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SENSITIVITY ANALYSIS OF A MATHEMATICAL MODEL FOR MICROBIAL DESALINATION CELLS

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ABSTRACT

Microbial Desalination Cell (MDC) is new developed technology that treats wastewater, generate electrical energy from it and desalinate saline water. However, this complicated technology faces many challenges to be implemented on a large scale that's why mathematical modelling for MDC is very essential. In this paper, A previous complex mathematical model was studied. Sensitivity analysis was conducted for model parameters to evaluate the influence of each parameter on the dynamics of MDC including electric current, desalination and COD removal to increase understanding of the relationships between input and output parameters in the model. Based on sensitivity results, the top effective parameters controlling the performance of MDC are maximum anodophilic microorganisms growth rate, maximum substrate consumption rate by anodophilic microorganisms and mediator yield.

INTRODUCTION

Bioelectrochemical systems (BES) are systems that their function is wastewater treatment and energy recovery through converting chemical energy embedded in wastewater to electrical energy through microbial-electrochemical reactions [1]. Microbial desalination cell (MDC) is one of bio electrochemical system types that desalinate salty water using current generated from oxidation of organic matter so it achieves three main goals: energy production, wastewater treatment and desalination [2].MDCs concept of operation is similar to electrodialysis desalination technology , however it uses electrical energy converted from chemical energy in wastewater [3]. Since BES are complicated systems , comprehensive mathematical models is important to understand the dynamic relation between physical , chemical , biological and electrochemical processes , so BES modelling is essential step towards optimization and scaling up [4] . However , Few MDC models are reported in the literature [5]. Ping Model is a MDC model with many parameters that increases the complexity of the model. In this paper, A sensitivity analysis was conducted for the parameters of Ping Model to determine the effect of each parameters on the MDC performance. The analysis was conducted using MATLAB and results of the most important parameters are presented.

Materials and Methods (MDC Model[6])

1. Mass Balances for Substrate

The following equations shows the mass balance for the substrate concentration in anode chamber

$$\frac{dS}{dt} = -\mu_{s,a}\, C_a - \mu_{s,m}\, C_m + \text{Danode (Sin-S)}$$

$$\mu_{s,a} = \mu_{s,a,max} \frac{S}{Ka + S} \frac{M_{OX}}{K_M + M_{OX}}$$

$$\mu_{s,m} = \mu_{s,m,max} \frac{S}{Km + S}$$

$$\text{Danode} = \frac{Qin}{Vanode}$$

Where t is time (d) ;S is substrate concentration (mg-S.L-1) ; Sin is influent substrate concentration (mg-S.L-1); Ca and Cm are concentrations for anodophilic and methanogenic microorganisms (mg-x.L-1); $\mu_{s,a}$ and $\mu_{s,m}$ are substrate consumption rate by anodophilic and methanogenic microorganisms (mg-S .mg-x-1 .d-1); Danode is dilution rate in anode chamber (day -1); Qin is the influent flow rate of substrate (L.day-1); Vanode is the volume of anode chamber (L); $\mu_{s,a,max}$ and $\mu_{s,m,max}$ are maximum substrate consumption rate by anodophilic and methanogenic microorganisms (mg-S .mg-x-1 .d-1) ;K,a and K,m are the half saturation constants for anodophilic and methanogenic microorganisms (mg-S.L-1); Mox is oxidized mediator fraction per anodophilic microorganisms (mg-M·mg-a−1); KM is half saturation constant for mediators (mg-M.L-1).

Mass Balances for Microorganisms

The following equations shows the mass balance for microbial population in anode chamber. The microbial population include anodophilic microorganisms that release electrons from consumption of organic matter and methanogenic microorganisms that convert substrate into methane:

$$\frac{dC_a}{dt} = \mu_a C_a - k_{d,a} C_a \text{-} \alpha_a D_{anode} C_a$$

$$\frac{dC_m}{dt} = \mu_m C_m - k_{d,m} C_m \text{-} \alpha_m D_{anode} C_m$$

$$\mu_a = \mu_{a,max} \frac{S}{Ka+S} \frac{M_{OX}}{K_M+M_{OX}}$$

$$\mu_m = \mu_{m,max} \frac{S}{Km + S}$$

$$\alpha_a = (\frac{1 + \tanh(K_{a,x} \left(C_a + C_m - C_{a,max}\right)\big)}{2}$$

$$\alpha_m = (\frac{1 + \tanh(K_{m,x} \left(C_a + C_m - C_{m,max}\right)\big)}{2}$$

Where µa and µm are growth rate of anodophilic and methanogenic microorganisms (d-1); Kd,a and Kd,m are decay rates of anodophilic and methanogenic microorganisms; $\mu_{a,max}$ and $\mu_{m,max}$ are maximum growth rate of anodophilic and methanogenic microorganisms (d-1) ; αa and αm are the dimensionless biofilm retention constants ; Ka,x and Km,x are steepness factors of anodophilic and methanogenic microorganism (L.mg-x-1); C a,max and C m,max are maximum attainable concentration for anodophilic and methanogenic microorganisms (mg-x.L-1)

2. Mass balance for Mediators

The intracellular mediator exists either in its oxidized and reduced form. The following equation shows the mass balance for oxidized mediators

M total=M red+Mox

$$\frac{dMox}{dt} = -Y\mu_{s,a} + \gamma \frac{I_{MDC}}{ne\ F} \frac{1}{VCa}$$

Where Mred and Mtotal are reduced and total mediator fraction per anodophilic microorganisms (mg-M·mg-a−1); Y is the mediator yield (mg-M .mg-S-1); IMDC is the MDC current (A) ; F is faraday constant (A. d. mole-1); γ is mediator molar mass (mg-M molmed -1); ne is the number of electrons transferred per mole of mediator (mole–e- .mole med -1)

3. Mass Balance for Salt concentrations

The following equations shows the mass balance for the salt concentration in the three chambers

$$\frac{dCsalt,m}{dt} = Dsalt(Csalt,in - Csalt,m) - d\left(C_{salt,m} - C_{salt,a}\right) - d\left(C_{salt,m} - C_{salt,c}\right) - \frac{I}{F\,Vsalt}$$

$$\frac{dCsalt,a}{dt} = d\left(C_{salt,m} - C_{salt,a}\right) \text{-Danode (Csalt,a)}$$

$$\frac{dCsalt,c}{dt} = d\left(C_{salt,m} - C_{salt,c}\right)$$

$$Dsalt = \frac{Qsalt}{Vsalt}$$

Csalt,a , Csalt,m, and Csalt,c are salt concentrations in anode , salt and cathode chambers (mol-salt.L-1) ; C salt, in is influent salt concentration (mol-salt.L-1) ;d is a membrane salt transfer coefficient (day−1); Dsalt is dilution rate in middle chamber (day -1) ; Q salt is salt flow rate (L.day−1); Vsalt is volume of salt chamber (L

4. Electrochemical equations

MDC current was determined by Ohm's law:

$$I_{\text{MDC}} = \frac{V_{OC} - \frac{RT}{F}\ln\left(\frac{M_{Total}}{M_{red}}\right)}{R_{int} + R_{ext} + Rsalt + Ranolyte + Rmembrane}$$

$$\text{Voc=Emin+ (Emax- Emin)}e^{-1/k_{\text{r}}\,C_a}$$

$$\text{Rint=Rmin+ (Rmax- Rmin)}e^{-k_{\text{r}}\,C_a}$$

Where Voc is open circuit voltage (V); Emin and Emax are minimum and maximum observed open circuit voltage (V); Rmin and Rmax are minimum and maximum observed internal resistances (Ω); kr is the constant that determines how fast the internal resistance respond to the change in anodophilic microorganisms' concentration (L·mg-a−1). R is ideal gas constant (J.K-1.mole -1); R salt is resistance of salt solution (Ω) ; R membrane is mass transfer resistance through an exchange membrane; Ranolyte is resistance of anolyte solution; Rext is the external resistance

RESULTS AND DISCUSSION

1. Base case results

The model differential-algebraic equations were solved using

MATLAB and parameters values were determined from previous studies [6], [7]. Substrate consumption increases by anodophilic and methanogenic microorganisms with decreasing rate until it reaches steady state after 8th day. Also, Current increases until it reaches the steady state after 8th day so consequently salt removal from middle chamber increases also with decreasing rate until it becomes constant starting from 8th day.

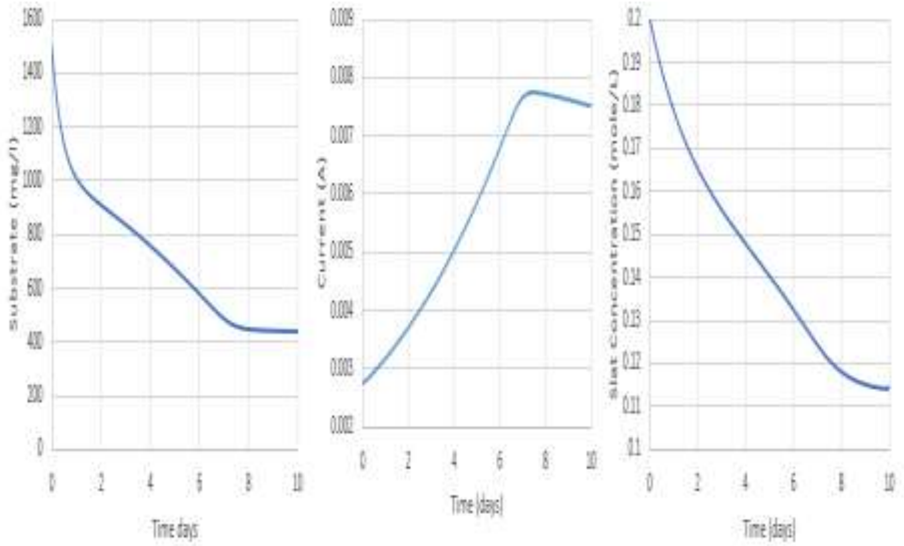

Figure 1 Change of substrate concentration, current produced and salt concentration in desalination chamber with time

2. Sensitivity analysis

The sensitivity analysis is conducted for MDC biological, operating and design parameters to determine the effect of parameters on the performance of MDC model. This analysis will use the local relative sensitivity analysis method in which it will be carried out on all parameters one by one by changing one of the parameters, while the other parameters were fixed without any change. Local relative sensitivity analysis [8] was used to determine the effect of changing the parameter value as ratio between change in output value to change in parameters value.

The following equation was used for each parameter:

$$T_j = \frac{P(t,x_j+\delta x_j)-P(t,x_j)}{\delta x_j} * \frac{x_j}{P(t,x_j)}, j = 1,2, \ldots$$

Where the dependent time sensitivity for any parameter 'j' is Tj ; the output value is P; the value of parameter j is xj ; the change in xj is δ xj;

the step of the change in this study is δ xj = 0.01xj.

3. Sensitivity analysis results

a) Maximum growth rate of microorganisms

The results of sensitivity analysis for the maximum growth rates effect on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 2 . It is clear that anodophilic and methanogenic microorganisms maximum growth rates (µa,max and µm,max) are effectual parameters but methanogenic microorganisms maximum growth rate is less effectual .The increase of anodophilic microorganisms maximum growth rate cause higher rate of substrate consumption so more decrease in substrate concentration until 7th day then substrate concentration increases due biofilm space limitation .Also, It cause increase in current produced and consequently the salt concentration decreases until 7th day since anodophilic microorganisms produce electrons from consumption of organic matter then after 7th day current produced decreases and salt concentration increases. On the other hand, the increase of methanogenic microorganisms' maximum growth rate cause decrease in substrate concentration and decrease in the current produced as the methanogenic organisms don't produce electrons from substrate oxidation and consequently, salt concentration increases.

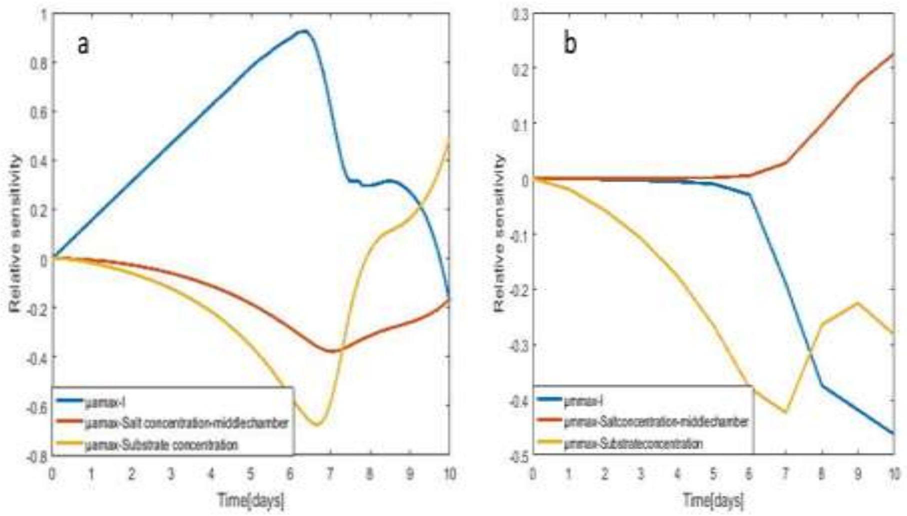

Figure 2 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to a) anodophilic maximum growth rates b) methanogenic maximum growth rates

4. Half rate constant

The results of sensitivity analysis for the half rates constant effect on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 3. It is clear that anodophilic microorganisms, methanogenic microorganisms and mediators half rate constant (Ka, Km and KM) are effectual parameters but mediators half rate constant is the most effectual. As Ka increases, anodophilic microorganisms growth rate and substrate consumption rate decrease until 9th day. Due to decrease of anodophilic growth rate, the biofilm space limitation effect is delayed so substrate concentration decrease and current increases from 9th to 10th day. As Km increase, methanogenic microorganisms' growth rate decrease, so substrate concentration increases, current decreases and salt concentration increases. As KM increases, anodophilic microorganisms growth rate and substrate consumption rate decrease, so substrate concentration increase and current decrease that cause increase in salt concentration.

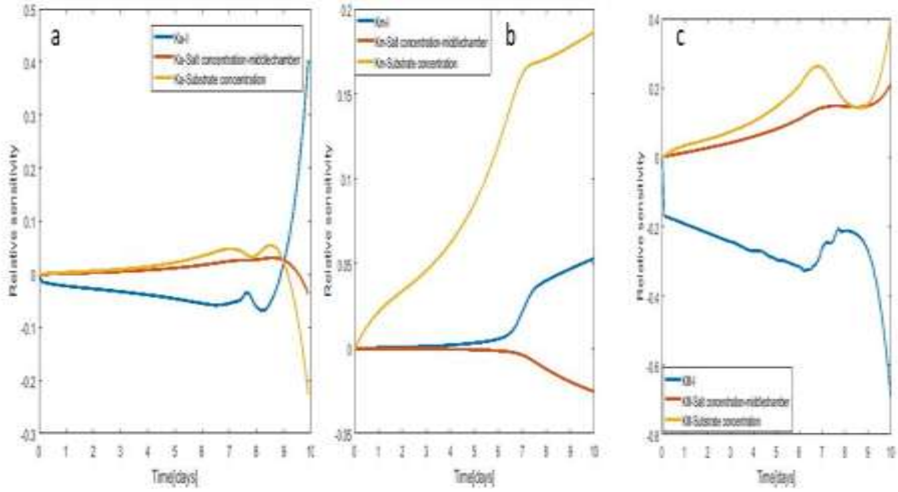

Figure 3 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to half rate constant of a) anodophilic microorganisms b) methanogenic microorganisms and c) mediators

5. Decay rates

The results of sensitivity analysis for the decay rate effect on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 4 . It is clear that the increase of anodophilic and methanogenic microorganisms decay rate are ineffectual parameters.

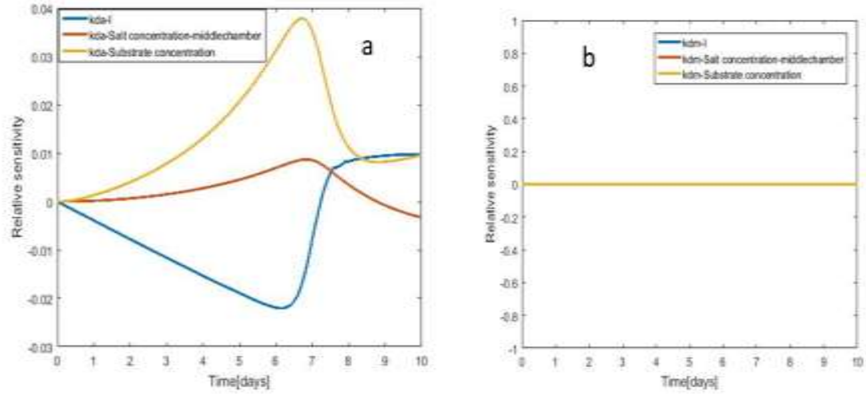

Figure 4 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to decay rate of a) anodophilic microorganisms and b) methanogenic microorganisms

6. Biofilm space limitation

The results of sensitivity analysis for the biofilm space limitation effect on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 5.It is clear that the anodophilic and methanogenic biofilm space limitation become more effectual from 7th to 10th day because when space limitation value increases, it allows more increase of anodophilic and methanogenic microorganisms concentration.

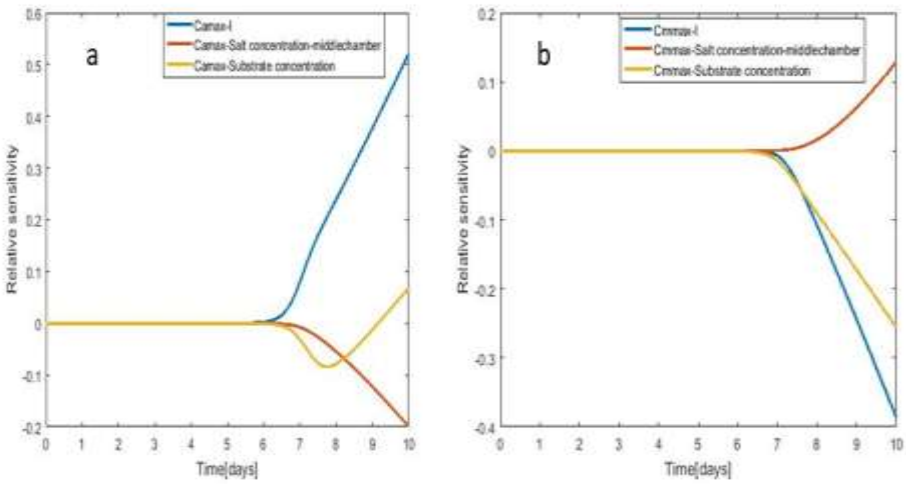

Figure 5 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to a) anodophilic biofilm space limitation and b) methanogenic biofilm space limitation

7.Maximum substrate consumption rate

The results of sensitivity analysis for the effect of maximum substrate consumption rate on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 6. The increase of methanogenic maximum substrate consumption rate has no effect on current production or desalination but it increases the rate of substrate oxidation by methanogenic organisms. However, the increase of maximum substrate consumption rate by anodophilic microorganisms cause sharp decrease in substrate concentration. Also, It cause increase in current and consequently decrease in salt concentration as increase of maximum substrate consumption rate reduce oxidized mediators concentration so it cause a decrease in concentration losses that leads to increase in current produced.

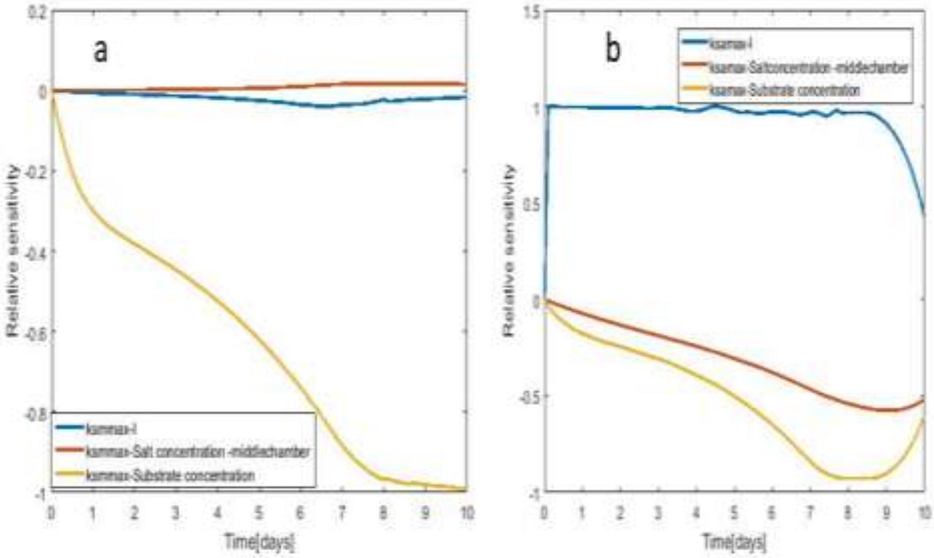

Figure 6 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to maximum substrate consumption rate by a) methanogenic microorganisms and b) anodophilic microorganisms

8.Mediator yield

The results of sensitivity analysis for the effect of mediator yield on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 7. Concerning the current and salt concentration in middle chamber, it is clear that mediator yield is very effectual parameter as it causes more current production and salt removal but it has minor effect on substrate concentration.

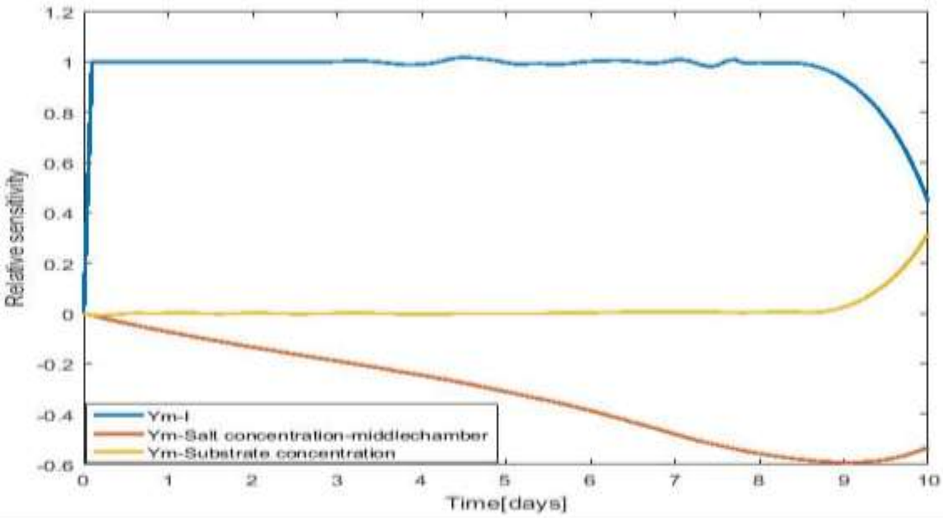

Figure 7 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to mediator yield

9.Diffusion coefficient

The results of sensitivity analysis for the effect of diffusion coefficient on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 8. It is clear that increase of diffusion coefficient is very effectual only in increasing salt removal in the middle chamber, however it has negligible effect on current.

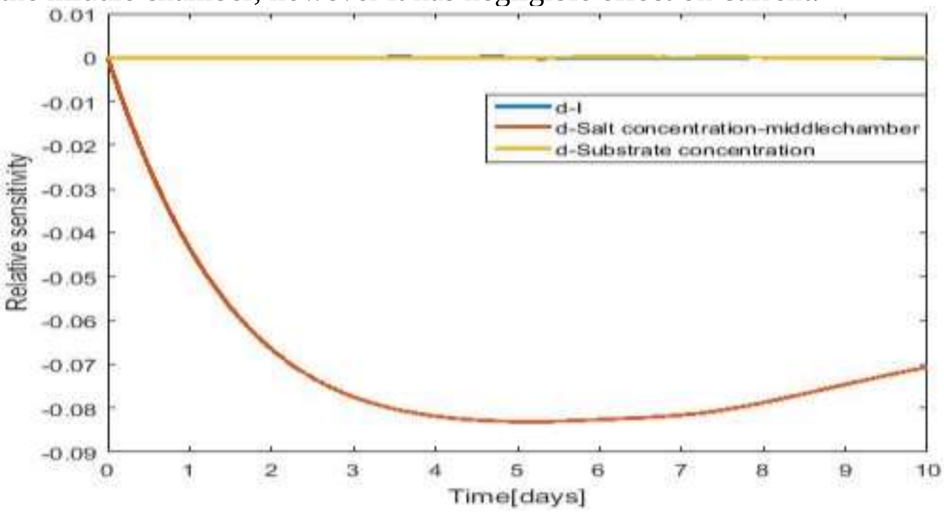

Figure 8 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to diffusion coefficient

10.Number of electrons transferred per mole of mediator

The results of sensitivity analysis for the effect of diffusion coefficient on current, substrate concentration and salt concentration in the middle chamber are shown in Figure 8 . It is very clear that number of electrons transferred per mediator is a very effectual parameter.

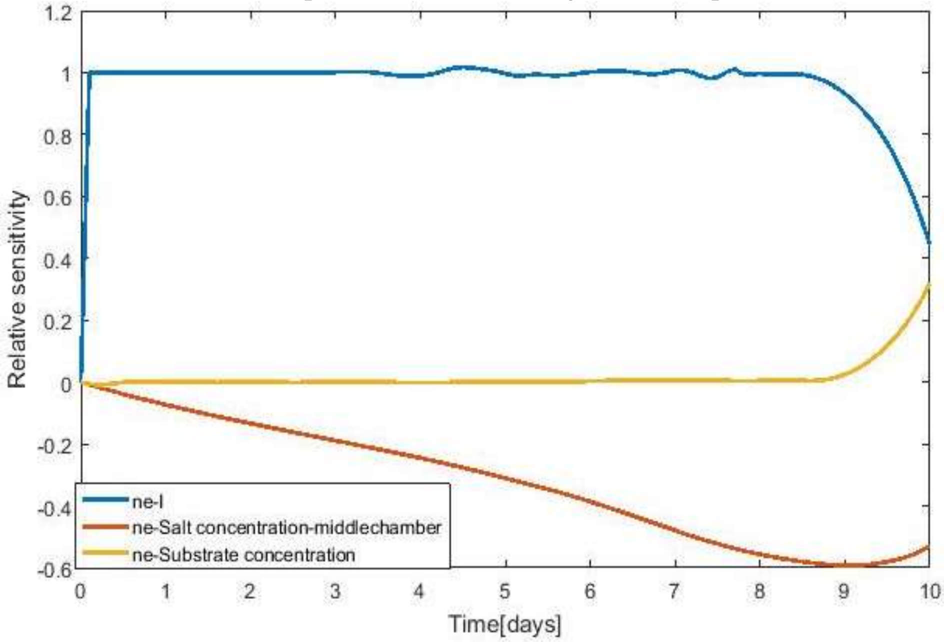

Figure 9 Relative sensitivity of current, substrate concentration and salt concentration in the middle chamber with respect to number of electrons transferred per mole of mediator

CONCLUSION

In this study, it is very clear that MDC model is very complicated and multivariable system that requires more analysis to be easily understood and used. Sensitivity analysis is one of the important tools that help to understand this system . Sensitivity analysis that was conducted for the MDC model shows the effect of each parameter on the performance of MDC inculding COD removal , desalination and electrical current produced . Top parameters that affect MDC performance are maximum substrate consumption rate by anodophilic microorganis, the maximum growth rate of these microorganisms and mediator yield so model users have to focus on reestimation of these parameters' values for better prediction of results.

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تحليل الحساسية لنموذج رياضي لخلايا تحلية المياه الميكروبية

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نبذة مختصرة

من تقنيات المعالجة الجديدة هي خلايا الوقود الميكروبية (**MFCs**)التي تحول المركبات العضوية في مياه الصرف الصحي إلى طاقة كهربائية من خلال سلسلة من العمليات الفيزيائية والكيميائية والبيولوجية والكهروكيميائية. خلية التحلية الميكروبية (**MDC**) تعد من التقنية الجديدة والمطورة لمعالجة مياه الصرف الصحي ، وتوليد الطاقة الكهربائية منها وتحلية المياه المالحة. تواجه هذه التكنولوجيا الجديدة العديد من التحديات لامكانية تنفيذها على نطاق واسع

ولهذا السبب في أن معرفة كاملة للنمذجة الرياضية لهذه التقنية **MDC** تعتبر ضرورية للغاية. في هذا البحث تم دراسة نموذج **MDC** باستخدام **Matlab** و تم دراسة تأثير كل متغير على أداء **MDC** ثم تم استخدام نتائج التحليل لتبسيط المعادلات من خلال استبعاد المتغيرات غير الفعالة. كما تم التحقق من صحة النموذج المخفض لتدفق الدفعات الدورية باستخدام نتائج اختبارات معملية تم الحصول عليها من المراجع المنشورة ثم تم مقارنته مع نموذج اخر باستخدام نفس النتائج المعملية. تمت دراسة تأثير متغيرات التشغيل المختلفة على أداء نظام **MDC** ثم تم إضافة بعض التعديلات على معادلات النموذج لتتوافق مع الاتجاهات الملاحظة في الدراسات التجريبية. يتم تقديم النموذج النهائي و الذي يمكن استخدامه في تصميم هذه **MDCs** لأهداف معالجة مختلفة

الكلمات الدالة: معالجة مياه الصرف الصحي – تحلية المياه،الطاقة – خلايا الوقود الميكروبية – خلايا التحلية الميكروبية