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An Optimization based Solution for Extended Spiegler-Kedem Model using Grey Wolf Optimizer

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Abstract— Extended Spiegler-Kedem (ESK) is an irreversible thermodynamics model that has been originally developed to predict the nanofiltration performance of multiple solutes systems by considering the osmotic coefficient in a membrane surface for non-ideal solutions. In the ESK model, the membrane is considered as a black box and all of the unknown parameters must be found by experimental data. Due to difficulties of doing enough precise experiments, traditional mathematical solutions such as Levenberg-Marquardt are not applicable. In this paper, at the first step, a modified ESK model for prediction of a high concentration solution is presented. Later, to compensate for the weakness of traditional mathematical methods, a solution based on optimization algorithms is proposed. Two optimization algorithms, Genetic Algorithm (as one of the most common algorithms) and Grey Wolf Optimizer (one of the most recent algorithms), are chosen and the results of ESK solution by them are provided and compared.

Keywords— Nano-filtration; Spiegler-Kedem; Negative Rejection; Grey Wolf Optimizer; Genetic Algorithm.

I. INTRODUCTION

The process of filtration through a membrane (reverse and forward osmosis) could be explained by the transport mechanism or irreversible thermodynamics. Solution-diffusion, Kimura-Sourirajan and extended Nerst–Plank are the models based on transport mechanism and the Spiegler-Kedem (SK) and Kedem-Katchalsky are based on irreversible thermodynamics. In irreversible thermodynamics, the membrane is considered as a black box, without considering the structure of membrane or mechanisms of transport. To simplify the modeling, the whole filtration is also considered as a slow process near the equilibrium. In this method of modeling, the flux of solvent and solute are only proportional to the chemical potential which is derived by pressure and concentration gradient.

Among these different methods, SK model has been widely used to predict the performance of single solutes in a Nanofiltration, reverse osmosis[1-3] and when one of the ions is impermeable to the membrane[4]. SK does not consider the interactions between the solutes and therefore, in many real practical filtrations, like water desalination, which the solution consists of more than two solutes, SK is not useful. To improve the model, Ahmad et al. developed SK for multiple solute systems by considering the solute-solute interactions. This model is named Extended Spiegler-Kedem (SKE) and can be summarized as the following equations:

$$J_v = \bar{L}_p\left(\frac{dP}{dx} - \sum_{s=1}^{n}\sigma_s\frac{d\pi_s}{dx}\right) \quad (1)$$

$$F_s = exp\left[\frac{-J_v(1-\sigma_s)}{P_{ss}}(1+\sum_{i=1}^{n}A_i)\right] \quad (2)$$

$$A_i = \frac{P_{si}(C_{pi}-C_{bi})\exp\left(\frac{J_v}{k_i}\right)}{J_v[C_{pi}-(1-\sigma_s)C_s]} \quad (3)$$

$$\frac{R_o}{1-R_o} = \frac{\sigma_s(1-F_s)}{1-\sigma_s}\exp\left(\frac{J_v}{k_i}\right) \quad (4)$$

$$R_o = 1-\left(\frac{C_p}{C_b}\right) \quad (5)$$

where F is driving force ($kWs/m\ mol$), A is osmotic constant ($m3Pa/g$), J_v is total volumetric flux ($m3/m2\ s$), C is concentration, σ is reflection coefficient and R_o is observed rejection. In all equations, the subscripts of b, p, s indicates bulk, permeate and i solute respectively.

In the ESK model, the solutes are considered ideal. In a non-ideal solution with a concentration of more than 1 molar on the membrane surface, the model must be modified using:

$$\Delta\pi_m = \varphi_m k(C_m - C_p)R_gT \quad (6)$$

where φ_m is the osmotic coefficient and k is the total number of constituent ions in the salt[5]. In this equation, by considering of the concentration on the solution on the membrane, φ_m, can be calculated for non-ideal solutions.

Ge et al. proposed a three-parameter model to calculate the osmotic coefficient[6]. In their model, the ion-ion distance, ion-solvent parameter, and solvent parameter are considered. In Ge's model, the two parameters of ion-ion and ion–solvent molecule interaction are not dependent to of the temperature of the solution and solvent[7]. The osmotic coefficient can be obtained from:

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$$\varphi = 1 - \frac{A|z_+ z_-|}{B^2 T^{\frac{1}{2}} a^2} \cdot \left[\frac{2}{I^{\frac{1}{2}}} - \frac{1}{(Ba)^{-1} T^{\frac{1}{2}} + I^{\frac{1}{2}}} - \frac{2\, ln\left(1 + BaT^{-\frac{1}{2}} I^{\frac{1}{2}}\right)}{BaT^{-\frac{1}{2}} I} \right] + \frac{S}{T} \cdot \frac{2n'}{2n'+1} \cdot \frac{I^{2n'}}{\nu'_+ + \nu'_-} \quad (7)$$

where φ is the osmotic factor, z is the ion charge, *A* and *B* are $6064.613\ kg^{1/2} mol^{-1/2} K^{3/2}$ and $56.827\ kg^{1/2} mol^{-1/2} K^{3/2}$ respectively. *T*, *a*, *n* and *S* show temperature, the parameter of ion-ion distance, the parameter of ion-solvent and salvation parameter respectively.

In equation 7, ν' is the stoichiometric number and can be calculated as:

$$\nu'_+ + z_+ = |\nu' - z_-| \quad (8)$$

I, ionic strength, can be calculated as

$$I = \frac{1}{2} \sum_i m_i . z_i^2 \quad (9)$$

where m is the molality (mol/kg).

II. FINDING UNKNOWN PARAMETERS

As it has been mentioned before, in the ESK model, the membrane is considered as a black-box. This means that there is a need for experimental data to find the unknown parameters. However, it should be considered that the number of unknown parameters in this model is relatively high. For instance, to predict the performance of the membrane in the four-solute solution, the unknown parameters of the model such as ρ_s, k_s, P_{ss}, P_{si} has to be found. The term P_{ss} is the solute permeability coefficient of solute *s* with the consideration of the interaction of solute *s* and the *Psi* is the solute permeability coefficient of solute s with the consideration of the interaction of solute *i*, *ss* is reflection coefficient and k_s is the mass transfer coefficient. In total, by considering *n* number of solutes in a system, the number of unknown variables will be $n^2 + 2n$. By considering *p* number of experimental data, we will have $n \times p$ equation that can be used to predict unknown variables. The mathematic solutions for such a problem like Levenberg-Marquardt, only work when $p \geq n + 2$. However, optimization algorithms can solve this equation. Optimization algorithms test different random values for all of the unknown variables and check the output of the model outputs with the experimental data. A set of random number for variables with the minimum acceptable difference between real condition and modeling can be considered as the correct answer. It should be considered that the optimization algorithms do not provide a certain answer for a specific question. They just try to be as close as possible to an optimum answer. This optimum finding is limited by processing time and resources. As much as process power increases or the period of the process be higher, the found answer will be closer to the optimum values. In a practical problem, the accepted closeness of the answer must be determined based on the nature and importance of the problem[8]. The better algorithm can find these optimum values in less time to save time and energy. Nowadays, there are different optimization algorithms[9-11]. From a well-known algorithm like Genetic Algorithm (GA) [12] to the most recent ones[13-15]. In this paper, GA as a complete famous algorithm in literature and a modern optimization algorithm named Grey Wolf Optimizer (GWO) are implemented. Due to the popularity of GA between researchers, there are many papers in the literature that used and discussed GA[16]. Therefore, in this paper GA principles and equations are not discussed and only the results and performance comparison between GA and GWO are provided.

III. GREY WOLF OPTIMIZER

GWO is an intelligent swarm-based algorithm developed by Mirjalili in 2014 [17]. The algorithm is inspired by the natural hunting behavior of the Grey wolf in nature as an apex predator on the top of the food pyramid. The algorithm simulates hunting (optimization of the cost function) with α male and female wolves which are followed by second and third top hunters (best solutions) named β and δ. The model of the optimization consists of searching for prey, encircling, hunting, and attacking.

A. Encircling prey

These steps are mathematically described as:

$$\vec{D} = \left|\vec{W}.\vec{X}_p(t) - \vec{X}(t)\right| \quad (10)$$

$$\vec{X}(t+1) = \vec{X}_p(t) - \vec{V}.\vec{D} \quad (11)$$

where t indicates the current iteration, *V* and *W* are coefficient vectors, $\vec{X}_p$ is the position vector of the prey, and *X* indicates the position vector of a grey wolf. The vectors V and W are calculated as follows:

$$\vec{V} = 2\vec{a}.\vec{r}_1 - \vec{v} \quad (12)$$

$$\vec{W} = 2\vec{r}_2 \quad (13)$$

where components of *v* are linearly decreased from 2 to 0 over the course of iterations and r_1, r_2 are random vectors in [0,1].

B. Hunting mechanism

In the hunting process, alpha, beta, and delta wolves lead the others to the prey position. In the mathematical simulation, we consider that alpha (the current best solution), beta and delta (the second and third top solutions) know the optimum solution (prey location). Therefore, the top best three solutions are saved and considered as the best potential of the optimum solution and the other search agents are obliged to update their position based on them. These equations simulate the search process.

$$\vec{E}_\alpha = \left|\vec{W}_1.\vec{X}_\alpha - \vec{X}\right| \quad (14)$$

$$\vec{E}_\beta = \left|\vec{W}_2.\vec{X}_\beta - \vec{X}\right| \quad (15)$$

$$\vec{E}_\delta = \left|\vec{W}_3.\vec{X}_\delta - \vec{X}\right| \quad (16)$$

$$\vec{X}_1 = \left|\vec{X}_\alpha(k) - \vec{V}_1.\left(\vec{E}_\alpha\right)\right| \quad (17)$$

$$\vec{X}_2 = \left|\vec{X}_\beta(k) - \vec{V}_2.\left(\vec{E}_\beta\right)\right| \quad (18)$$

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$$\vec{X}_3 = \left|\vec{X}_\delta(k) - \vec{V}_3.\left(\vec{E}_\delta\right)\right| \quad (19)$$

and rest of the wolves update their position as the following equation:

$$\vec{X}(k+1) = \frac{\vec{X}_1 + \vec{X}_2 + \vec{X}_3}{3} \quad (20)$$

C. Searching for and attacking the prey

Searching (exploration) and attacking (exploitation) are two abilities that grey wolves use in hunting. Grey wolves search for prey by diverging and attack prey by converging. Diverge and converge can be simulated mathematically by using $\vec{V}$ factor. $\vec{V}$ is a random number in the interval of $[-2v, 2v]$. $|\vec{V}| \leq 1$ forces the search agents toward the current optimum points and $|\vec{V}| \geq -1$ forces them to spread for fittest value. Exploration and exploitation make sure that the algorithm moves toward the optimum values and don't be trapped in a local optimum value[18].

IV. RESULTS AND DISCUSSION

The ESK model is tested with experimental data of Wadley et al. [19]. The data consists of the laboratory scale Nano-filtration experiments of the solution consists of 1-1-1 ternary mixture of $NaNO_3$, NaCl, $CaCl_2$. The total concentration of feeding solution is 0.0015 kg/m^3. In total, system contains of Na^+ of 0.69 kg/m^3, NO^{-3} with 0.93 kg/m^3, Cl^- with concentration of 1.5957 kg/m^3 and Ca^{2+} with the concentration of 0.6 kg/m^3. The membrane used as a filter is NF200 and all the tests are done at 35 ˚C with the range of pressure from 2.0 to 3.5 MPa.

The unknown parameters of the model with four solutes, ρ_s, k_s, P_{si}, have to be found by the optimization algorithm. To have a better understanding of the performance of each algorithm in finding the optimum values of unknown parameters, both algorithms are run in Matlab 2017, by a 2670 core i7® CPU without pooling process. Both algorithms used the same cost function and the tests are done in the same number generation or process time. However, based on the fundamental differences between the two algorithms, process time and convergence rate are so different for them. While each generation of GA needs a shorter period of time than GWO, the overall trend of convergence in GWO is much faster. To have a better understanding of the performance in solving ESK, both of them are run in an equal period of time [7].

TABLE I. THE ESTIMATED FACTOR OF ESK MODEL BY GA

Factor	*Na+*	*No3-*	*Cl-*	*Ca2+*
ρ_s	0.9886	0.7499	0.80877	0.8597
k_s	4.12e–05	7.26e–5	4.44e–3	3.62e–3
P_{s1}	1.54e–5	9.22e–8	8.77e–8	4.19e–8
P_{s2}	1.17e–7	1.20e–5	1.02e–5	6.81e–8
P_{s3}	1.96e–6	1.21e–6	1.79e–6	5.60e–8
P_{s4}	7.51e–7	6.29e–8	6.63e–8	9.56e–7
R2	0.9423	0.9030	0.8779	0.5374

TABLE II. THE ESTIMATED FACTOR OF ESK MODEL BY GWO

Factor	*Na+*	*NO3-*	*`Cl-*	*Ca2+*
ρ_s	0.9889	0.7489	0.8159	0.8485
k_s	4.13e-05	7.27e-05	4.45e-3	6.27e-3
P_{s1}	1.53e-05	9.31e-08	8.85e-08	4.18e-08
P_{s2}	1.26e-07	1.20e-05	1.01e-05	4.10e-08
P_{s3}	2.45e-06	1.21e-06	1.76e-06	8.65e-08
P_{s4}	6.45e-07	6.27-08	6.57-08	1.27e-06
R2	0.9623	0.9010	0.9236	0.8277

The results of the optimization show a significant improvement in the coefficient of determination (R^2) for Ca^{2+} and an overall improvement for the others. Fig. 1 shows the ion rejection of the system versus volumetric flux for all four ions. As it can be seen in the figure, the Na^+ shows negative rejection which the models and the algorithms could predict completely. The mechanism of this rejection can be explained by the effect of Donnan. Based on this effect, the negative rejection of Na is because of the negative charges of the surface of the membrane[20-25].

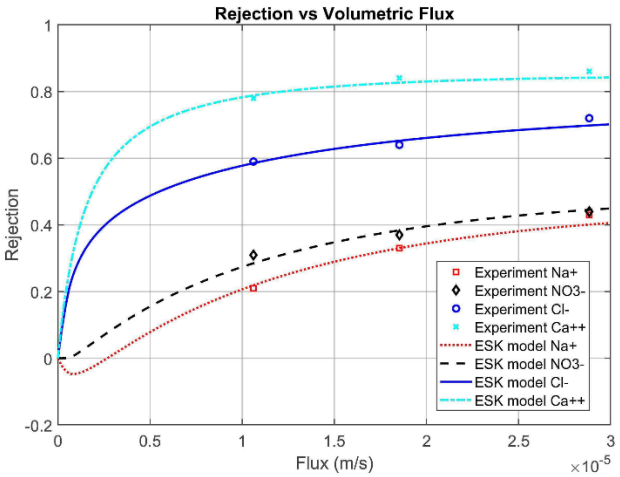

Fig. 1. Ions rejection of system versus volumetric flux (GWO).

V. CONCLUSION

Spiegler–Kedem model is a useful method to predict the behavior of single solutions in the reverse, forward osmosis, and Nano-filtration. An extended version of Spiegler–Kedem (ESK) can be implemented to estimate the performance of multiple solutes in the filtration. In the ESK model, the membrane is considered as a black-box and unknown parameters can be found by mathematical calculation over experimental data. Solving the equations using traditional mathematical solutions like Levenberg-Marquardt needs an adequate number of experimental data points. In the solutions with a high number of solvents, having an adequate number of experimental points is not easy to access. In this paper, we present an optimization solution to find the unknown parameters of the ESK model. Genetic Algorithm (one of the most common) and Grey Wolf Optimizer (one of the most recent ones) are implemented and the results of the solution with them are compared and presented. The results show that while GA and GWO are both able to move toward the better

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answers for the equations, GWO shows better improvement in the accuracy of the answers. Lower process time of this algorithm makes it a more desirable option for finding the solutions in such problems.

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