.
- No drop interaction or back mixing effects.
- Local mass transfer coefficients may be averaged over the total time of contact of the drop with the continuous phase.
- Perfect mixing in the horizontal plane of the continuous phase.

4.1. Dispersed Phase Mass Transfer:

The solute differential mass balance on a horizontal section of column with height dZ for the dispersed phase fraction with drop diameter, d_i and drop velocity, $V_{d,i}$ is given below,

$$g_i W_D y_i + N_i a_i S dz = g_i W_D (y_i + \frac{dy_i}{dz} dz) \quad (8)$$

$$N_i a_i S dz = g_i W_D \frac{dy_i}{dz} dz = f_i \phi V_{d,i} S \rho_D \frac{dy_i}{dz} dz \quad (9)$$

Where $a_i = \frac{6\phi f_i}{d_i}$ (10)

$V_{d,i}$ is the drop velocity with respect to the column wall and can be calculated through the drop slip velocity $V_{s,i}$. Drop slip velocity was predicted using the hydrodynamic model proposed by Olney [31]. In this model $V_{s,i}$ should be calculated from the following relation:

$$V_{s,i} = C_R V_{t,i}(1-\phi) = V_{d,i} + \frac{V_C}{1-\phi} \quad (11)$$

$V_{t,i}$ is the drop terminal velocity and can be predicted using correlations proposed by Klee and Treybal [32].

The interphase flux is given by:

$$N_i = K_{OD,i} \rho_D (y^* - y_i) \quad (12)$$

Combining equations (9) and (10) gives:

$$\frac{dy_i}{d\eta} = \frac{6K_{OD,i}Z}{V_{d,i}d_i}(y^* - y_i) = \frac{Z}{H_i}(y^* - y_i) \quad (13)$$

$\eta = \frac{z}{Z}$ and $\frac{1}{H_i} = \frac{6K_{OD,i}}{V_{d,i}d_i}$

Where i is the number of the dispersed phase drop size fraction, ranging from i=1 for the smallest to i=N for the largest, and z is the column vertical position.

4.2. Continuous Phase Mass Transfer:

The transport equations describing hydrodynamics and the solute concentration, x, in the continuous phase taking into account the interphase mass transfer from the continuous to the dispersed phase could be written as:

$$\frac{dx^2}{d\eta^2} + pe_c \frac{dx}{d\eta} = \frac{6 pe_c \phi Z \rho_D}{V_c \rho_c} \sum_{i=1}^{N} \frac{K_{OD,i} f_i}{d_i} (y^* - y_i) \quad (14)$$

$pe_c = \frac{V_c Z}{E_c}$ (Peclet number)

Where: $V_C = \frac{W_C}{\rho_C S} = \frac{Q_C}{S}$ $V_D = \frac{W_D}{\rho_D S} = \frac{Q_D}{S}$

In the above equations Z and S are the total column height and its cross-sectional area, respectively. The boundary conditions to solve the equation are:

$$B.C.1 \qquad At\ \eta=0 \quad x=x_1 \qquad \frac{dx}{d\eta}=0 \quad and \quad y_i = y_1$$

$$B.C.2 \qquad At\ \eta=1 \qquad x = x_2 - \frac{1}{pe_c}\frac{dx}{d\eta}$$

Where x_1 and x_2 are the outlet and inlet continuous phase solute concentrations. y_1 is the inlet dispersed phase solute concentration. By defining a new variable as:

$$X = x + \frac{1}{pe_c}\frac{dx}{d\eta}$$

Which represents what would be the plug flow concentration in the continuous phase; equation (14) is reduced to two first order differential equations:

$$\frac{dx}{d\eta} = pe_c(X - x) \qquad (15)$$

$$\frac{dX}{d\eta} = \frac{6\rho_D \phi Z}{V_c \rho_c}\sum_{i=1}^{N}\frac{K_{OD,i} f_i}{d_i}(y^* - y_i) \qquad (16)$$

4.3. Mass Transfer Coefficient:

The dispersed phase individual mass transfer coefficient is found dependent on the behavior of the single droplet in the sense whether it is stagnant, circulating or oscillating [33]. In the present work, the simplified model of Handlos and Baron [22] as used by many researches [34], [35] was used. In turbulent circulating drop model, a system of circulation tori is assumed with random displacement of particles in the radial direction. The average concentration in the torus may be obtained as follows:

$$y(z) = 2y\sum_{1\ n=1}^{\infty} B_n^2 \exp\left[-\lambda\frac{V_S Z}{128\, d V_d (1 + \mu_D / \mu_C)}\right] \qquad (17)$$

By applying equation (17) the local overall dispersed phase coefficient may be obtained as below:

$$K_{OD}(z) = \frac{dV_d}{6(y^* - y)}\frac{dy}{dz} \qquad (18)$$

And integrating equation (18) over the column height, Cruz-Pinto [21] obtained the average overall mass transfer coefficient as:

$$K_{OD,i} = -\frac{d_i V_{d,i}}{6Z}\ln\left\{2\sum_{n=1}^{\infty} B_n^2 \exp\left[-\lambda_n \frac{V_S Z}{128\, d_i V_{d,i}(1 + \frac{\mu_D}{\mu_C})}\right]\right\} \qquad (19)$$

Where the eigenvalues, λ_n and constants, B_n are dependent on the continuous phase mass transfer coefficient, K_C. This gives an average value of $K_{OD,i}$ over the column height, Z, which gives a sufficiently accurate prediction of mass transfer rates for this model.

5. Solutions of the Column Model Equations

The column-averaged overall mass transfer coefficients, $K_{OD,i}$, were calculated from equation (19) for Handlos-Baron drop model. The calculated average mass transfer coefficients were then substituted directly into equations (13) and (16) which were solved to obtain the dispersed and continuous phase concentration profiles. At this stage it was necessary to solve a system of N+2 first order ordinary differential equations (N is the number of drop size fractions in the distribution). For solving that system, a very accurate and fast Runge-Kutta type integration method was used. From the predicted concentrations and experimental extraction efficiencies, the predicted and experimental plug flow number of transfer units were calculated as follows:

-Predicted Extraction Efficiencies (dispersed phase basis):

$$P_{E_{OD}} = \frac{y_2 - y_1}{y^*(x_2) - y_1} = \frac{y_2 - y_1}{mx_2 - y_1} \tag{20}$$

-Predicted Plug-Flow Number of Transfer Units (dispersed phase basis):

$$P_{N_{ODP}} = \frac{1}{\frac{1}{\Lambda} - 1} \ln \frac{1 - P_{E_{OD}}}{1 - \frac{P_{E_{OD}}}{\Lambda}} \tag{21}$$

-Experimental Plug-Flow Number of Transfer Units

$$E_{N_{ODP}} = \frac{1}{\frac{1}{\Lambda} - 1} \ln \frac{1 - E_{E_{OD}}}{1 - \frac{E_{E_{OD}}}{\Lambda}} \tag{22}$$

$E_{E_{OD}}$: Experimental extraction efficiencies.

Where m is the solute distribution coefficient and Λ, the extraction factor, is given by:

$$\Lambda = \frac{\rho_C Q_C}{\rho_D Q_D m}$$

For calculating model parameters, mass transfer and axial dispersion coefficients, GA approach was applied; this routine was used to find the minimum of the sum of squared concentration deviations between the experimental and the theoretical generated profiles.

To apply the NAG library, initial values for E_c and K_c should be introduced within a given range. These initial values were predicted using correlations proposed by Misek [36, 37] for E_c and Calderbank & Moo Young [38] for K_c whereas in GA approach randomly initial values for E_c and K_c between the specified lower and upper limits are sufficient.

Owing to the more pronounced effect of the number of transfer units, especially very close to equilibrium conditions (i.e, when the extraction efficiency approach to one) these, rather than extraction efficiencies, were employed for quantitative analysis of the results in this work.

A full detail of E_c and K_c values using NAG library and the effect of operating conditions on them is given elsewhere [18, 39].

6. Results and Discussion

The results obtained using NAG software and Genetic Algorithm are summarized in Table 3.

Table .3.Experimental operating conditions and predicted values of parameters

Run No.	QC cm^3s^{-1}	QD cm^3s^{-1}	d_{32} cm	Hold-up (ϕ)	$E_{N_{ODP}}$	$K_c \times 1000$	E_c	$SSD \times 10^6$	$P_{N_{ODP}}$	$K^*_c \times 1000$	E_c^*	$SSD^* \times 10^6$	$P^*_{N_{ODP}}$
1	20.20	26.70	0.1964	0.038	2.237	1.016	1.38	3.04	2.349	0.922	1.3	1.31	2.259
2	20.20	26.70	0.1743	0.045	2.402	1.470	2.64	0.07	2.581	1.33	2.56	0.0345	2.409
3	20.20	26.70	0.1672	0.063	2.895	2.018	2.75	1.64	2.676	2.2	2.88	1.09	2.847
4	29.50	50.80	0.1995	0.063	2.338	1.055	1.44	0.91	2.108	1.095	1.608	0.825	2.349
5	29.50	50.80	0.1862	0.070	2.301	1.006	1.75	0.57	2.419	1.072	1.956	0.512	2.364
6	29.50	50.80	0.1843	0.078	2.671	1.748	2.60	1.61	2.460	1.72	2.701	1.132	2.678
7	48.20	80.0	0.2064	0.093	2.146	1.015	1.71	1.27	1.837	1.02	1.954	1.057	2.105
8	48.20	80.0	0.2153	0.107	2.355	1.308	2.86	0.08	2.244	1.22	2.642	0.0714	2.362
9	48.20	80.0	0.1977	0.116	2.316	1.195	3.33	0.30	2.421	1.095	3.072	0.198	2.314
10	20.20	26.70	0.2462	0.029	1.622	0.977	1.45	0.40	1.664	1.02	1.651	0.384	1.646
11	29.50	50.80	0.2930	0.048	1.247	0.955	1.77	0.91	1.265	0.924	1.751	0.796	1.255
12	48.20	80.0	0.2921	0.067	1.206	0.997	2.01	0.23	1.110	0.924	1.751	0.136	1.165
13	5.80	7.30	0.1347	0.069	1.614	1.183	1.27	1.20	1.606	1.169	1.260	1.446	1.628
14	5.80	7.30	0.1372	0.069	1.691	1.322	1.19	4.55	1.733	1.326	1.252	5.03	1.759
15	5.80	7.30	0.1529	0.083	2.081	1.629	1.29	3.05	2.072	1.655	1.376	4.69	2.109
16	5.80	7.30	0.1229	0.139	2.552	1.798	2.23	8.37	2.525	2.2	2.549	9.312	2.619
17	21.23	21.23	0.1946	0.028	2.159	2.381	1.67	0.06	2.318	2.7	1.987	0.0426	2.183
18	21.23	21.23	0.1685	0.032	2.605	3.180	1.69	0.32	2.707	2.93	1.741	0.114	2.597
19	21.23	21.23	0.1007	0.047	3.394	3.996	1.99	0.84	3.664	4.5	2.097	0.789	3.350
20	38.67	31.64	0.1846	0.039	2.753	2.556	1.54	0.01	2.717	2.22	1.354	0.00959	2.738
21	38.67	31.64	0.1351	0.044	3.458	3.733	2.09	0.14	3.490	3.8	2.222	0.196	3.537
22	57.41	41.43	0.1379	0.056	3.259	2.425	2.73	0.03	3.547	2.5	3.009	0.0192	3.292
23	38.67	31.64	0.1321	0.045	3.618	4.089	2.27	0.05	3.646	4.2	2.402	0.0636	3.654
24	2.57	2.57	0.1192	0.019	1.682	2.294	0.49	0.34	1.622	2.29	0.555	0.23	1.669
25	2.57	2.57	0.1305	0.026	1.788	2.661	0.64	0.53	1.770	2.522	0.674	0.578	1.768
26	2.57	2.57	0.1010	0.028	2.023	2.701	0.64	0.59	2.291	2.97	0.719	0.576	2.271
27	4.68	3.83	0.1188	0.037	1.922	2.461	0.79	0.31	1.882	2.4	0.813	0.256	1.938
28	4.68	3.83	0.1306	0.039	2.011	2.854	0.80	0.17	1.956	2.4	0.655	0.189	2.087
29	4.68	3.83	0.1077	0.045	2.540	3.485	0.80	0.69	2.522	3.802	0.915	0.854	2.645
30	4.68	3.83	0.0857	0.054	2.713	5.374	1.69	7.60	3.100	5.48	1.762	4.32	2.764
31	6.93	5.02	0.1037	0.059	2.516	2.513	0.91	0.94	2.347	2.3	0.947	0.821	2.437
32	6.93	5.02	0.1121	0.064	2.653	3.286	0.94	0.98	2.428	3.33	1.039	0.708	2.677
33	6.93	5.02	0.0891	0.070	3.186	3.507	1.23	0.38	3.317	3.331	1.257	0.369	3.252
34	2.57	2.57	0.1305	0.025	1.744	2.507	0.60	0.17	1.753	2.355	0.580	0.149	1.75
35	4.68	3.83	0.0894	0.044	2.924	3.316	0.78	0.26	2.889	3.8	0.915	0.364	3.03
36	2.57	2.57	0.1503	0.026	1.242	1.380	0.52	0.82	1.219	1.461	0.609	0.89	1.291
37	4.68	3.83	0.1325	0.041	1.499	1.258	0.44	2.11	1.371	1.3	0.531	1.93	1.439
38	6.93	5.02	0.1413	0.047	1.512	1.441	0.66	0.65	1.272	1.33	0.575	0.613	1.400
39	21.23	21.23	0.2182	0.024	1.915	2.226	1.39	0.15	1.910	2.3	1.539	0.24	1.946
40	38.67	31.64	0.2244	0.038	2.230	2.348	1.45	0.001	2.121	2.36	1.546	0.00098	2.225
41	57.24	41.44	0.1650	0.053	2.840	2.445	2.94	0.03	2.932	2.11	2.688	0.0216	2.815
42	21.23	21.23	0.2138	0.029	2.014	2.032	1.46	0.02	2.101	1.9	1.486	0.0123	2.0198

*: predicted by GA method

In figures 6 and 7 E_c and K_c values are shown and compared, respectively. Comparison between E_c values shows maximum deviation of about 30% and K_c values about 15%.

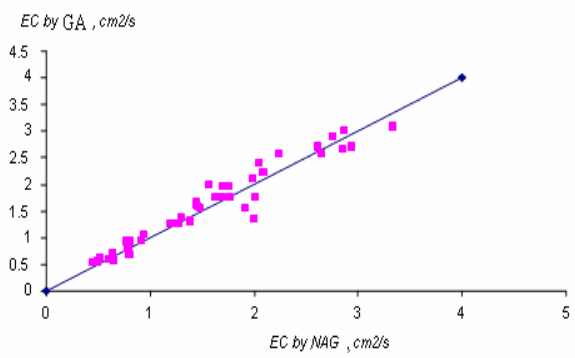

Fig .6 . Comparison between E_c values predicted by NAG and GA

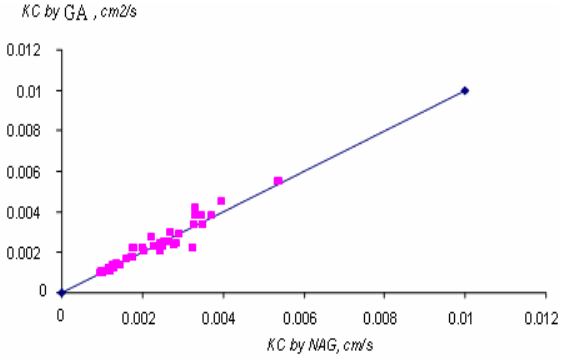

Fig .7. Comparison between K_c values predicted by NAG and GA

In figures 8 and 9 the predicted and experimental plug flow number of transfer units using GA approach and NAG library are compared. As these figures show, more agreements between $P_{N_{ODP}}$ and $E_{N_{ODP}}$ values are attained when Genetic Algorithm was applied, although this trend can be seen when the sum of squared differences (SSD) values are compared in Table 3. Another criterion to distinguish that this approach is more applicable is the calculation of 95% confidence limit in plug flow number of transfer units. The less 95% confidence limit means the more accurate prediction. This parameter is calculated using the following relation:

$$95\%\ \text{Confidence Limit} = 2 * \sqrt{\frac{\sum \left(\frac{EN_{ODP} - PN_{ODP}}{EN_{ODP}} \right)^2}{n-1}} \qquad (23)$$

Where $E_{N_{ODP}}$ and $P_{N_{ODP}}$ are the experimentally measured and predicted plug flow number of transfer units calculated from equations 21 and 22, and n is the number of experiments.

Predicted 95% confidence limit in plug flow number of transfer units (that is obtained from predicted concentration profile and consequently originated from predicted mass transfer and axial dispersion coefficients) when Genetic Algorithm and NAG library were applied, were 6.02%and 13.21% respectively. Comparison between these two values demonstrates much more applicability of Genetic Algorithm.

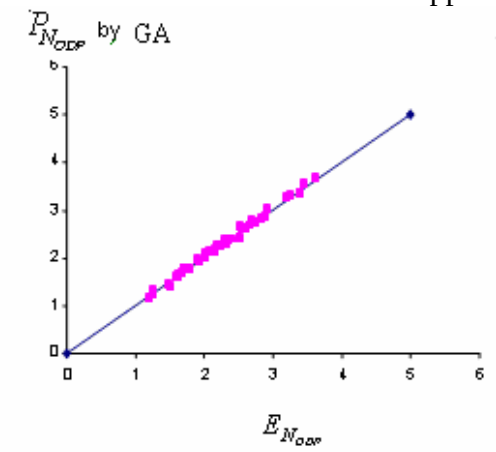

Fig.8. Comparison between experimental and predicted values of N_{ODP} , using GA.

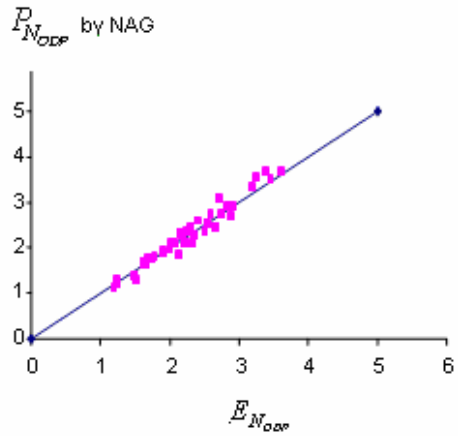

Fig.9. Comparison between experimental and predicted values of N_{ODP} , using NAG

7. Conclusions

Results obtained in this study which can lead to better prediction of RDC column performance and design, show the following:

- Comparing the results obtained by GA method to those obtained through the classical identification method (NAG library) demonstrates the feasibility and advantage of proposed approach.
- More precise operating conditions, drop size distribution, concentration profile… measurement and more realistic assumptions will lead to more accurate mass and axial dispersion parameters.

Nomenclature

B_n Eigen values of Strum-lioville Equation

C_R Constriction factor

d_i Drop diameter, ith fraction (cm)

d_{32} Sauter-mean drop diameter (cm)

E_c Continuous phase axial dispersion coefficient $(cm^2 s^{-1})$

E_{OD} Extraction efficiency, dispersed phase based

f_i Static volume fraction of dispersed phase, drop diameter, d_i

N Number of drop size fractions

K_c Continuous phase mass transfer coefficient (cms^{-1})

$K_{OD,i}$ Overall mass transfer coefficient ith fraction, dispersed phase based, (cms^{-1})

m Solute distribution coefficient , y^* / x

N_{ODP} Plug flow number of transfer units, dispersed phase based

Q_C, Q_D Volumetric flow rates, continuous and dispersed phases $(cm^3 s^{-1})$

S Column cross-sectional area for flow (cm^2)

V_C, V_D Superficial velocities, continuous and dispersed phase (cms^{-1})

$V_{d,i}$ Drop vertical velocity respect to column wall, *i*th fraction (cms^{-1})

$V_{S,i}$ Drop slip velocity, *i*th fraction (cms^{-1})

$V_{t,i}$ Drop terminal velocity (cms^{-1})

x Weight fraction solute, continuous phase

y_i Dispersed phase solute weight fraction, *i*th fraction, average

y^* Weight fraction solute, at equilibrium with continuous phase bulk

z Column vertical position (cm)

Z Column height (cm)

μ_C, μ_D Viscosity, continuous and dispersed phases $(gcm^{-1}s^{-1})$

ρ_C, ρ_D Density, continuous and dispersed phases (gcm^{-3})

δ Interfacial tension (gs^{-2})

ϕ Dispersed phase volume fraction

λ_n Eigen value

Λ Extraction factor $(\rho_C Q_C / m\rho_D Q_D)$

t,T Temperature $(^{\circ}C, K)$

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