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Optimization of Extended UNIQUAC Parameter for Activity Coefficients of Ions of an Electrolyte System using Genetic Algorithms

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Abstract – In the present research, in order to predict activity coefficient of inorganic ions in electrolyte solution of a petroleum system, we studied 13 components in the electrolyte solution, including H_2O, CO_2 (aq), H^+, Na^+, Ba^{2+}, Ca^{2+}, Sr^{2+}, Mg^{2+}, SO_4, CO_3, OH^-, Cl^-, and HCO_3. To predict the activity coefficient of the components of the petroleum system (a solid/liquid equilibrium system), activity coefficient model of Extended UNIQUAC was studied, along with its adjustable parameters optimized based on a genetic algorithm. The total calculated error associated with optimizing the adjustable parameters of Extended UNIQUAC model considering the 13 components under study at three temperature levels (298.15, 323.15, and 373.15 K) using the genetic algorithm is found to be 0.07.

Key words: Mineral ions, Optimization, Genetic Algorithms, Extended UNIQUAC Model

1. Introduction

Optimization is the process of maximizing the desirable efficiency. Optimization techniques implement this process by undertaking some modifications on an initial assumption. To increase the efficiency, optimization algorithms should apply operators on initial points to produce new points within the search space for objective function (to gradually move toward the optimal locations within this space). In most of these search techniques (gradient method), the algorithm proceeds from one point to another; in most cases, this point-by-point approach ends up with optimization errors as they converge to a local maxima. This drawback in optimization of nonlinear models leads to complex issues in the process of problem solving. To overcome this drawback [1-3] powerful algorithms such as genetic algorithms (GA) are proposed. Electrolyte solutions are listed among the most important aqueous systems in chemical industries, such as petroleum systems, due to the electrostatic and short-range forces established between ions and solvent. Either high or low concentration can lead to a non-ideal behavior in the electrolyte systems. In this regards it is necessary to investigate all inter-particle forces. Due to the dependence of saturation index of mineral sediment formation in chemical systems, such as oil, on the mineral ions of aqueous solutions, the importance of their activity factors increases; thus it is being used in modeling thermodynamic prediction of mineral sediment formation during industrial processes. In studies predicting mineral sediments in electrolytic aqueous solutions, two terms of thermodynamic equilibrium constant and activity factor of water-soluble mineral components are considered. Mineral sediments are one of the main problems of oil facilities, and the formation of these deposits is one of the fundamental challenges the water feeding systems confront. Depending on the conditions (changes in water pressure and temperature alone or in combining two incompatible water) during an operation when these mineral ions are dissolved in the system (in a state of saturation), these deposits can cause major problems by reducing the inner diameter of extraction pipe, increasing repair and maintenance costs and causing overall decline in the exploitation of oil of underground reservoirs. Therefore, considering the importance of mineral sediment formation based on the nature and activity of mineral ions in water systems of industrial operations such as oil, in this research in order to predict activity factor of mineral ions in oil systems, 13 components of electrolytic solutions have been studied: H_2O, CO_2 (aq, H^+, Na^+, Ba^{2+}, Ca^{2+}, Sr^{2+}, Mg^{2+}, SO_4, CO_3, OH^-, Cl^- and HCO_3. Considering the satisfying efficiency of the activity coefficient model of Extended UNIQUAC with its adjustable parameters optimized using genetic algorithms, we used this method to investigate the activity coefficient of the ions in this study.

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2. Theoretical Section

2-1. Extended UNIQUAC Model

Thomsen and Rasmussen (1999)[4] exercised Extended UNIQUAC model to study the electrolytic systems. Satisfying results were

acquired for the solid-liquid, liquid-liquid and liquid-vapor equilibrium systems. The model is a combination of local composition model (UNIQUAC) and Debye-Hückel term. UNIQUAC model was suggested by Abrams and Prausnitz [5] to describe the Gibb's additional energy of the mixture, and includes two parts: one part of the compound is related to the entropy of the system and is determined according to the size and shape of molecule, the remaining part considers the intermolecular forces involved in mixing enthalpy and depends on molecular forces.

UNIQUAC equation has adjustable parameters and is expressed as follows for the equilibrium of liquid-solid systems (multi-part) [4-6]:

$$G^E = G^E_{combinatorial} + G^E_{Residual} + G^E_{Debye\text{-}HucKel} \quad (1)$$

$$\frac{G^E_{combinatorial}}{RT} = \sum x_i \ln\left(\frac{\varnothing_i}{x_i}\right) - \frac{Z}{2}\sum q_i x_i \ln\left(\frac{\theta_i}{\varnothing_i}\right) \quad (2)$$

In the upper equation, G^E is Gibbs free energy, z is coordination number with a value of 10; x_i is mole fraction; φ_i is mole fraction; φ_i is volume fraction and θ_i is the surface area fraction of ions in the liquid-solid or liquid-vapor equilibrium system which is expressed as:

$$\varnothing_i = \frac{x_i r_i}{\sum_l x_l r_l} \quad (3)$$

$$\theta_i = \frac{x_i r_i}{\sum_l x_l r_l} \quad (4)$$

where r_i and q_i are the volume and surface area parameters for each ion. Also, for the residual term, the following equation holds:

$$\frac{G^E_{Residual}}{RT} = -\sum_i q_i x_i \ln\left(\sum_k \theta_k \varphi_{ki}\right) \quad (5)$$

$$\varphi_{ij} = \exp\left(-\frac{u_{ij} - u_{ii}}{RT}\right) \quad (6)$$

where u_{ii} is the interaction energy between similar ions in an equilibrium system of solid-liquid and vapor-liquid. u_{ij} is the interaction energy between different ions in an equilibrium system. The interaction energy is a function of temperature and is defined as:

$$u_{ij} = u^0_{ij} + u^t_{ij}(T - 298.15) \quad (7)$$

where u_{ij}^0 and u_{ij}^t are two adjustable parameters for interaction energy between the ions in the equilibrium system.

The Debye-Hückel contribution (to the Gibb's excess energy) of the extended UNIQUAC model is given by the expression:

$$\frac{G^E_{Debye-HucKel}}{RT} = -x_w M_w \frac{4A}{b^3}\left[\ln\left(1 + bI^{\frac{1}{2}}\right) - bI^{\frac{1}{2}} + \frac{b^2 I}{2}\right] \quad (8)$$

where M_w is the molar mass of water, x_w is the mole fraction of water, A is a Debye-Hückel parameter, b is a constant value equal to 1.5 $(\frac{Kg}{mol})^{0.5}$, and I is the ionic strength.

$$I = 0.5\sum m_i Z_i^2 \quad (9)$$

In Eq. 9, z_i is the charge and m_i is the molality (mol $(kg\ H_2O)^{-1}$) of ion i. Considering the relationship between excess Gibbs free energy and basic equations of thermodynamics, by differentiation of Equation 1 with respect to the mole fraction of different species, the activity coefficient for each ion is derived:

$$\ln\gamma_i = \left[\frac{\partial\left(\frac{nG^E}{RT}\right)}{\partial n_i}\right] \quad (10)$$

$$\ln\gamma_i = \ln\gamma_i^{Residual} + \ln\gamma_i^{combinatorial} + \ln\gamma_i^{Debye\text{-}Hückel} \quad (11)$$

To normalize Equation 11 for electrolyte system, considering water existence (as a solvent) and its ions of solute, we have:

$$\gamma_i \to 1 \ \text{ as } \ x_i \to 0 \quad (12)$$

$$\gamma_i^* = \frac{\gamma_i}{\gamma_i^\infty} \quad (13)$$

In Eq. 13, for y_i^∞ (act ivity coefficient of ion at infinite dilution), we have:

$$\gamma_i^\infty = \lim_{x_i \to 0}\gamma_i \quad (14)$$

And finally, we have:

$$\ln\gamma_i^* = \ln\left(\frac{\varnothing_i}{x_i}\right) + 1 - \left(\frac{\varnothing_i}{x_i}\right) + \frac{z}{2}\cdot q_i\left[\ln\left(\frac{\varnothing_i}{\theta_i}\right) + 1 - \frac{\varnothing_i}{\theta_i}\right] - \ln\left(\frac{r_i}{r_w}\right) + 1 - \frac{r_i}{r_w}$$
$$+ \frac{z}{2}\cdot q_i\left[\ln\left(\frac{r_i \cdot q_w}{r_w q_i}\right) + 1 - \frac{r_i \cdot q_w}{r_w q_i}\right] + q_i\left[1 - \ln\left(\sum_k \theta_k \varphi_{lk}\right) - \sum_k \frac{\theta_k \varphi_{lk}}{\Sigma\theta_l \varphi_{lk}}\right]$$
$$- q_i[1 - \ln(\varphi_{wi}) - \varphi_{iw}] - Z_i^2 \frac{AI^{1/2}}{1 + bI^{1/2}} \quad (15)$$

2-2. Genetic Algorithms

First introduced by John Holland, the genetic algorithm is indeed a special case of evolutionary algorithm. It only requires some information about the quality of generated solutions using each set of variables, whereas some other optimization techniques require detailed information and recognition of the problem structure and variables [7,8].

As a numerical optimization technique, genetic algorithms considers a set of points within the solution space and searches different points across this space at each iteration. This algorithm works without any limitation regarding the function to be optimized (e.g., differentiability) and, in the process of searching for a solution, it only requires the evaluation of the objective function at different points. According to these features genetic algorithms can be considered as a reliable technique in case of different linear and non-linear problems. In each iteration, each string in the set of available strings will be decoded and its value is evaluated using the objective function. Based on the evaluated values, a fitness value is assigned to each string. This fitness value determines the probability for each string to be selected among the population of the strings.According to the selection probabilities, a set of strings is selected. By applying genetic operators on the selected strings, new strings are selected to replace some of the strings from the initial population; this is done to keep

the number of strings constant at different iterations. In genetic algorithms, not only genetic operators search for new points in the solution space at each iteration, but also the selection process searchs the regions within the solution space where the statistical average of the objective function considered by the user is higher in value [8,9]. In genetic algorithms, using strings of either constant or variable lengths, a set of design variables is coded, with each string representing a solution point in computational search space.

These algorithms begin with producing a generation where a so-called "initial population" is generated either selectively or randomly. The existing population is selected according to the fitness of each individual in the population for the next generation. Thereafter, genetic operators, such as selection, crossover or mutation, are applied and finally a new population is established. Consequently, new generations replace older ones and the cycles continue until a solution is reached [8-10]. Theh genetic algorithm does not require detailed information about the problems under study. Considering that its decisions are principally made randomly, all possible solutions are achievable theoretically. Among other strengths of genetic algorithm, one can refer to the following [8-11]:

1. It does not need to calculate derivatives of functions.
2. It can undertake the optimization process using either continuous or discrete variables.
3. It can undertake the optimization process using a large number of variables.
4. It is capable of obtaining several solutions at the same time.
5. It is applicable on sets of solutions.

Many researchers have made use of genetic algorithms to solve complex linear or non-linear engineering and chemical problems and issues, including Agrawal *et al*. [12] (in optimizing low-density polyethylene reactor), Cao *et al*. [13] (in optimizing the minimum consumption of fresh water), Elliot *et al*. [14] (in optimizing aviation fuel combustion), Jezowski *et al*. [15] (in optimizing retrofitting thermal transducer) and Masoori *et al*. [16] (in optimizing reaction rate in reactive systems), and the results demonstrate the efficiency of using genetic algorithms in optimization and objective function problems. System problems and industrial and chemical process optimization are among the other usages of genetic algorithms as stated by Till *et al*. [17], Young *et al*. [18] and Lepar *et al.* [19].

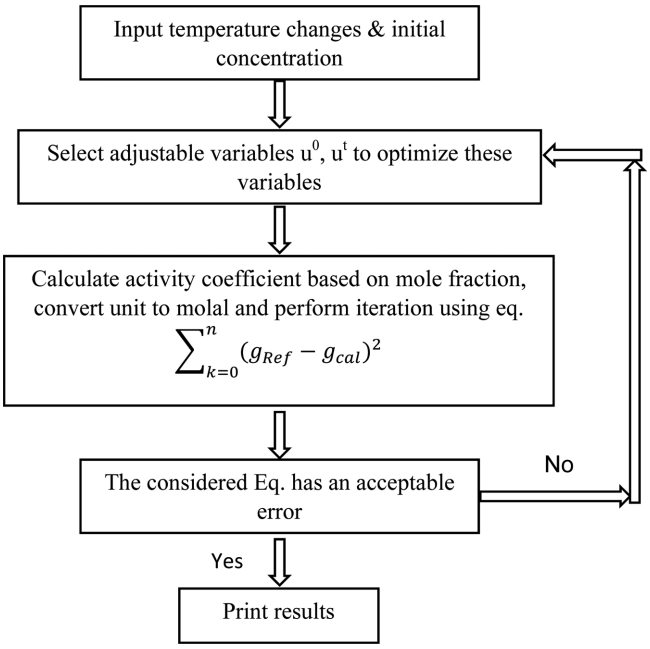

Fig. 1. A flowchart for the optimization process of the activity coeefficient of inorganic ions using Extended UNIQUAC model based on Genetic Algorithm.

Fig. 1 provides a flowchart of optimization and calculation of activity coefficient of ions in a petroleum system (under solid/liquid equilibrium) using genetic algorithm. According to this flowchart, we begin with calling three constant terms, R, temperature variations, and initial concentration in molality. Since the activity coefficient model of Extended UNIQUAC is calculated based on molar ratios, the initial concentration should be unit-converted from molality to molar ratio. In Extended UNIQUAC model, three important parameters comprise the main axis of the model: *u* with all of them being optimizable and adjustable. However, the parameter *u* is more important than the others due to its dependence on temperature con-

Table 1. Initial Concentration values for calculation of activity coefficient

Components of Electrolytic system	Initial concentration (molality)	Activity Coeeficient at 298.15 k	Activity Coeeficient at 323.15 k	Activity Coeeficient at 373.15 k
H_2O	55.5	0.8506	0.8507	0.8554
CO_2(aq)	0.00867	1.8095	1.8091	1.8088
H^+	0.00401	1.9810	1.3059	0.9719
Na^+	3.14	0.7263	0.7373	0.6649
Ba^{2+}	0.000112	0.1510	0.1326	0.0793
Ca^{2+}	0.311	0.4019	0.3199	0.1876
Sr^{2+}	0.0172	0.3578	0.2679	0.1312
Mg^{2+}	0.0981	0.6378	0.4617	0.2359
OH^-	2.96E-12	0.3631	0.3471	0.2818
Cl^-	4.05	0.9317	0.9327	0.8462
SO_4^{2-}	0.00406	0.0233	0.0272	0.0227
CO_3^{2-}	2.92E-13	0.0160	0.0138	0.0052
HCO_3	0.0113	0.7098	0.7218	0.5851

ditions. The three parameters u were used in the optimization algorithm and then, the activity coefficient was calculated in molar ratio, and once unit-converted to molality, it was fed into a trial and error loop. The optimization process stops as soon the error satisfies the predefined error criterion and the results are printed. The computation process continues until the error criterion is met.

3. Data Used in this Study

In this research, in order to investigate activity coefficient of ions in a petroleum system, the activity coefficient model of Extended UNIQUAC was studied. The adjustable parameters of this model were optimized according to the equilibrium concentration and activity coefficient (according to Pscalsim[1] Software of The Research Institute of Petroleum Industry of Iran) presented in Table 1.

4. Results and Discussion

4-1. Results of parameter optimization of the model

The process denoted in the flowchart in Fig. 1 was performed on the data. After running the application for the equilibrium concentrations presented in Table 1 and temperature variations of 298.15, 323.15, and 373.15 K, the error equation ($\sum_{k=0}^{n}(g_{Ref}-g_{cal})^2$) represents a total calculated error equal to 0.07. Fig. 2 shows the trend of GA iterations as the optimization process continued to reach a desirable total error (at three temperature levels of 298.15, 323.15, and 373.15 K). Table 2 represents optimal values of the parameters r and q. Tables 3 and 4 represent the values of u^o and u^t, respectively.

In Figs. 3~5, the trend of the GA iteration is represented for the 13 components in the electrolyte solution including water, dissolved carbon dioxide, hydrogen, sodium, barium, calcium, strontium, magnesium hydroxide, chloride, sulfate, carbonate and bicarbonate at three different temperatures (298.15, 323.15, and 373.15 K).

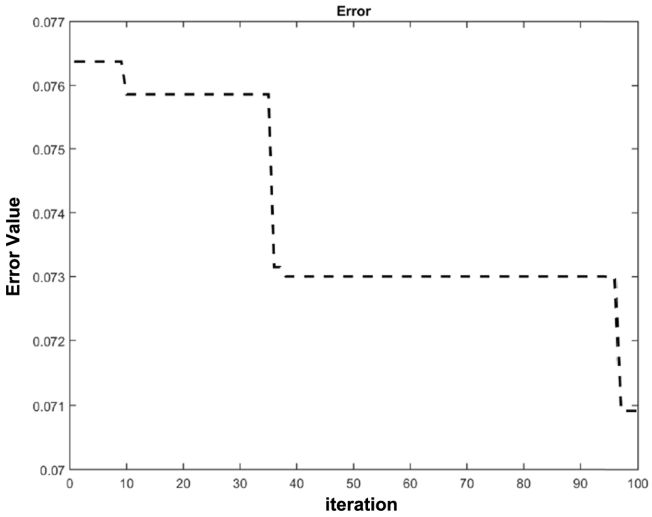

Fig. 2. Calculation of total error associated with the optimization of activity coefficient of ions in electrolyte solution of Extended UNIQUAC model at three temperatures of 298.15, 323.15, and 373.15 K and the pressure of 1 bar by implementing Genetic Algorithms in Matlab Software (reference activity coefficient, activity coefficient of inorganic ions in Pscalsim Software).

Table 2. Optimization of parameters r and q for UNIQUAC equation fitted to experimental data [6,20]

Electrolyte solution components	r	q
H_2O	0.92	1.4
CO_2	0.75	2.45
H	0.14	0.1E-15
Na	1.4	1.2
Ba	15.67	14.48
Ca	3.87	1.48
Sr	7.14	12.89
Mg	5.41	2.54
OH	9.4	8.88
Cl	10.39	10.2
SO_4	12.79	12.44
CO_3	10.83	10.77
HCO_3	8.08	8.68

Table 3. $u^o_{ij} = u^o_{ji}$ parameter of energy interaction between ions for aqueous electrolyte systems in UNIQUAC equation

Solution components	H_{2O}	CO_2	H	Na	Ca	Ba	Sr	mg	OH	Cl	So_4	Co_3^{2-}	Hco_3^-
H_{2O}	0												
$CO_{2(aq)}$	778.4	0											
H	1106.6	1954.4	0										
Na	1655.3	1816.93	1260.2	0									
Ca	1320.01	2175.9	1535.3	1248.4	0								
Ba	1253.3	1434.6	1076.25	1339.9	2309.9	0							
Sr	1556.8	1610.7	2003.3	1679.7	1583.1	1611.6	0						
Mg	1400.94	1576.4	851.1	1304.02	1159.4	1262.4	1603.7	0					
OH	1274.7	1843.04	562	1684.2	1446.7	1502.3	1639.4	216.848	1283.2				
Cl	1056.9	2215.2	1368.7	1528.2	1458.1	1585.25	1568.8	65.83	1550.6	1131.2			
So_4	1527.5	1618	877.6	1432.8	822.6	1290.2	732.1	161.3	1920.9	1328.5	1370.9		
Co_3^{2-}	1846.8	1623.4	1835.4	1321.8	1755.7	1168.2	994.35	1589.9	1952.6	1278.2	1657.6	1693.4	
HCO_3^-	2000	2222	2233	1333	1590	2500	3100	1991	2001	1223	2876	2223	2099

[1]Pars Scale Simulator

Table 4. $u^{t}_{ij} = u^{t}_{ji}$ parameter of energy interaction between ions for aqueous electrolyte systems in UNIQUAC equation

Solution components	H_{2O}	CO_2	H	Na	Ca	Ba	Sr	mg	OH	Cl	So_4	CO_3^{2-}	Hco_3^-
H_{2O}	0.0001												
$CO_{2(aq)}$	2.01	0.002											
H	−5.66	−2.06	0.0012										
Na	1.9	−2.83	5.001	0.00203									
Ca	5.81	−6.03	4.28	−0.062	0.032								
Ba	24.75	−6.2523	−6.624	1.47	2.63	0.0001							
Sr	8.4	1.9343	4.34	−4.5	−2.88	6.97	0.0011						
Mg	7.97	−4.711	−2.23	5.7	4.73	12.4	5.62	0.0025					
OH	−1.97	4.75	−4.02	−3.27	3.95	5.96	1.35	7.9	1.54				
Cl	−2.95	−2.04	−5.411	−1.46	9.16	0.93	−5.4	6.77	−5.2	7.3			
So_4	−2.64	1.34	−5.2	−2.463	−1.069	−0.54	1.25	2.44	14.98	2.44	6.7		
Co_3^{2-}	−6.54	−6.25	0.004	2.5113	7.64	6.59	−4.5	0.03	−0.4	7.7	−6.56	−0.46	
HCO_3^-	2	3.1	−2.3	1.3	−1.9	2.5	3.1	1.91	1	1.23	2.6	2.3	2.9

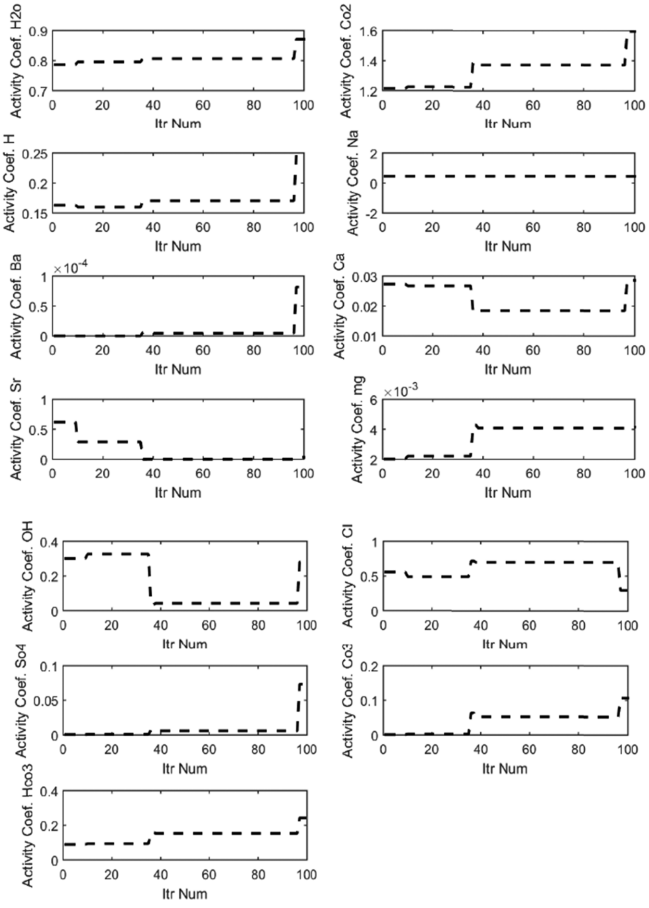

Fig. 3. Optimization of activity coefficient of components of electrolyte solution using genetic algorithms (GA) at 298.15 K.

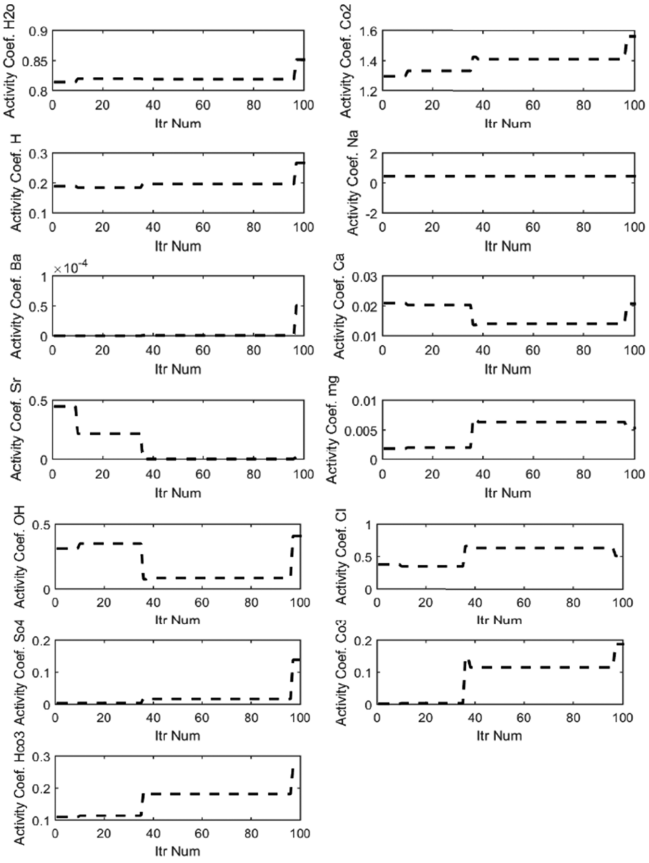

Fig. 4. Optimization of activity coefficient of components of electrolyte solution using genetic algorithms (GA) at 323.15 K.

4-2. Comparing the results of genetic algorithms with other algorithms

Fig. 6 provides a comparison between the optimization of Extended UNIQUAC model based on three algorithms: Imperialist Competitive Algorithm (ICA) [21], Particle Swarm Optimization Algorithm (PSO) [22-23] and Artificial Bee Colony Algorithm (ABC) [24-26]. Based on the flowchart in Fig. 1, the associated error with the optimization of the parameters of the considered model in this research using IC, PSO and ABC algorithms was found to be 0.054, 0.1045, and 0.089, respectively. Whereas, the associated error with the application of the proposed GA in the present research was 0.07, emphasizing superior quality and accuracy of the genetic algorithms compared to the aforementioned algorithms.

4-3. Comparing the optimized theoretical model with experimental results

Fig. 7 compares solubility predictions of three electrolyte systems

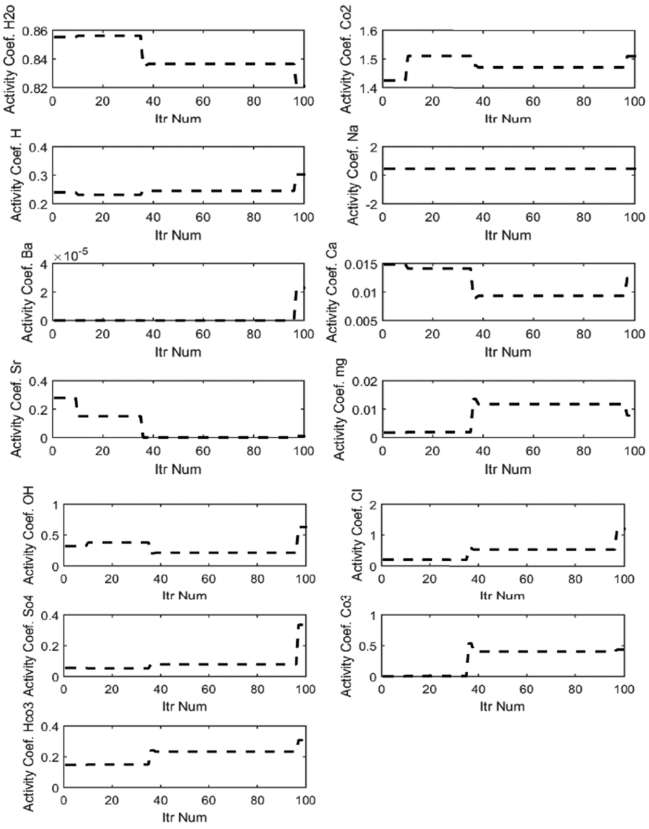

Fig. 5. Optimization of activity coefficient of components of electrolyte solution using genetic algorithms (GA) at 373.15 K.

at the constant pressure of 1 bar and two different temperatures of 323 and 368 K using the theoretically optimized model in this research to experimental results. According to the results of Fig. 7, solubility of barium sulfate at 323 K increases as does the concentration of sodium chloride. This is also true for the solubility of strontium sulfate in presence of magnesium chloride and calcium chloride at 368 K, as the increase in the concentration of magnesium chloride and calcium chloride leads to an increase in the concentration of strontium sulfate. Comparing the results demonstrated in Fig. 7 emphasizes that the optimized model in this research is significantly acceptable.

5. Conclusion

Considering the efficiency of the activity coefficient model of Extended UNIQUAC with optimized parameters was studied to predict activity coefficient of inorganic ions in petroleum systems (under solid-liquid equilibrium). The parameters of Extended UNIQUAC model were optimized by using genetic optimization algorithm. To apply trial and error on the results, the Pscalsim Software released by Research Institute of Petroleum Industry (RIPI) was used as the comparison reference. The total error calculated for the 13 ions under three temperatures of 298.15, 323.15, and 373.15 K using the genetic algorithm was found to be 0.07, and the iteration trend of the algorithm was reported for the 13 components of the system under study at three temperatures of 298.15, 323.15, and 373.15 K. The results obtained

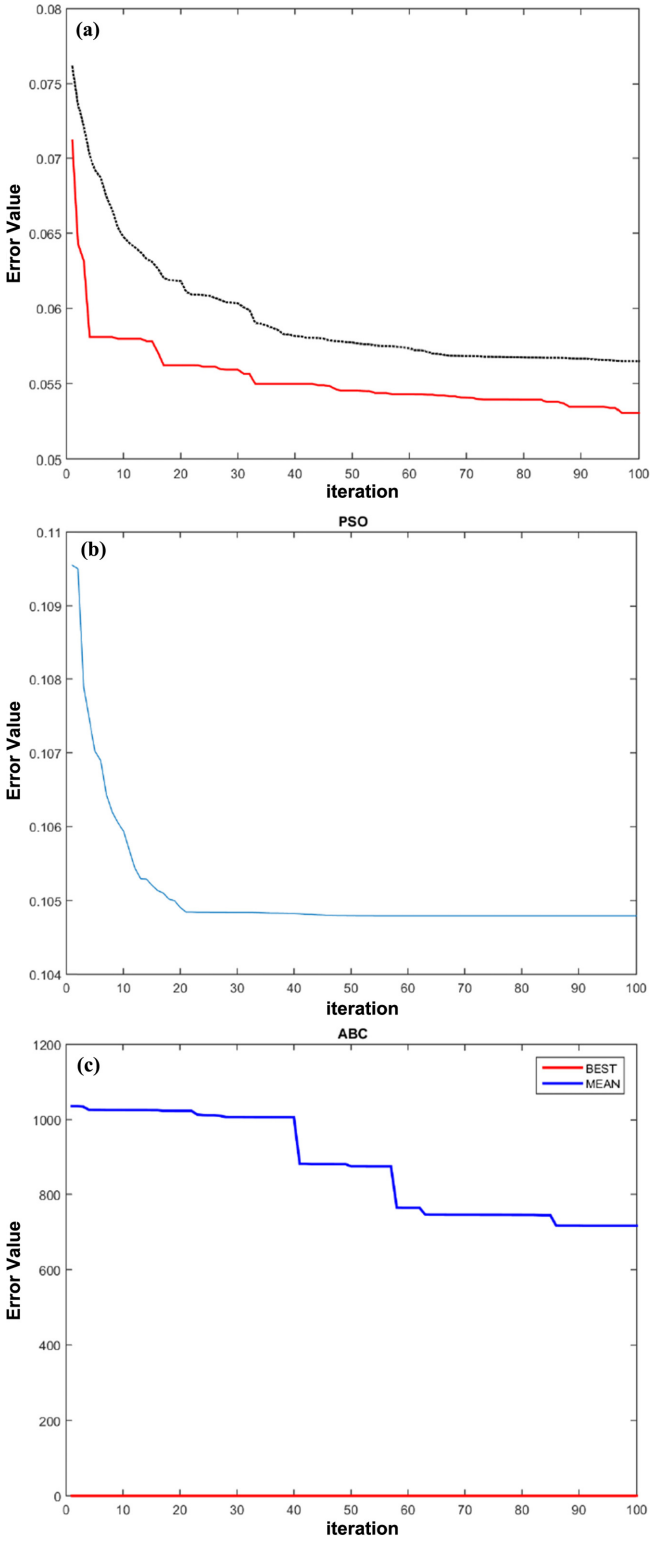

Fig. 6. Comparison between the optimization of Extended UNIQUAC model based on three algorithms: imperialist competitive (a) Particle Swarm Optimization (b) and Artificial Bee Colony (c).

using the genetic algorithm demonstrate the importance and priority of exploiting the optimized Extended UNIQUAC model in case of investigating saturation index of inorganic precipitates.

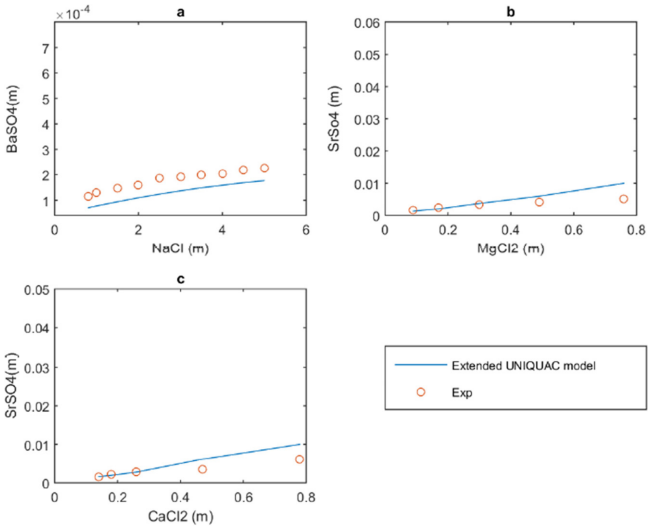

Fig. 7. Comparison between solubility values ((molality) predicted by Extended UNIQUAC model and experimental data: a) $BaSO_4$-NaCl-H_2O (at pressure: 1 bar and Temperatures : 323.15 K & Experimental reference [27]). b) $SrSO_4$-$MgCl_2$-H_2O (at pressure: 1 bar and Temperatures: 368.15 K & Experimental reference [28]). c) $SrSO_4$-$CaCl_2$-H_2O (at pressure: 1 bar and Temperatures: 368.15 K & Experimental reference [28]).

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