



Modeling of solute transport in multi-component solution for reverse osmosis membranes

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ABSTRACT

The model of salt transport through the membrane in multi-component system was developed with the irreversible thermodynamics theory considering the effect of the interaction between the salt ions. With the proposed transport model, the model for spiral-wound module was built based on the mass conservation law and concentration polarization derived by film theory. Through the parameter estimation, the frictional coefficients related to permeability of water and each ion was determined and then phenomenological analysis was conducted. The simulation results show that the salt rejection is increasing as the applied pressure and feed flow rate increasing. Also, the predictions by present model are in good agreement with the experimental data in the literature.

Keywords: Desalination; Spiral-wound reverse osmosis membrane; Membrane transport modeling

1. Introduction

Reverse osmosis (RO) process has become very popular and important as a separation technique during the past decade. This process can be applied to various fields such as desalination of seawater, wastewater treatment, chemical and biological industry and food and agricultural industries [2].

Many studies have been published to explain the mechanism of salt transport through the membrane, which has dependence of membrane properties and operation conditions [2–6]. In particular, both mechanistic and thermodynamic models have been used for explaining the transport phenomena of the salt: one of the most popular and frequently used among the mechanistic

models is the solution-diffusion model, in which the salt is assumed to pass through the membrane independently with the water. During the diffusion process across the membrane, there exists a difference in diffusion rates between the different species. Therefore, the separation is accomplished due to the concentration gradient formed across the membrane [2]. The thermodynamic models also have been used widely and developed by many authors [3,4]. They do not require the mechanistic view of the salt transport, rather use the linear phenomenological law of the irreversible thermodynamics. The following two thermodynamic models are based on the friction model, which explains the transport of the single salt solution through the membrane using two types of the frictions existing: One is between the salt and the membrane, and the other is between the solvent and the

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membrane. Kedem and Katchalsky first developed the transport model based on the irreversible thermodynamics which describes systems at non-equilibrium [3]. The Kedem–Katchalsky model takes account of the dissipation function composed of flows and forces in the case of the solution separated into the solute and the solvent by the membranes. The flows and the forces are also linearly related by adding the phenomenological coefficients, and consequently the fluxes across the membrane are calculated using the relationships. The Spiegler–Kedem model is an improved version of the Kedem–Katchalsky model [4]. Instead of the whole membrane, the infinitesimally divided elements of the membrane are considered since the salt concentration change across the membrane is continuous. Those models mentioned above can be used for the systems in which the coefficients, such as permeability, reflection coefficients, etc., are known.

However, these results have investigated under the single salt condition. Several studies have been proposed to describe the salt transport in multi-component system, and one of the most widely known methods is Kimura–Sourirajan analysis (KSA) [5]. The work of Kimura and Sourirajan mainly demonstrates how the permeation through the membrane is carried out by considering the behaviours of multi-component solution, especially electrolytes. Kimura–Sourirajan analysis explains the transport phenomena of the various salts under the assumption that each permeating salt uses distinct parameters for the each equation. The performance of the model has been verified in the sense that the result agreed with the one observed by experiments. However, it is reported that some discrepancy is shown between the expectations and the experimental results since the convective terms for the flux are neglected. Apart from the KSA, a number of approaches to describe the transport of the multi-component systems have been reported including Nernst–Planck equations, Ficks' law, a generalized form of Fick's law, and Stefan–Maxwell equation [6]. Among those, the Stefan–Maxwell equation is the mostly preferred in the aspect of capability of explaining not only the interactions between the salts but also the effects of those inter-frictions by the interactions. In the same manner with the thermodynamic models for the single salt solution, the Stefan–Maxwell equation is first derived for the multi-component electrolyte solution based on the linear phenomenological relation and extended to the various equations for each component of the non-electrolyte salts. Thus, the permeation process through the membrane can be described by applying the Stefan–Maxwell form for

$$\begin{aligned}
 F_w &= R_{11}J_w + R_{12}(J_w - J_{s1}) + R_{13}(J_w - J_{s2}) \dots + R_{1n}(J_w - J_{sn-1}) \\
 F_{s1} &= R_{21}(J_{s1} - J_w) + R_{22}J_{s1} + R_{23}(J_{s1} - J_{s2}) \dots + R_{2n}(J_{s1} - J_{sn-1}) \\
 F_{s2} &= R_{31}(J_{s2} - J_w) + R_{32}(J_{s2} - J_{s1}) + R_{33}J_{s2} \dots + R_{3n}(J_{s2} - J_{sn-1}) \\
 &\vdots \\
 F_{sn-1} &= R_{n1}(J_{sn-1} - J_w) + R_{n2}(J_{sn-1} - J_{s1}) + R_{n3}(J_{sn-1} - J_{s2}) \dots + R_{nm}J_{sn-1}
 \end{aligned} \tag{3}$$

the pressure-driven process with either the electrolyte or the non-electrolyte.

The objective of this work is the modelling of salt transport model and evaluation of the transport parameters in multi-component system. The salt transport model was developed with using the irreversible thermodynamic theory. The model for spiral-wound module was built with developed the salt transport model and then proposed the algorithm for solving the equations of the model numerically. Through the parameter estimation, the permeability coefficients of each ion were determined and analysed the physical meaning of the parameters.

2. Model development

2.1. Membrane transport model

In the irreversible thermodynamic theory, the flows are assumed to be a linear function of all the driving forces at near of thermodynamic equilibrium. However, the driving forces can be expressed as linear functions of the fluxes for clear implication of coefficients. The transport model for reverse osmosis membrane based on irreversible thermodynamics can be expressed as follows:

$$\begin{aligned}
 F_w &= \bar{R}_{11}J_w + \bar{R}_{12}J_{s1} + \bar{R}_{13}J_{s2} \dots + \bar{R}_{1n}J_{sn-1} \\
 F_{s1} &= \bar{R}_{21}J_w + \bar{R}_{22}J_{s1} + \bar{R}_{23}J_{s2} \dots + \bar{R}_{2n}J_{sn-1} \\
 F_{s2} &= \bar{R}_{31}J_w + \bar{R}_{32}J_{s1} + \bar{R}_{33}J_{s2} \dots + \bar{R}_{3n}J_{sn-1} \\
 &\vdots \\
 F_{sn-1} &= \bar{R}_{n1}J_w + \bar{R}_{n2}J_{s1} + \bar{R}_{n3}J_{s2} \dots + \bar{R}_{nm}J_{sn-1}
 \end{aligned} \tag{1}$$

where F and J denote the driving force and flux across the membrane respectively, and the subscripts w and si implies pure water and i -th ion species, respectively. The coefficients \bar{R}_{ij} are the resistances through the membrane. In the physical meaning of each coefficient, the diagonal coefficients, \bar{R}_{ii} are the resistances between the membrane and water/ion, and the off-diagonal coefficient, \bar{R}_{ij} are the resistances due to the interaction between salt species. Especially \bar{R}_{ij} 's imply the resistances between water and ions. From Onsager's relation, off-diagonal coefficients obey the following relationships:

$$\bar{R}_{ij} = \bar{R}_{ji} \tag{2}$$

In order that the meaning of coefficient has the resistance, however, the flux, J should be changed as the relative flux term since component flows through the membrane simultaneously. Therefore, Eq. (1) is changed as:

The diagonal coefficients have always positive but off-diagonal coefficients may be either positive or negative since ion has negative or positive charge and interact by electric force each other. If the coefficient R_{ij} is negative, the flow of species j increases the flow of species i as reinforcing the driving force to transport through the membrane.

Simply, Eq. (3) is written as matrix form

$$\begin{pmatrix} F_w \\ F_{s1} \\ \cdot \\ \cdot \\ \cdot \\ F_{sn-1} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n R_{1i} & -R_{12} & \dots & -R_{1n} \\ -R_{12} & \sum_{i=1}^n R_{2i} & \dots & -R_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ -R_{1n} & -R_{2n} & \dots & \sum_{i=1}^n R_{ni} \end{pmatrix} \begin{pmatrix} J_w \\ J_{s1} \\ \cdot \\ \cdot \\ \cdot \\ J_{sn-1} \end{pmatrix} \quad (4)$$

The driving forces can be expressed as the free energy difference across the membrane. The following equations are the driving force of water and ions [2]:

$$F_w = x_w (RT \Delta \ln(a_w) + \bar{V}_w \Delta P) \quad (5)$$

$$F_{si} = x_{si} (RT \Delta \ln(a_{si}) + \bar{V}_{si} \Delta P) \quad (6)$$

where x is the molar fraction, a is activity and V is molar volume. The physical meaning of F_w and F_{si} are the free energy difference when x_w moles of water or x_{si} moles of salt ion is transported from the feed solution to permeate through the membrane, respectively. Then, Eqs. (5) and (6) can be derived as follows:

$$\begin{aligned} F_w &= x_w (RT \Delta \ln(a_w) + \bar{V}_w \Delta P) \\ &= x_w (RT \Delta \ln(\gamma_w x_w) + \bar{V}_w \Delta P) \\ &\approx x_w (RT \Delta(-x_s) + \bar{V}_w \Delta P) \\ &\approx x_w (-\bar{V}_T RT \Delta(c_s) + \bar{V}_w \Delta P) \\ &\approx -\bar{V}_T \Delta \pi + \bar{V}_w \Delta P \approx \bar{V}_T (\Delta P - \Delta \pi) \end{aligned} \quad (7)$$

$$\begin{aligned} F_{si} &= x_{si} (RT \Delta \ln(a_{si}) + \bar{V}_{si} \Delta P) \\ &= x_{si} (RT \Delta \ln(\gamma_{si} x_{si}) + \bar{V}_{si} \Delta P) \\ &= \bar{V}_T (c_{si} RT \Delta \ln(c_{si}) + \bar{V}_{si} c_{si} \Delta P) \end{aligned} \quad (8)$$

Eqs. (7) and (8) can be simplified by assuming that the activity coefficients, γ are unity and the partial molar volume of water, \bar{V}_w is equal to partial molar volume of whole solution, \bar{V}_T .

The membrane transport model can be obtained by combining Eqs. (4), (7) and (8) as a result.

2.2. Salt rejection

To solve the membrane transport model, it is more convenient to use salt rejection since the concentrations of permeate side are unknown. The salt rejection is defined as follows:

$$r = 1 - \frac{C_s^P}{C_s^F} \quad (9)$$

where superscripts P and F denote the permeate side and feed side, respectively.

The terms, $\Delta(C_s)$ and $\Delta \ln(C_{si})$ in Eqs. (7) and (8) are related to the salt rejection and can be written as

$$\Delta(c_s) = C_s^F - C_s^P = C_s^E \left(1 - \frac{C_s^P}{C_s^F}\right) = C_s^E r = \sum C_{si}^F r_i \quad (10)$$

$$\Delta \ln(c_{si}) = \ln\left(\frac{C_{si}^F}{C_{si}^P}\right) = \ln\left(\frac{1}{1-r_i}\right) = -\ln(1-r_i) \quad (11)$$

Substituting Eqs. (10) and (11) into Eqs. (7) and (8) results in

$$F_w = x_w (-\bar{V}_T RT \sum C_{si}^F r_i + \bar{V}_w \Delta P) \quad (12)$$

$$F_{si} = \bar{V}_T (\bar{V}_{si} c_{si} \Delta P - c_{si} RT \ln(1-r_i)) \quad (13)$$

With inverse matrix form, Eq. (4) can be written as

$$\mathbf{J} = \mathbf{R}^{-1} \mathbf{F} \quad (14)$$

where \mathbf{R} is the coefficient matrix, \mathbf{J} is the vector for fluxes and \mathbf{F} is the vector for driving forces.

The salt rejection can be also determined from fluxes and expressed as:

$$r_i = 1 - \frac{J_{si}}{\bar{V}_w J_w + \sum \bar{V}_{si} J_{si}} \quad (15)$$

Substituting Eq. (14) with Eqs. (12) and (13) into Eq. (15), the salt rejection can be expressed as

$$r_i = 1 - f(r_i, P, T, c_s^F) \quad (16)$$

The above equation is an implicit function of the salt rejection. Although an explicit expression is preferable, it is difficult to derive if some assumptions such as very dilute solution of permeate side are not valid. Therefore, Eq. (16) should be calculated iteratively under the given operating conditions such as applied pressure, feed temperature and concentration of feed. The iteration scheme is shown as Fig. 1.

2.3. Model for spiral-wound module

In this section, the model equations for the spiral-wound module are derived. The schematic drawing of spiral-wound module is shown in Fig. 2.

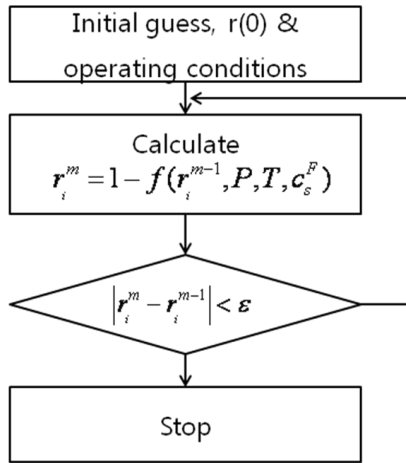


Fig. 1. Iteration scheme for calculating the salt rejection.

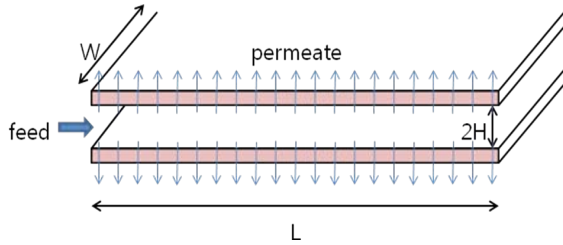


Fig. 2. Schematic drawing of stretched spiral-wound module.

The mole or volumetric fluxes of water and all ions, J_i through the membrane are given by Eq. (14) as a matrix form.

At steady state, the mass of all components should be conserved anywhere. Therefore, the following equations are valid:

$$Q(x) = Q(0) - \int_0^x W \sum_{i=1}^n J_i(x^*) dx^* \quad (17)$$

$$Q(x)c_{si}(x) = Q(0)c_{si}(0) - \int_0^x W J_{si}(x^*) (1 - r_i(x^*)) c_{si}(x^*) dx^* \quad (18)$$

where W is membrane width and Q is the axial flow rate of whole solution.

To describe the concentration polarization phenomena, a film theory approach developed by Michaels and others was used [30]. The relationship between concentration polarization and permeate flux can be expressed as:

$$\frac{c^w - c^p}{c^b - c^p} = \exp\left(\frac{J_w \delta}{D}\right) \quad (19)$$

where c^w is the concentration at the membrane surface, c^b and c^p are concentrations at the bulk and permeate side, respectively. Also, δ is film layer thickness and \bar{u} is

average axial flow velocity. Assuming constant diffusivity, a local mass transfer coefficient in a thin rectangular channel is described by

$$k(x) = \frac{D}{\delta(x)} = \frac{1}{1.475} \left(\frac{3\bar{u}}{2H} \frac{D^2}{x} \right)^{1/3} \quad (\text{laminar flow}) \quad (20)$$

$$k(x) = \frac{D}{\delta(x)} = \frac{0.04 \text{Re}^{0.75} \text{Sc}^{0.33} \cdot D}{d_h} \quad (\text{turbulent flow})$$

Substituting Eq. (19) into Eq. (20) and applying the salt rejection, the following equation can be obtained.

$$\frac{c_{si}^w(x)}{c_{si}^b(x)} = 1 - r_i(x) + r_i(x) \exp\left(\frac{J_w(x)}{k_i(x)}\right) \quad (21)$$

The driving pressure in the module decreases along the membrane channel due to the friction loss of the feed stream through the membrane wall and spacers. The pressure drop along the axial direction of membrane is simply described by [1]

$$\Delta P(x) = \Delta P(0) - k_f \frac{12\bar{u}(x)\eta dx}{H^2} \quad (22)$$

where k_f is the friction coefficient in the feed channel related to the pressure drop along the channel and η is the viscosity of solution in the feed side.

The derived model for spiral-wound module cannot be calculated analytically. Therefore, a numerical approach is used in this study. The filtration channel is divided into m segments of equal interval, Δx , and then the concentrations of each component, driving pressure, permeate flux and axial flow velocity are calculated. In the first segment, the following equations are assumed, in which concentration polarization is neglected and rejections are assumed unity.

$$\begin{aligned} \mathbf{J}(1) &= \mathbf{R}^{-1}\mathbf{F}(1) \\ Q(1) &= Q(0) \\ u(1) &= u(0) \end{aligned} \quad (23)$$

$$\begin{aligned} c_{si}(1) &= c_{si}(0) \\ \Delta P(1) &= \Delta P(0) \end{aligned}$$

For segments from 2 to m

$$Q(i) = Q(i-1) - W\Delta x \sum_{i=1}^n J_i(i-1) \quad (24)$$

$$\bar{u}(i) = Q(i)/(HW) \quad (25)$$

$$c_{si}(i) = \frac{Q(i-1)c_{si}(i-1) - WJ_{si}(i-1)(1 - r_i(i-1))c_{si}(i-1)\Delta x}{Q(i)} \quad (26)$$

$$\Delta P(i) = \Delta P(i-1) - k_f \frac{12\bar{u}(i-1)\eta\Delta x}{H^2} \quad (27)$$

$$k(i) = \frac{1}{1.475} \left(\frac{3\bar{u}(i) D^2}{2H i \Delta x} \right)^{1/3} \quad (28)$$

$$\frac{c_{si}^w(i)}{c_{si}^b(i)} = 1 - r_i(i) + r_i(i) \exp\left(\frac{J_w(i-1)}{k_i(i)}\right) \quad (29)$$

$$r_i(i) = 1 - f(r_i^*(i), P(i), T, c_{si}(i)) \quad (30)$$

$$J(i) = \mathbf{R}^{-1} \mathbf{F}(i) \quad (31)$$

The algorithm of numerical procedure is shown in Fig. 3. With the above equations and algorithm, the numerical solution of the model for spiral-wound module can easily be determined.

3. Results and discussion

3.1. Parameter estimation

The parameters in the presented multi-components model are estimated with using experimental data from literature [5]. In this literature, they have carried out experiments which are desalination of wastewater with various applied pressures and feed flow rates in the spiral-wound module. For the estimation of the ion rejection, 5 different ions are measured in both the feed and permeate solution. Experimental data from literature are shown in Table. 1.

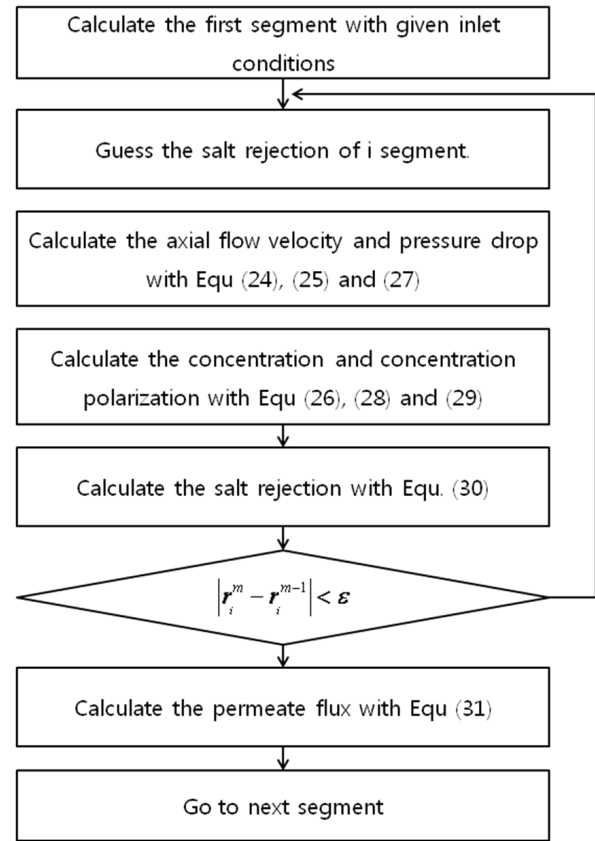


Fig. 3. Numerical procedure for calculating equations of spiral-wound module.

Table 1
Experimental data from literature [5]

Applied pressure (bar)	Permeate flow rate (l/h)	Feed flow rate (l/h)	Mole fraction × 1e6				
<i>P</i>	<i>D</i>	<i>F</i>	Ca ²⁺	Mg ²⁺	Na ⁺	Cl ⁻	HCO ₃ ⁻
25	23.8	204	4.6	7.9	71	92	7.2
30	29.1	202	4.2	7.5	66	86	6.5
35	34.4	202	3.7	7.1	61	81	5.8
40	39.8	201	3.3	6.7	57	76	5.0
25	23.7	268	3.9	7.1	62	82	6.9
30	29.4	269	3.6	6.7	55	74	6.6
35	35.3	272	3.3	6.3	49	67	6.3
40	41.1	276	3.1	5.9	42	59	6.0
25	23.6	334	3.6	6.9	58	79	6.7
30	29.3	332	3.4	6.4	52	71	6.4
35	35.2	335	3.1	5.9	46	63	6.1
40	41.0	343	2.8	5.4	40	54	5.8
25	23.3	395	3.4	6.7	54	75	6.6
30	29.2	395	3.2	6.1	47	67	6.2
35	34.9	395	3.0	5.7	40	59	5.8
40	40.8	395	2.7	5.3	33	52	5.4

In the case of water system with 5 ions, it is not easy to estimate parameters since there are 21 parameters in the present model. Therefore, the least-square solution may be used for decision of initial guesses to estimate parameters. Using the least-square solution, the order of magnitude for each parameter can be inferred. However, the coefficient matrix from least-square estimate is not a symmetric form. The least-square solution can be easily obtained by following equations.

$$\begin{aligned}
 \mathbf{F} &= \mathbf{R}\mathbf{J} \\
 \mathbf{F}\mathbf{J}^T &= \mathbf{R}\mathbf{J}\mathbf{J}^T \\
 \mathbf{R} &= \mathbf{F}\mathbf{J}^T (\mathbf{J}\mathbf{J}^T)^{-1}
 \end{aligned}
 \tag{32}$$

where \mathbf{F} and \mathbf{J} are matrix constructed from the set of all experimental data. With the initial guesses for the parameters, parameter estimation is conducted to minimize sum of error square by adjusting the parameters value with an optimization technique until the error is below a tolerance level, where the error is defined as a sum of square differences between experimental data and simulated values. The objective function is as following,

$$\min_{R_{ij} (i \leq j)} \sum_{k=1}^N (\mathbf{R}^{-1}\mathbf{F}_k - \mathbf{J}_k^{\text{exp}})^T (\mathbf{R}^{-1}\mathbf{F}_k - \mathbf{J}_k^{\text{exp}})
 \tag{33}$$

where J_k^{exp} is the measured permeate flux and subscript, k means experiment's number.

In Figs. 4, 5 and 6 the permeate fluxes and salt rejections of each component are presented as a function of the applied pressure for various feed flow rates. For the

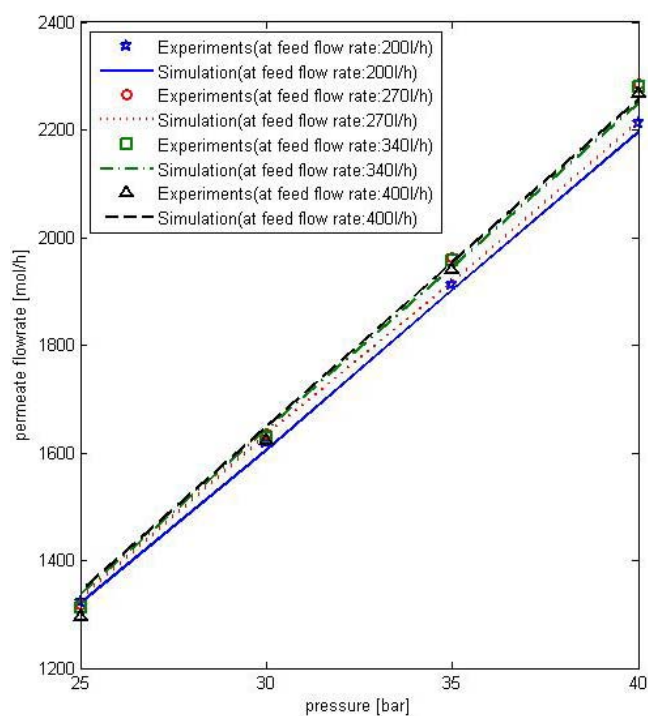


Fig. 4. Permeate flow rate of water with various feed flow rate.

comparison, both simulation results and experimental results are plotted simultaneously.

The results show that the salt rejection is increasing as the applied pressure and the feed flow rate are increasing. As shown in Table 2, the relative error of permeate flux of water and ions are below 2% and the 10%, respectively. The predictions by present model are in good agreement with the experimental data.

The obtained optimal parameters are shown in Table 3. As mentioned above, the physical meaning of parameters, R_{ii} 's are the resistances of ion component and membrane and they should be positive. Also, R_{ii} 's depend on the membrane property, but they may not depend on operating variables except the temperature. Parameters, R_{ij} on the other hand, may be either positive or negative and they are independent of membrane property and operating conditions.

Table 2
Relative errors for parameter estimation

Error of $J_{w'}$ %	1.2174
Error of $J_{Ca'}$ %	5.0959
Error of $J_{Mg'}$ %	2.2080
Error of $J_{Na'}$ %	9.6413
Error of $J_{Cl'}$ %	6.1231
Error of $J_{HCO_3'}$ %	4.6712

Table 3
Optimal frictional coefficients

Coefficient	Value	Sign
R11	3.5094e-4	+
R22	4.1463	+
R33	6.0501	+
R44	0.2309	+
R55	0.5886	+
R66	1.6486	+
R12	-6.7734e-6	-
R13	-1.0525e-5	-
R14	-1.0649e-5	-
R15	-5.4724e-5	-
R16	6.0029e-6	+
R23	-0.2086	-
R24	-0.0901	-
R35	0.0315	+
R26	0.0373	+
R35	0.0291	+
R36	0.0717	+
R45	0.3079	+
R46	0.1301	+
R56	-0.0719	-

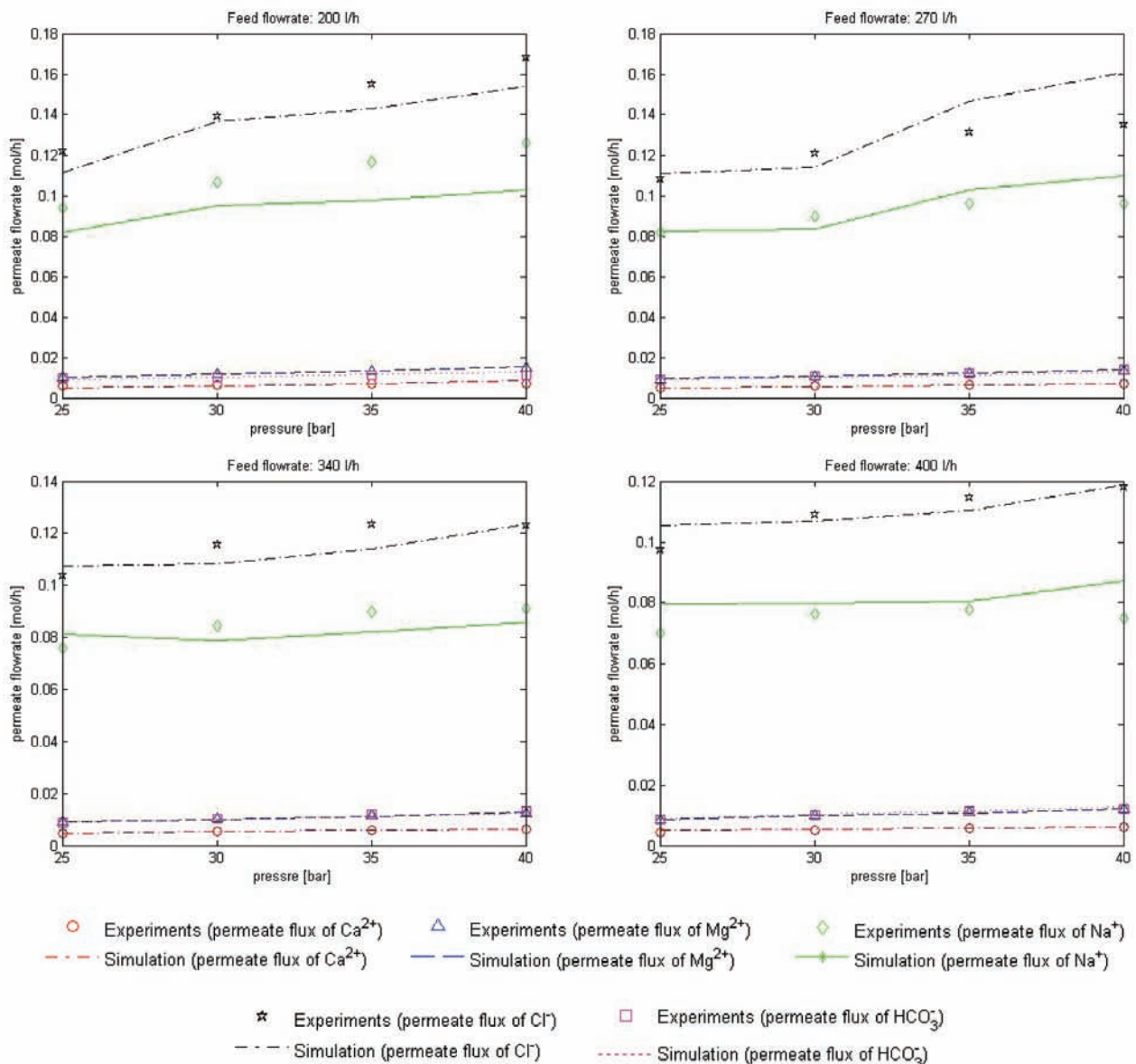


Fig. 5. Permeate flow rate of ions with various feed flow rate.

As shown in Table 3, R_{ij} 's are either positive or negative. When the i -th ion has different charge with j -th ion, the coefficient, R_{ij} has positive sign and conversely, when the i -th ion has equal charge with j -th ion, the coefficient, R_{ij} has negative sign. The reason for this seems to be the repulsion and attraction of charged ion by electric force. If the i -th and j -th ions have same charge, they repulse each other and there is no friction between the i -th and j -th ions. On the other hand, if they have different charge, there is high friction between the i -th and j -th ions because of attraction forces. In the case of water and ion, the frictional coefficients, R_{ij} 's have small value compared to R_{11} with 2-orders of magnitude difference.

Therefore, water and salt fluxes are not significantly affecting each other.

4. Conclusions

In this study, the model of salt transport through the membrane in multi-component system was developed with the irreversible thermodynamics theory. The proposed model considered the effects of the interactions between the salt ions. The transport model was expressed as matrix form for compact representation. Then, using the proposed transport model, the model for spiral-wound module was built based on the mass conservation law

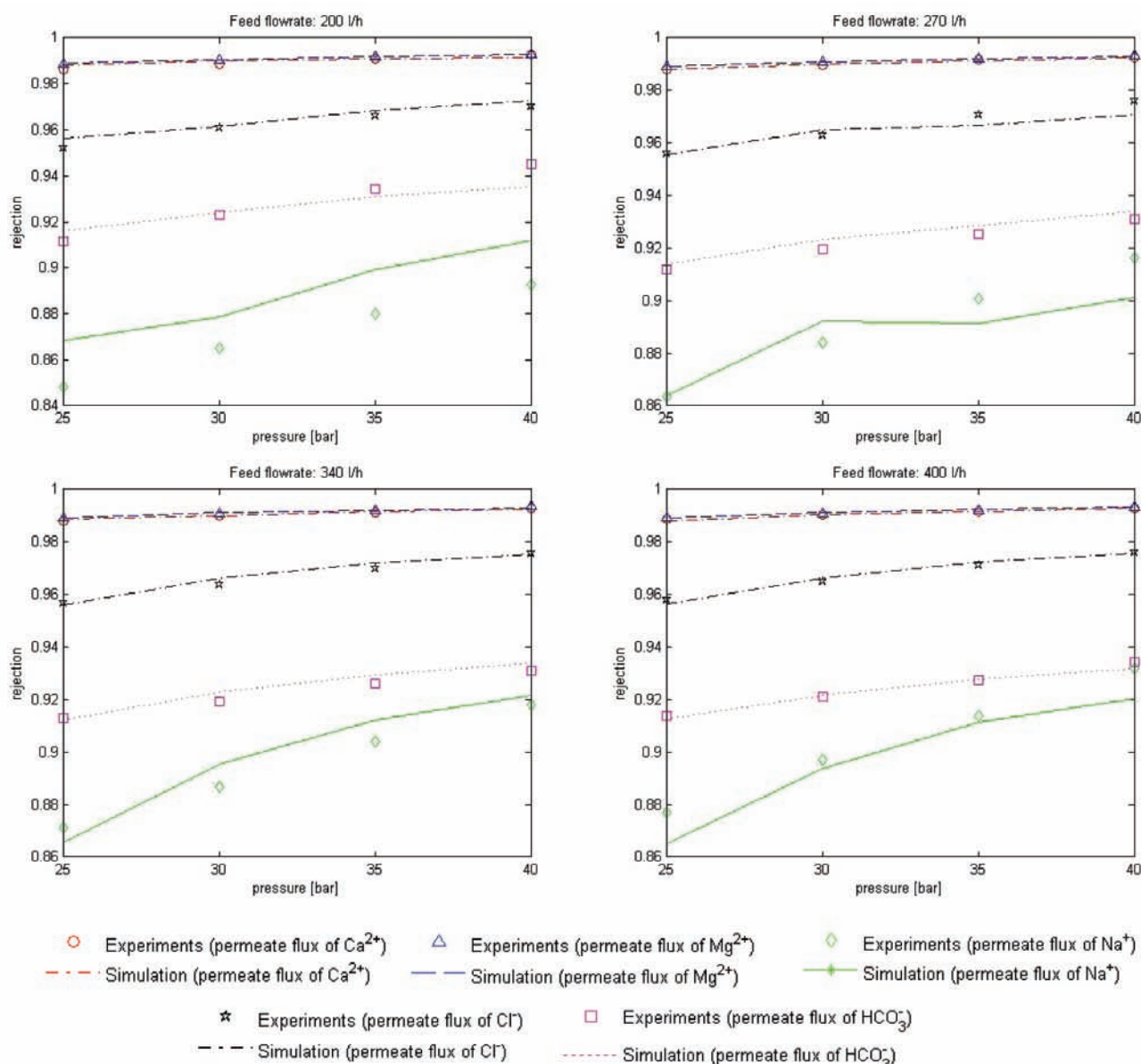


Fig. 6. Salt rejection of ions with various feed flow rate

and concentration polarization derived by film theory. Through the parameter estimation, the frictional coefficients related to permeability of water and each ion were determined. The obtained coefficients were analysed for the physical meaning of the parameters. When one ion has different charge with another ion, the coefficient has positive sign and when ion has equal charge with another ion, the coefficient has negative sign, conversely. Although the proposed salt ion transport model has relatively many parameters than other models, most parameters except of the diagonal parameters in the matrix, \bar{R} may be set a constant because they are independent of the membrane property. The predictions by present model are in good agreement with the experimental data in the literature.

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Symbols

- a — Activity
- c — Concentration, mol/l
- D — Diffusivity, dm
- H — Height of the channel, dm
- J — Flux across the membrane, dm/h
- k — Mass transfer coefficient, dm/h

k_f	— Friction coefficient
P	— Pressure, bar
Q	— Axial volumetric flow rate, l/h
R	— Gas constant, bar·l/mol·K
r	— Salt rejection
R_{ij}	— Resistance through the membrane, bar·dm ² ·h/mol
T	— Temperature, K
\bar{u}	— Average axial flow velocity, dm/h
\bar{v}	— Molar volume, l/mol
W	— Membrane width, dm
x	— Molar fraction, mol/mol

Greek

γ	— Activity coefficient
δ	— Film layer thickness, dm
Δx	— Segment interval, dm
η	— Viscosity of solution, bar h
π	— Osmotic pressure, bar

Subscripts

k	— Number of experiment
s	— Salt
si	— i -th ion species
T	— Total
w	— Pure water

Superscripts

b	— At the bulk side
exp	— Measured in experiments
F	— At feed side
P	— At permeate side
w	— At the membrane surface

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