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NOTE

Three Phase Flash Calculations Using Genetic Algorithm Approach

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A new approach based on the genetic algorithm has been proposed for solving three phase flash calculations containing two liquid phases and one vapour phase. Based on this approach choosing the initial guess for the compositions of the involved phases is not an important step, which in the ordinary three phase algorithms affects directly the convergence of the calculations. A real problem has been solved with this approach and good results have been obtained in comparison with the experimental data. ϕ-ϕ approach has been adopted for vapour-liquid-liquid equilibrium (VLLE) calculations based on Peng-Robinson equation of state.

Key Words: Genetic algorithm, Three phase flash calculations.

Information about vapour-liquid-liquid equilibrium (VLLE) is essential for many chemical processes and the separation operations[1]. Among these industrial processes the recovery of organic acids from dilute solution resulting from fermentation processes and the extraction of aromatic compounds from petroleum fluid fraction are only two examples of the potential of VLLE operations in the chemical and petrochemical industries[2-5]. For designing and optimization of the liquid extraction processes as well as various separation equipments one has to know the equilibrium conditions due to complex nature of the VLLE calculations. It can be said that for obtaining reliable results one has to examine every specific case to check its convergence. To confirm this point one may refer to the works of Liu *et al.*[6] and Yokozeki[7]. Therefore as an important result it may be mentioned that presentation of unique algorithm for VLLE calculation is a crucial step in the subject. In this work a simple and efficient approach based on the genetic algorithm has been proposed for VLLE calculations and good results have been obtained for a ternary system.

Problem statement: The compositions of the liquids and vapour phases are given by the following equations:

$$\mathrm{X1(I)} = \frac{\mathrm{s(I)}}{\mathrm{x(1)\times(1-R1(I))+x(2)\times(R1(I)/R2(I)-R1(I))+R1(I)}} \quad (1)$$

$$\mathrm{X2(I)} = \frac{\mathrm{(s(I)\times R1(I)/R2(I))}}{\mathrm{x(1)\times(1-R1(I))+x(2)\times(R1(I)/R2(I)-R1(I))+R1(I)}} \quad (2)$$

$$\mathrm{Y(I)} = \frac{\mathrm{(s(I)\times R1(I))}}{\mathrm{x(1)\times(1-R1(I))+x(2)\times(R1(I)/R2(I)-R1(I))+R1(I)}} \quad (3)$$

x(1) and x(2), equals to the number of moles of the liquid phases No. 1 and 2, respectively.

Considering the above relations, it is obvious that in a three-phase system the value of x(1) and x(2) must be known. These values will be the answers of a nonlinear system of equations which will be obtained from the following equations:

$$\sum_{\mathrm{i=1}}^{3} \mathrm{x2(i)} = 1 \quad (4)$$

$$\sum_{\mathrm{i=1}}^{3} \mathrm{(x1(i)-Y(i))} = 0 \quad (5)$$

Using these two relations, the system of equation will be obtained:

$$\mathrm{f_1} = \sum_{\mathrm{k=1}}^{3} \frac{\mathrm{s(k)\times R1(k)/R2(k)}}{\mathrm{x(1)\times(1-R1)k))+x(2)\times(R1(k)/R2(k)-R1(k))+R1(k)}} - 1 = 0 \quad (6)$$

$$\mathrm{f_2} = \sum_{\mathrm{k=1}}^{3} \frac{\mathrm{s(k)\times(1-R1(k))}}{\mathrm{x(1)\times(1-R1(k))+x(2)\times(R1(k)/R2(k)-R1(k))+R1(k)}} = 0 \quad (7)$$

where, R1(I) = [1.4529 0.2103 0.0001], R2(I) = [0.1518 0.2876 0.0009].

R1 and R2 are the K-values of different components in the mixture. These values have been calculated by the Peng-Robinson equation of state. Now by considering the above equations we can carry out the VLLE calculations for ternary system. The feed consists of methane(1)-ethane(2)-*n*-octane(3). In this work, we have chosen the composition of feed as s(1) = 0.8054, s(2) = 0.1385, s(3) = 0.0560.

Genetic algorithm: The genetic algorithm (GA) is a stochastic search technique based on the mechanism of natural selection and natural genetics to imitate living beings for solving difficult optimization problems with high complexity and an undesirable structure. The genetic algorithm approach represents a powerful, general-purpose optimization paradigm in which the computational process mimics the theory of biological evolution[8,9]. It has been successfully used in job-shop scheduling, production planning, line balancing and process optimization. Goldberg[10] proposed the most common and useful form of genetic algorithm. Different from traditional point-to-point descending and ascending search techniques, a genetic algorithm starts from one set of random solutions called a population. Each individual solution in the population is called a chromosome. At each generation, the genetic algorithm performs genetic operations such as crossover and mutation on the selected chromosomes to yield offspring to produce the next generation. During each generation, these chromosomes evolve into better fitness by applying an evolution operation, called the selection. From generation to generation, eventually, the chromosomes in the population will converge. In this case, the best chromosome is found. Generally, the basic steps of a genetic algorithm approach in solving an optimization problem can be summarized as follows:

Genetic Algorithm Steps

1. Represent the problem variable as a chromosome of a fixed length and choose the size of a chromosome population, the crossover probability and the mutation probability.
2. Define a fitness function to measure the fitness of an individual chromosome in the problem domain.
3. Randomly generate an initial population of chromosomes.
4. Calculate the fitness of each individual chromosome.
5. Select a pair of chromosomes for mating from the current population. Parent chromosomes are selected with a probability related to their fitness. Highly fit chromosomes have a higher probability of being selected formatting. The roulette wheel method is usually applied in chromosome selection.
6. Create a pair of offspring chromosomes by applying the genetic operators: crossover and mutation.
7. Place the created offspring chromosomes in the new population.
8. Repeat step 5 until the size of the new chromosome population is equal to the size of the initial population.
9. Replace the initial (parent) chromosome population with the new (offspring) population.
10. Repeat steps 4-9 until the termination criterion is satisfied.

Implementation: In this work, the genetic toolbox in MATLAB® has been used[11]. Eqns. 6 and 7 are the objective functions (f_1 and f_2) which have been combined to form a unique objective function or fitness function. This function may be read as:

$$F = \frac{w_1 f_2 + w_w f_2}{w_2 + w_2}$$

As X1, X2 and Y are mole fractions they must be in the interval [0, 1] the nonlinear constraints have been considered. The genetic algorithm toolbox uses the Augmented Lagrangian genetic algorithm (ALGA) to solve nonlinear constraint problems.

The genetic algorithm in MATLAB was run with below parameters:

Population size	20
Parameters	2
	$0 \le x(1) \le 1$, $0 \le x(2) \le 1$
Generation	30
Nonlinear constraints	$X_2(i) - 1 \le 0$
	$X_1(i) - 1 \le 0$
	$Y_1(i) - 1 \le 0$, for i = 1:3
Hybrid with local optimization	Pattern search
Encoding	Real value

The best solution in last generation is x(1) = 0.4132 and x(2) = 0.2095 which by these value the composition of two liquid phases and one vapour phase are as follows:

X1 = 0.657123 0.214483 0.128288
X2 = 0.828907 0.156835 0.014254
Y = 0.954734 0.045106 0.000013

The experimental data on the liquid phases are as follows:

X1 = 0.682 0.187 0.131
X2 = 0.806 0.158 0.036

In comparison with these data, it is found that the method handled the relevant calculations very well.

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