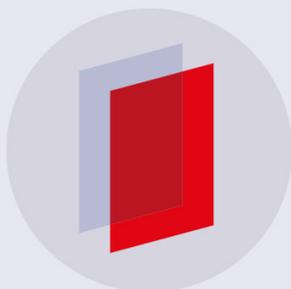


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Model assessment of a nanofiltration membrane for the removal metal ions from simulated wastewater

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Abstract

This paper accords the likelihood of applying Donnan and Steric Partitioning Pore Model (DSPM) together with extended Nernst-Planck model to elucidate the capacity of charge and Donnan exclusion mechanisms in removing ions from simulated wastewater in Nano-Pro-3012 membrane filtration process. The extended Nernst-Planck model reports the transportation of cations across Nano-Pro-3012 with respect to electrical potential gradient, movement of solutes and pressure difference through the membrane. The working principle of these two equations is dependent on the adsorption of the charged surface, diffusion and convective transport. This principle was established with a software called Comsol multi-physic 4.3b to explain the capacity of charge and Donnan exclusion mechanism of Nano-Pro-3012. The extended Nernst-Planck model and the Darcy law model were applied to evaluate the physical interrelationship amidst Nano-Pro-3012 and ionic solutions with the aim of having a good understanding of the transport and rejection working operation of the ions. The principle of these equations was first used to envisage the capability of Nano-Pro-3012. The data obtained were validated with the laboratory data. There was an establishment that movement of solutes across the membrane bring about diffusion transport. The total flux in solution increases due to the working operation of the diffusion which in turns reduces the electrical potential, as a result, reduces the flux in the membrane. Ions smaller than pore sizes are rejected and the theoretical data is in conformity with the experimental data.

Keywords: Nanofiltration membrane. Extended Nernst-Planck equation. Donnan exclusion. Concentration gradient. Electrical potential. Zeta potential. Rejection of ions. Comsol multi-physic 4.3b

1. Introduction

The obtainability of clean water has come to be a serious global challenge confronting the mankind as a result of water contamination by human activities [1]. Therefore, the provisions for clean water are under constraint because contaminated water from homes and diverse industries has resulted to a major issue on the surroundings globally. The separation process by nanofiltration (NF) is known to be one of the latest processes utilized in eliminating pollutants from contaminated water. The operation of NF membrane is a pressure-driven partitioning operation and its features rest in the middle of reverse osmosis and ultrafiltration [2, 3]. It is a propitious technical knowledge to partition neutral and stimulating saline in solutions [4]. Retention of metal ions by NF is principally guided by the movement of ions across



concentration polarization stratum, partitioning phenomenon at membrane intersections together with the movement of solute across the pores [5]. Hence, modeling of the movement of ions across nanofiltration is very important in envisaging the capability of membrane for the removal of ions. Such knowledge will assist in the interpretation of the principle of separating various salt/metal; therefore, choosing a proper membrane for a precise process. For the purpose of envisaging the partitioning capability of NF membranes, diverse models were exploited. Some of the models are the non-equilibrium, the space charge, Teorell-Meyer-Sievers, electrostatic and steric-hindrance together with semi-empirical models [6, 7].

Wu et al. [8] used a non-equilibrium model to investigate NF of aqueous solutions of some ionic liquids. The data generated from nanofiltration experiments were examined by the non-equilibrium thermodynamics approach for the purpose of finding out the factors of empirical movement. Empirical transport factors for the ionic liquids-water system were compared with factors of an inorganic electrolyte-water system. Data obtained suggested that an exceedingly effective procedure for ionic liquids separation can possibly be developed as long as the states of operation are further enhanced. Yang et al. [9] developed a non-equilibrium theory for polydimethylsiloxane membrane pervaporation of acetone, butanol and ethanol. The dissolution and desorption procedures conducted were done as quasi external response activities founded on the theory of non-equilibrium dissolution at the boundary of solutes and membrane. Quasi-practical theory depended on stable transmission of mass, disregarding the concentration polarization and adsorption at the imbuing side. The diffusion factors together with the rate constants of the adsorption kinetic of the theory were attained by a straight line connection of the flux with diverse thickness of the membrane including equilibrium partition coefficient. The values calculated through the theory were in agreement with the practical flux. The authors recommended that there should be further application of the non-equilibrium theory and the modeling parameters with an aim of envisaging the partitioning ability and choosing of working settings for the membrane.

With respect to the theory of space charge, surplus electric charge was conducted for the range of charge circulated above the zone of space by the capacity. Here, the membrane is presumed to have similar cylinder-shaped pores. The charges of the membrane are evenly circulated on the interior hedge of the pores. Radially and axially resultant circulation of electrical potential and concentration of ion are presented depending on the Poisson-Boltzmann model [10]. The three significant factors of the space charge theory are surface charge density of the capillaries, pore radius and the electrolyte concentrations. Nernst-Planck model for the movement of ions, the Navier-Stokes model for volumetric flow and the Poisson-Boltzmann model for radially circulation of the electric potential together with ion concentration are considered fundamental equations that governs the mechanism of the space charge theory [11]. The most predominant models for nanofiltration obtainable from space charge theory assumes radial uniformity of the concentration of ions and potential across the pores, which is effective for modest surface charge densities and suitably contracted pores [5]. Kristensen et al. [12] used the accustomed space-charge concept for a joint movement model of solutes across cylinder-shaped nano-pores in order to develop models for counter-ion transport numbers capacity. For a zero and non-zero gradient of concentration together with the application of current density, the calculations of the transport number from the space-charge model was equated to an equivalent calculation from the

constant potential and Teorell-Meyer-Sievers theories. With this approach, the authors suggested that the best conditions for carrying out membrane potential tests are dependent on a straightforward membrane feature, known as the volumetric charge density.

With hypothesizing a homogeneous fixed charges radial dispersion and moveable species, Teorell-Mayer-Sievers model (TMS) is a demanding method extensively utilized to evaluate electrical features of a negatively charged membrane [11, 13]. The essential mechanisms that characterized TMS model are the potential of the membrane, coefficient of diffusion, electric conductivity and transport number with the assumption that the movement of ions and activity coefficient are constant [14]. The main models of TMS theory are the Donnan model for the partition coefficients of concentrations of ion between membranes and outward solution, the Nernst-Planck model together with diverse states of electro-neutrality for the interior part of a membrane and outward solutions [15]. The transport features and the occurrence of electrokinetic of charged capillaries has been illustrated by Teorell-Mayer-Sievers model [16, 17]. Elsherif et al. [18] used Teorell-Mayer-Sievers model to study the fixed charge density in corresponding/L solution with mobility ratio cation to anion in a membrane phase. Several approaches were applied for the purpose of estimating the effective charge density with the aid of membrane potential measurements. The data obtained from membrane potential was used to estimate the action of the number of ions and perm-selectivity. The authors concluded that the approach of Teorell-Mayer-Sievers is unreliable to evaluate the fixed charge density for ion-exchange membranes having an elevated fixed group concentration. However, the movement of ion in the interior part of the membrane is presupposed to be equivalent to the mobility of ion in the free volume. Furthermore, the transport of ion is dependent on the moment related to the frictional model. The presumption is specifically challenging; hence, resulted in establishing a hybrid equation which takes into account a reduction in ion movement as a result of the interference in the interior pores of a membrane such as Donnan-steric partitioning pore model (DSPM) [10].

DSPM serves as an amplification of the TMS equation [19]. It takes into consideration a charged porous stratum of the membrane and it is designated by three modifiable factors; the mean radius of the pore, the volumetric charge density, and membrane active thickness [20]. The interference of the pore such as the interrelationship between the movement of ions and the membrane material can be rated by interference characteristics for diffusion and convection and is dependent on the active pore radius [10]. The model is dependent on the extended Nernst-Planck model [21]. Imbuing of ions via the nanofiltration membrane can be illustrated by Extended Nernst-Planck model. Extended Nernst-Planck model illustrates the diffusion, convection, and electro-migration triggered by electrical potential and concentration gradients [22]. Ions convention through the membrane, the concentration and the electrical potential gradients are as a result of the pressure variance through the membrane. This leads to ionic diffusion through the nanofiltration membrane [23]. The two methods often used for simulation are Monte Carlo method and molecular dynamic [24]. Nonetheless, the measure of Monte Carlo method and molecular dynamic is not enough to predict the transportation of ions at macro scale technology like NF process. DSPM has also been successfully used in modeling NF membrane performance without the extended Nernst-Planck model [25]. However, in spite of the attainment of Donnan Steric pore model, a remarkable condemnation concerning DSPM is the difficulty in the computational method of solving the equation and the repetition pattern needed to work out the

combined differential equations. Therefore, the incorporation of DSPM in extended Nernst Planck equation will be applied for this work to resolve the difficulty in the computational method and the repetition pattern needed to work out the coupled differential equations [26]. This work is done to test the capacity of charge and Donnan exclusion mechanism during Nano-pro-3012 filtration process using DSPM in conjunction with extended Nernst Planck equation.

1.1 Donnan Steric pore model and Extended Nernst Planck model

Utilization of Donnan Steric Partitioning Pore equation and the extended Nernst-Planck model was presented to illustrate the movement of ion through the pores. Extended Nernst-Planck model envelopes the three essential parts of mechanisms of ion movement across NF membrane [11], which brings about diffusion, electro-migration and convection [22]. Subject to the hypothesis of Donnan equilibrium, the interface of membrane-solution was utilized by a 1-D method and the mean of the impacts of radial were taken. The gradients of concentration across the membrane thickness were taken into account. Following the work of [27], the separation principle of ion linking membrane and solution at the circumferences of the membranes (feed part and infiltrate part) was described by the steric-Donnan equilibrium. The gradient of the concentrations was obtained through the synthesis of the mathematical statement of extended Nernst-Planck and the working principle of electro-neutrality. The influence of Donnan is due to the polarities of the charge linking the solute and the membrane. These factors governed how a membrane is selected based on the following four assumptions: (1) it was hypothesized that the solution is ideal. (2) It was hypothesized that the amplitude of the membrane charge is fixed and even. (3) It was hypothesized that the entire ions in the membrane have the capacity to move from one side of the membrane to the other. (4) It was hypothesized that Donnan equilibrium transpires at the membrane/feed border and the membrane/infiltrate border [11].

At this point, the presence of the membrane fixed charges have the capacity to govern the circulation of ions. Fig. 1 displays an outline of the concentration of solute in membrane and the feed circumference stratum. The circumference stratum is taken to be a concentrated solution where the solvent molecule infuses; the penetrability of static stratum is intensely governed by the concentration and the molecular weight of the solute [28]. The flow path of diffusion was created owing to the gradient of concentration in the circumference stratum. The coordinate distance x was the basis of the solute concentration in the circumference stratum. Hence, nanofiltration models are envisioned to achieve infiltrate composition on the basis of feed composition and the working conditions [27].

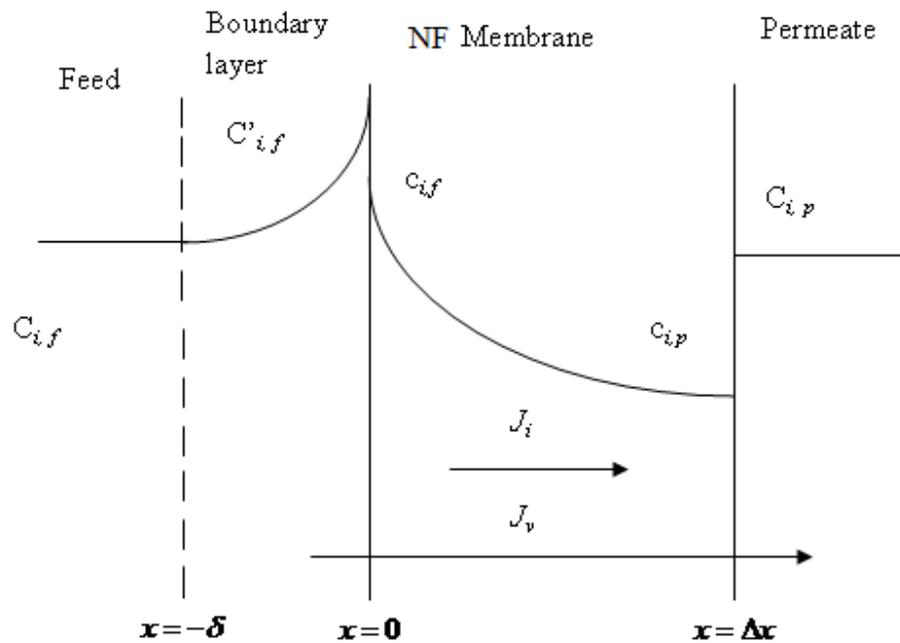


Fig. 1 The outline of the concentration of solute in the membrane/feed boundary stratum [27].

2. Theory and Experimental Method

2.1 The Model Equations

The purpose of modeling a membrane is to get solute concentrations from the infiltrate $C_{i,i}$, from identified concentrations of solute in the feed partition $C'_{i,f}$ [27]. Hence, these concentrations are connected via the concentrations of solute c_i in the NF membrane, and they are considered to represent the state variables of this work. Movement of the solvent and the solute that transpires in the pores with a active radius r_p and active length Δx together with membrane effective charge X_d were taken into account by Donnan-Steric Pore model. Darcy law states that in steady porous media flows, the macroscopic velocity is assessed by the gradient of pressure, the viscosity of fluid and the assembly of the permeable medium which is responsible for the motion [29]. The total flux through membrane surface is written in Eq. 1. Solute flux, J_i is obtained by sapping solutes via diffusion, convection and electrical forces from one side of the membrane to the other. The movement of solute across the membrane was described by Nernst Planck model written in Eq. 2 [27]. Arrays of constraints, states of the circumference and the electro-neutrality represented by Eqs. 4-6, governed the transport equation. Eqs. 4-6 serves as controls that are essential in the feed, membrane and infiltrate correspondingly.

$$u = -\frac{\kappa}{\mu} \nabla P \quad (1)$$

here, u stands for the Darcy velocity (m/s), κ denotes permeability (m^2), μ denotes liquid dynamic viscosity (Pa.s), ρ denotes density (kg/m^3), P denotes pressure of the fluid (Pa).

$$J_i = K_{i,c} c_i J_v - D_{i,p} \frac{dc_i}{dx} - \frac{z_i c_i D_{i,p}}{RT} F \frac{d\psi}{dx} + R_i \quad (2)$$

here R_i ($\text{mol}/(\text{m}^3 \cdot \text{s})$) represents the response term, J_i denotes flux of ion (i) centered on the area of Nano-Pro-3012 membrane ($\text{mol}/\text{m}^2 \cdot \text{s}$), $D_{i,p}$ signifies hindered diffusivity (m^2/s), c_i denotes concentration of ion in the membrane (mol/m^3), z_i signifies valence of ion (i), $K_{i,c}$ denotes hindrance factor for convection in the structure of Nano-Pro-3012 membrane, J_v signifies volume flux ($\text{m}^3/\text{m}^2/\text{s}$), R denotes universal gas constant ($\text{J}/\text{mol} \cdot \text{K}$), T stands for absolute temperature (K), F denotes Faraday constant (C/mol), and ψ stands for electrical potential (V) in the pores [30]. The velocity, u , is equivalent to that of the solvent [31]; hence, the input of solute to the velocity of solvent, via any kind of force, is insignificant when compared to the input of solvent to the solute. Eq. 2 presents one variable for the concentration of individual dissolved ions and the electric potential, ψ . In furtherance of attaining the gradient of concentration, taking cognizance that the ion flux is associated to its concentration is very important [11]; and the relationship is written as:

$$J_i = J_v C_{i,p} \quad (3)$$

Electro-neutrality in the bulk solution is represented by:

$$\sum_i z_i C_i' f = 0 \quad (4)$$

Electro-neutrality in the infiltrate solution is represented by:

$$\sum_i z_i C_{i,p} = 0 \quad (5)$$

$$\sum_i z_i c_i + X_d = 0 \quad (6)$$

here X_d stand for active membrane charge density (mol/m^3).

By utilizing the states given in Eqs. (4), (5) and (6) for Eq. (2) and repositioning it, the gradient of the electrical potential attained is given in Eq. 7.

$$\frac{d\psi}{dx} = \frac{\sum_{i=1}^n \frac{z_i J_v}{D_{i,p}} (K_{i,c} c_i - C_{i,p})}{\frac{F}{RT} \sum_{i=1}^n z_i^2 c_i} \quad (7)$$

It was hypothesized that the Donnan equilibrium was utilized at the feed/membrane border and at the membrane/infiltrate border. The Donnan equilibria are represented by:

$$\left(\frac{\gamma_{i,0} c_{i,0}}{\gamma_i C_{i,f}} \right) = \phi_i \exp\left(-\frac{z_i F}{RT} \Delta\psi_D \Big|_{x=0} \right) \quad (8)$$

$$\left(\frac{\gamma_{i,\Delta x} c_{i,\Delta x}}{\gamma_{i,p} C_{i,p}} \right) = \phi_i \exp\left(-\frac{z_i F}{RT} \Delta\psi_D \Big|_{x=\Delta x} \right) \quad (9)$$

here γ_i and $\gamma_{i,0}$ denote the activity coefficient of ion (i) in the membrane and the bulk solution, ϕ denotes the steric segregating term. Eqs. 8 and 9 described the settings of the circumference at the membrane sides. The gradient of concentration for individual component i may be represented in accordance with the state variables from Eq. 2.

$$\frac{dc_i}{dx} = J_v \left\{ \frac{K_{i,c}c_i - C_{i,p}}{K_{i,d}D_{i,\infty}} - z_i c_i \frac{\sum_{i=1}^n \frac{K_{i,c}c_i - C_{i,p}}{K_{i,d}D_{i,\infty}}}{\sum_{i=1}^n z_i^2 u_{m,i} c_i} \right\} \quad (10)$$

Eq. 10 illustrates the sub-domain of the membrane. Eqs. 8 and 9 denote to the states of the circumference at both sides of the membrane [27]. The hindered diffusivity ($D_{i,p}$) in Nernst-Planck is obtained from the following equation:

$$D_{i,p} = K_{i,d} * D_{i,\infty} \quad (11)$$

The migratory in electric field mobility is based on Nernst-Einstein relation, written as:

$$u_{m,i} = \frac{D_{i,p}}{RT} \quad (12)$$

here $D_{i,\infty}$ denotes the bulk diffusivity (m^2/s), $K_{i,d}$ represents the hindrance factor for diffusion and $u_{m,i}$ represents the mobility ($s*mol/kg$).

2.2 Comsol multi-physic and definition of constant

Extended Nernst-Planck equation was solved using Comsol multi-physic. The sub-scope of the study was identified for every state variable based on their modes [27]. The problem identification is shown in Table 1. The identified problem consists of the following factors: the concentrations of ion in the feed, feed temperature, Darcy velocity, fluid dynamic viscosity and the permeability. These factors are relevant in applying Comsol multi-physic with regard to a certain pressure written in Eq. 1. The Nano-Pro-3012 parameters for the Donnan-Steric Pore equation applied in Comsol multi-physic simulation are given in Table 2. Scanning electron microscopy was used in obtaining the active pore radius. A micro gauge thickness tester was used in obtaining the membrane thicknesses (Δx). A minimized cost function founded on the model solution by employing information obtained from experiments was applied to fit the active membrane charge X_d into Comsol multi-physic. Table 3 displays other working variables of the model.

Table 1 The description of problem

Parameters	Values	Description
$C'_{1,f}$	11.1	Iron concentration (mol/m^3)
$C'_{2,f}$	0.18	Nickel concentration (mol/m^3)
$C'_{3,f}$	0.12	Cobalt concentration (mol/m^3)
$C'_{4,f}$	2.81	Manganese concentration (mol/m^3)
$C'_{5,f}$	4.114	Magnesium concentration (mol/m^3)
T	298.15	Working temperature (K)
u	0.00478	Darcy velocity (m/s)
μ	0.00089	Fluid dynamic viscosity (Pa.s)
k	$3.56e^{-15}$	permeability (m^2)

Table 2 DSPM membrane parameters

Parameters	Values	Description
r_p	28.7	Membrane pore radius (nm)
A	0.01076	Membrane area (m ²)
Delta	0.01161	Membrane thickness (m)

Table 3 DSPM working variables

Parameters	Descriptions
ΔP	Pressure difference (Pascal)
ψ_m	Electrical potential (V)
μ	Dynamic viscosity of the solution (kg.m.s ⁻¹)

2.3 The definition of the sub-scope for the Nernst Planck model without electroneutrality mode

The ion concentrations in the feed and infiltrate do not independently satisfy the condition of electro-neutrality from the membrane charge; hence, Nernst Planck model in the absence of electro-neutrality must be applied [27]. The Nernst Planck model was utilized for each ion i , it is given in Eq. 13.

$$\nabla \cdot (-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V) = R_i - u \nabla c_i \quad (13)$$

Eq. 13 can be compared with Eq. 2; however, D was used as a modified diffusivity in Eq. 11 and the mobility of ion was computed with Eq. 12. The remaining data needed for the simulation are the ions charge numbers and x-Velocity (V). However, Nernst Planck model will not precisely equate the extended Nernst Planck model owing to the fact that the extended Nernst Planck model put into consideration the corrected convective term. Hence, R_i was responsible for the addition of the correction for the convective term [27].

2.4 Experiment using simulated wastewater

A mixture with common divalent ions (FeSO₄, NiSO₄, CoSO₄, MgSO₄, and MnSO₄) similar to the water sample obtained from Rand Uranium water treatment plant, South Africa [32], was simulated using the concentration of divalent ions in the Rand Uranium wastewater treatment plant. The salt mixture experiment was carried out at 30 bar at pH value of 2.2 and the temperature was retained to 25°C.

2.5 Filtration experiment

1 L stirring cell membrane filtration device was used for the study. Nano-Pro-3012 was positioned in the stirring cell. The experiment was done with 1 L of solution of different concentrations of metal ions. The membrane area was around 0.01075 m². A Nano-pro-3012 was cut and fixed into the stirring apparatus. The salts solution was positioned in the stirring apparatus at the feed inlet. A working pressure of 30 bar was used by means of a nitrogen gas cylinder. The pure water permeate was obtained by taking the mass of the obtained infiltrate in the course of a preset time. The infiltrate permeate and retention were examined as a function of operating time as a working parameter. The infiltrate flux J_v (L/m²/h) was obtained using Eq. (14) [33].

$$J_v = \frac{FR_i}{SA} \quad (14)$$

where, FR_i and SA denote the flow rate of infiltrate and the membrane surface area, correspondingly. The retention detected was computed by Eq. 15 [33].

$$\%R = \left(1 - \frac{C_i}{C_{if}}\right) \times 100 \quad (15)$$

2.6 Inductively Coupled Plasma/Optical Emission Spectrometry (ICP-OES) Arcos

The application of ICP for analyzing the concentration of ions depended on the unconstrained photons emission from atoms and ions that have been triggered in a radio frequency discharge. The samples were directly injected into the instrument, while solid samples were extracted in order for the analytes to be present in a solution. The sample solutions were changed to an aerosol and routed into the central channel of the plasma. The cation concentration in the feed and infiltrate were evaluated by utilizing ICP-OES. The instrument was equipped with a water crossflow nebuliser and a Scott double-pass spray chamber.

3. Discussion of Results

3.1 The motion of ion through the membrane

For the purpose of having an acumen in the characteristics of ion-transport via the membrane, influence of membrane electrical potentials on fluxes were studied and displayed Fig 2. Concentration gradient through the membrane result in diffusion transport. This upsurges the entire flux in solution and decreases the electrical potential; in so doing reduces the flux in the membrane. Hence, it could be concluded that the flux is dependent on its internal and its external concentrations together with the electrical potential difference through the membrane [34]. It should be pointed out that membrane potentials hinge on the diverse mobilities of the different ions and their concentration gradients. The cations were noted to be initially positioned at one side of the solution and diffused through the solution heading to the areas of lower concentration as time increases.

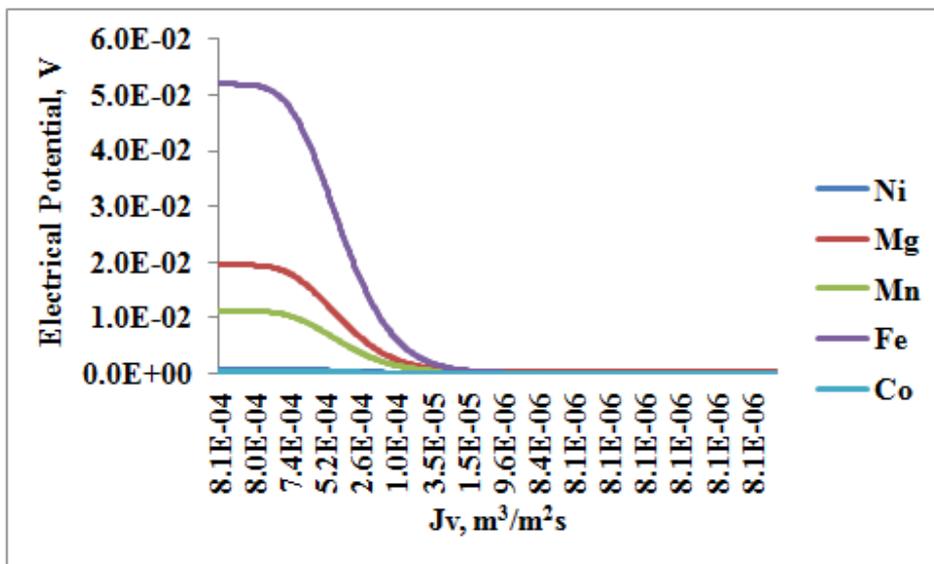


Fig. 2 Membrane potential as a function of flux of various cation solutions [34].

3.2 The outline of concentration along the membrane thickness

In order to envision the outline of cations decontamination, the distribution outline of the cation concentrations was displayed in Fig. 3 for 1-D configuration channel through the membrane thickness. Cation concentrations were graphically assessed by displaying the concentration distribution through the membranes. The feed bulk side solution configuration has a circumference layer with interval of 0, 0.01. The concentration outline was formed with the dereliction of the suspended species. The effective membrane thickness (Δx) comprises of different level of porosity. This influenced the selection of pore radius; hence, the separation of ions takes place here [34]. Fig. 3 displays the positive charges of Nano-Pro-3012, which instigated a severe reduction of cations concentration in the membrane. The influence possess some critical impacts on the movement of ions across the membrane. It could be envisaged that Nano-Pro-3012 will be effective in removing metal ions from wastewater.

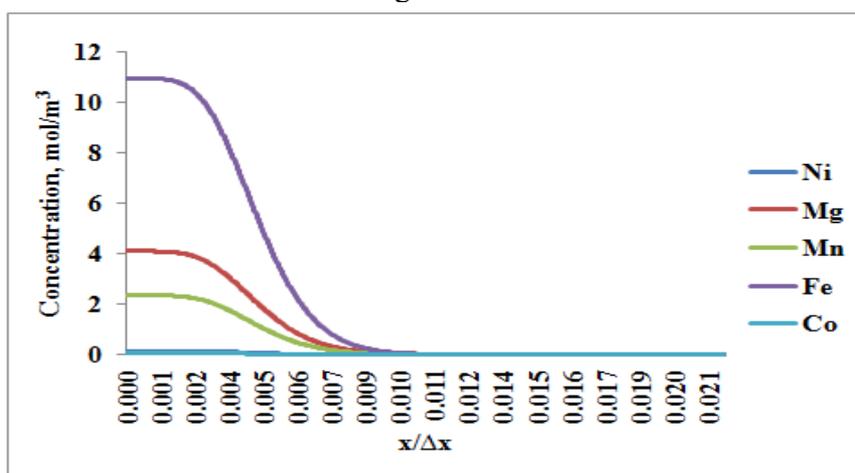


Fig.3. Concentrations of ions through the membrane thickness in the course of filtration [34]

3.3 Conformity of experimental data with theoretical data

The theory and simulation of a well effectuate NF membrane for the separation of electrolyte mixtures needs a pure understanding of motion of ion characteristics in the membrane with reverence to the removal of single ions. The variance linking the membrane pore the solute ion radii resulted to the steric impact and charge polarities in the membrane; and the solute resulted to Donnan effect. The combination of these impact have a powerful effect on the rejection of ions. The characteristics of membrane transport with reverence to ions are entwined as a result of the impulsive rising of electric fields, at the time that the features of NF membrane are gotten from the estimations of retention of salts [35]. The effects of charge relatively led to the rejection of ions as a result of the correlation amid charged particles and charged membrane [36]. The reliance of the retention of ion on the membrane flux is well clarified based on Extended Nernst Planck model which establishes the foundation of illustrating the motion of solute ions across the membrane. The model hypothesizes that the movement of solute takes place through convection, diffusion and electric passage across the double stratum of the membrane surface. The experimental data were conformed to the theoretical data of single ions, as shown in Fig. 4. The figure makes known the inclination of the retention of five mixture of salts on the membrane flux. The retention of ions increases as the infiltrate flux increases; this reflection embraces the support of the transmembrane pressure with a founded theory that the retention of ions would increase as transmembrane pressure increase [37-40]. The study has shown that Donnan exclusion mechanism had solid influence with the cations when operated at low flux. Nonetheless, the overall ions retentions were high as a result of the influence of dielectric exclusion. The mixed ions were rejected and solution was analyzed for each ion. A very good conformity was observed between the predicted and the laboratory data (see Fig. 4).

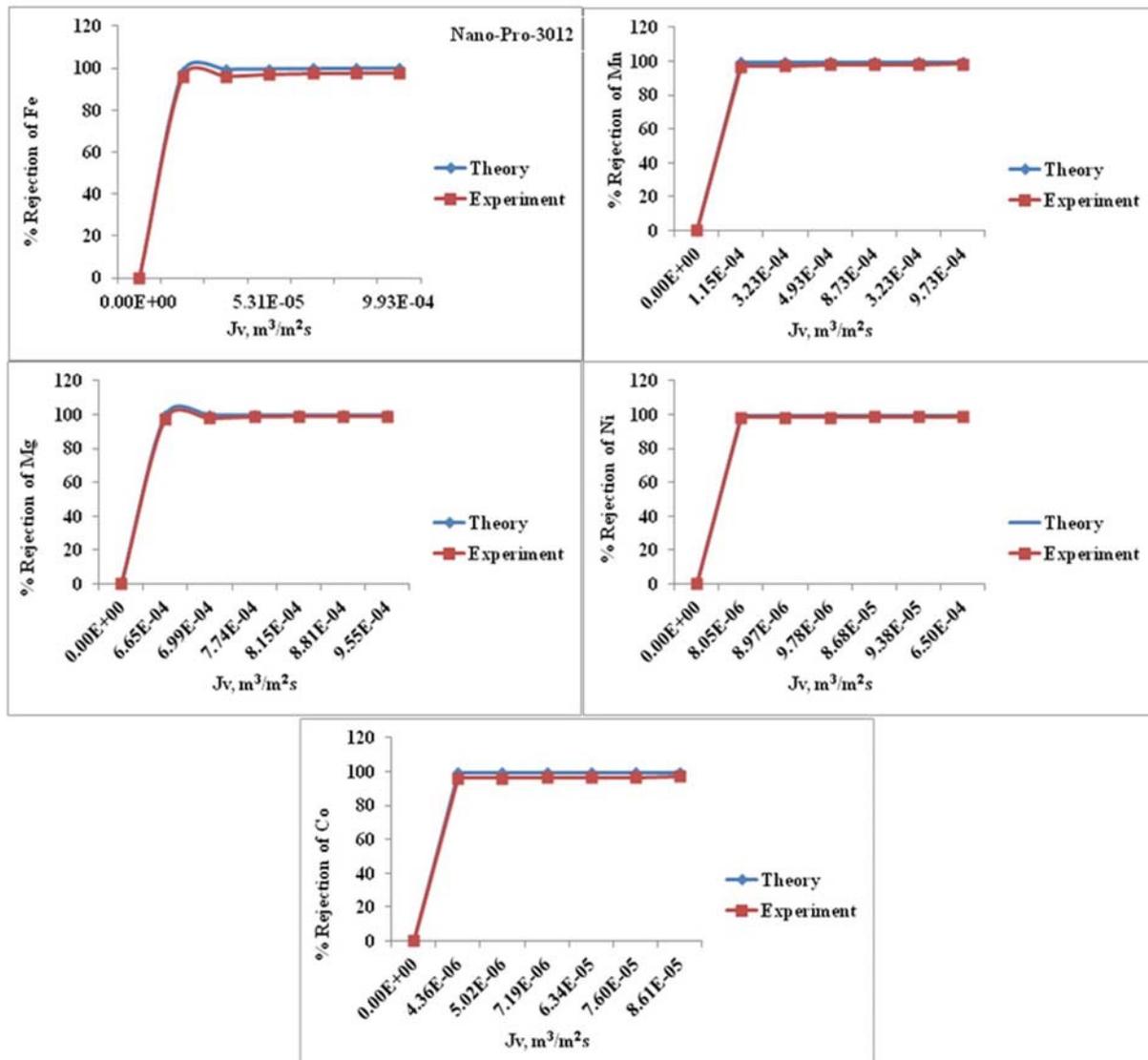


Fig. 4 The anticipated and laboratory retention of single salts vs permeate flux for Nano-Pro-3012. [34].

4. Conclusion

Nano-Pro-3012 membrane was theoretically evaluated with the utilization of extended Nernst Planck model as a result of its illustration with ionic motion mechanisms through the membrane. Donnan steric pore model uses the extended Nernst-Planck model in combination with Darcy law model to illustrate the ion transport inside the pores. The study gave the capability to accurately envisage the occurrence that takes place close to the surface of the membrane in an effort to deduce the capacity and role of charge and Donnan exclusion mechanism during Nano-Pro-3012 filtration process. The model equations were solved with the utilization of Comsol multi-physics software. The model was solved for five different cations at different concentrations (similar to the concentrations of ions in acid mine water). Conclusion made from

the model was that flux is governed by internal and external concentrations and on the electrical potential difference through the membrane. Result shows that the potential of Nano-Pro-3012 is subjected to the diverse mobilities of ions and on their gradients of concentration. A very good conformity was observed between the predicted and the laboratory data.

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