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تصدر في جامعة مؤتة

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مؤتة للبحوث والدراسات

"سلسلة العلوم الطبيعية والتطبيقية"

مجلة علمية محكّمة مفهرسة

تصدر عن جامعة مؤتة

تصدر المجلة مجلداً سنوياً يضم أعدادا

شروط النشر:

1- تنشر المجلة البحوث العلمية الأصيلة التي تتوافر فيها شروط البحث في التحديد والإحاطة والاستقصاء والتوثيق في العلوم الطبيعية والتطبيقية للباحثين من داخل جامعة مؤتة وخارجها، مكتوبة باللغة العربية أو الإنجليزية، ويشترط في البحث ألا يكون قد نُشِرَ أو قدِم للنشر في أيّ مكانٍ آخر، وأن يوقع الباحث الرئيسي خطياً أنموذج (إقرار وتعهد النشر) المدرج ضمن موقع المجلة الإلكتروني na_darmutah@mutah.edu.jo

2- تخضع البحوث المقدمة للتحكيم المكتوم من أساتذة مختصين حسب الأصول العلميّة المتبعة في المجلة.

تعليمات النّشر:

1- يُطبع البحث باستخدام البرنامج الحاسوبي (MS Word) بمسافات مزدوجة بين الأسطر وهوامش 2,5 سم، وعلى وجه واحد من الورقة (A4)، بحيث لا تزيد عدد صفحاته عن (20) صفحة وفي حدود (6000) كلمة، ونوع الخط وحجمه (Traditional Arabic 14) للبحوث المطبوعة باللغة العربية، و (Times New Roman 14) للبحوث المطبوعة باللغة الإنجليزية، بما في ذلك الأشكال والرسومات والجداول والهوامش والملاحق، وترسل منه أربع نسخ ورقية ونسخة إلكترونية على (CD).

2- أن يستخدم الباحث الأرقام العربية ونظام الوحدات الدولي ومختصرات المصطلحات العلمية المعروفة، شريطة أن تُكتب كاملة أوّل مرة تردُ في النصّ.

3- أن يكتب ملخص للبحث باللغة العربية وآخر بالإنجليزية بما لا يزيد عن (150) كلمة لكل منهما، وعلى ورقتين منفصلتين بحيث يكتب في أعلى الصفحة عنوان البحث واسم الباحث (الباحثين) من ثلاثة مقاطع مع العنوان (البريد والإلكتروني) والرتبة العلمية، وتكتب الكلمات الدالة (Keywords) في أسفل صفحة الملخص بما لا يزيد على خمس كلمات بحيث تعبر عن المحتوى الدقيق للمخطوط.

4- أن تُرقم الأشكال والجداول والرسومات والخرائط على التوالي حسب ورودها في البحث، وتُزود بعناوين، ويُشار إلى كل منها بالتسلسل نفسه في متن البحث، وتقدم بأوراق منفصلة.

5- أن يعتمد الباحث في التوثيق أسلوب هارفارد وذلك على النحو الآتي:

أ. يشار إلى المراجع في متن البحث باسم العائلة للمؤلف الواحد/ الاثنين وسنة النشر. مثال: (هولمز، 1991). (سميث وهوتون، 1997). وإذا زاد عدد المؤلفين عن اثنين فيكتب الاسم الأخير للمؤلف الأول وآخرون، ثم سنة النشر. مثال: (مور وآخرون، 1990). وتكتب الأسماء الكاملة للمؤلفين في قائمة المراجع بغض النظر عن عددهم. وفي حال الإشارة إلى المؤلف في بداية الفقرة فيكتب اسم المؤلف ثم تليه سنة النشر بين قوسين. مثال: هالام (1990)

ب. إذا وردت عدة مراجع للمؤلف نفسه وأنجزت في السنة نفسها فتميز بإضافة حروف هجائية بعد السنة مباشرة (ويلسون، 1994أ. ويلسون، 994 ب).

ج. يمكن استخدام الحواشي من أجل توضيح أي غموض أو شرح مبهم كما في حالة المصطلح الذي يتطلب التوضيح، في هذه الحالة تدرج الحواشي بقائمة بعد انتهاء البحث مباشرة بأرقام متسلسلة حسب ورودها في متن البحث.

د. تدرج المراجع والمصادر المستخدمة في البحث في قائمة واحدة في نهاية البحث (بعد قائمتي الحواشي والملاحق) وترتب هجائياً وفق اسم العائلة للمؤلف وعلى النحو التالي:

الكتب:

هانت، ج. 1996. البترول الجيوكيمياء والجيولوجيا، الطبعة الثانية. جورج فريمان وشركاه، نيويورك.

فصل في كتاب:

شين، أ. ي. 1983. بيئة المد والجزر المستوية، المنشور في: بيئات ترسيب الكربونات، الذي حرره بيبوت، د. ق. ومور، سي. هـ، الجمعية الأمريكية لعلماء جيولوجيا البترول، تولسا، أوكلاهوما، الولايات المتحدة الأمريكية، ص 171-210.

الدوريات:

قندلفت، ف. ب.، ويلسون، أ. ب.، وبيرسون، ب. ن. 2006. البيئة القديمة لعوالق المنخربات من الإيوسين الأوسط المتأخر وتطورها. المستحاثات المجهرية البحرية. 60 (1): 1-16.

المؤتمرات والندوات:

هوبر، ب. ت. 1991. دراسة الطبقات الحيوية للعوالق من مواقع 738 و744، كيرغولن هضبة (جنوب المحيط الهندي). من العصر باليوجين والنيوجين المبكر. والمنشور في: بارون، ج.، لارسن، ب.، وآخرون. (تحرير): وقائع برنامج حفر المحيطات، النتائج العلمية، المجلد، 119. محطة الكلية، ص: 427-449.

الأطروحات:

ثوابته، س. م. 2006. دراسة صخرية ورسوبية وجيوكيميائية الحجر الجيري على طول الجانب الشرقي من وادي الأردن والبحر الميت. أطروحة ماجستير، الجامعة الهاشمية.

تقارير غير منشورة:

مخلوف، ع. م. والحداد، أ.ج. 2006. البيئات الترسيبية والسحنات من تشكيل أبو رويس التابع لأواخر العصر الترياسي، الأردن. مجلة علوم الأرض الآسيوية. انكلترا، في النشر.

لا تعاد المخطوطات المقدمة للنشر في المجلة إلى أصحابها سواءً قُبلت للنشر أم لم تُقبل كما تحتفظ الهيئة بحقها في عدم نشر أي بحث دون إبداء الأسباب، وتُعد قراراتها نهائية.

تحتفظ المجلة بحقها في أن تختزل أو تُعيد صياغة بعض الجمل لأغراض الضبط اللغوي ومنهج التحرير.

يُهدى إلى الباحث (الباحثين) نسخة واحدة من العدد المنشور فيه البحث و(20) مستلة منه، ويتحمل الباحث (الباحثون) نفقات أي مستلات إضافية.

تتم المراسلات جميعها باسم:

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مجلة علمية محكّمة ومفهرسة تصدر عن

عمادة البحث العلمي

جامعة مؤتة

قسيمة اشتراك

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التاريخ :   /   /   200 التوقيع :............ ....

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للمؤسسات (11) ديناراً أردنياً.

ب – خارج الأردن (للأفراد والمؤسسات): (30) دولاراً أمريكياً.

ج– للطلبة: (5) دنانير سنوياً

د – تضاف أجرة البريد لهذه الأسعار.

تُملأ هذه القسيمة، وترسل مع قيمة الاشتراك إلى العنوان التالي:

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المحتويات

حلول عددية شرائحية لمنظومات من المعادلات التفاضلية الجبرية غير الخطية

سليمان محمد محمود *

محمد علي

بشار جديد

ملخص

يهدف هذا العمل إلى دراسة وتقديم طريقة عددية لحل منظومات من المعادلات التفاضلية الجبرية غير الخطية. تستخدم الطريقة المقترحة كثيرات حدود شرائحية من الدرجة الثامنة وخمس نقاط تجميع لتقريب الحل للمسألة المطروحة. تم إثبات أن الطريقة موجودة وتقدم حل وحيد، وتبين الدراسة أن الطريقة تكون مستقرة ومتقاربة وهذا التقارب من الرتبة السابعة عند تطبيقها لحل منظومة من المعادلات التفاضلية الجبرية غير الخطية أيّا كان دليلها.

وقد تم اختبار فعالية الطريقة المقترحة بحل ثلاث مسائل اختبار، وتشير النَتائِج العددية إلى فعالية وكفاءة الطريقة الشرائحية المقدمة بالمقارنة مع بعض الطرائق الأخرى.

الكلمات الدالة: منظومة تفاضلية جبرية غير خطية، دليل عال، كثيرة حدود شرائحية، نقاط تجميع، الخطأ المقتطع، مرتبة التقارب.

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* **العنوان:** قسم الرياضيات، كلية العلوم، جامعة تشرين، اللاذقية، سوريا

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Spline Numerical Solutions for Systems of Nonlinear Differential Algebraic Equations

Suliman M Mahmoud

Mohamad Ali

Bashar Gdeed

Abstract

In this paper, a numerical method is presented for solving systems of nonlinear differential algebraic equations. This method is based on spline polynomials of degree eight with five collocation points to approximate the solution of the proposed problem. The study shows that the method when applied to nonlinear differential-algebraic systems for any index is existent and unique. Moreover, this method is stable and convergent of order seven.

Numerical experiments for three test problems and comparisons with other available results are given to illustrate the applicability and efficiency of the presented method.

Keywords: Nonlinear Differential-Algebraic Systems, Higher Index, Spline Polynomials, Collocation Points, Truncation Error, Order of Convergence.

1- مقدمة: Introduction

اهتم الباحثون بدراسة المعادلات التفاضلية بأنماطها وأشكالها المختلفة نظراً لأهميتها الكبيرة في عصرنا الحاضر. فهي تصف العديد من المسائل الفيزيائية والكيميائية والهندسية والميكانيكية الخ، نذكر على سبيل المثال: نمذجة الشبكات الالكترونية، محاكاة العمليات الكيميائية، مسائل التدفق للسوائل غير القابلة للانضغاط في الهيدروليك و للهواء في التكييف وللغازات في الأجهزة الكهربائية، في العلوم الطبية ردود أفعال الأجسام في ممانعة الأمراض والفيروسات. في الهندسة المدنية اهتزاز الجسور البيتونية والحديدية ومقاومة الانقطاع، والجدير بالذكر إن معظم هذه النماذج تعطى بمعادلات تفاضلية جبرية غير خطية(Benhammouda, 2018)

نقدم معالجة عددية لجملة من المعادلات التفاضلية الجبرية غير الخطية ذات دليل عال من الشكل(Benhammouda, 2015):

$$\begin{aligned} u' &= f(t,u,v,w), \\ v' &= g(t,u,v), \\ 0 &= q(t,v) \ . \end{aligned} \qquad (1)$$

حيث إن جداء مصفوفات جاكوبي $(\frac{\partial q}{\partial v})(\frac{\partial g}{\partial u})(\frac{\partial f}{\partial w})$ للدوال الثلاث f, g, q غير شاذ.

تدعى المنظومة التفاضلية الجبرية (1) بصيغة هيسنبيرغ (Hessenberg) غير الخطية ذات دليل يساوي3، وهي إحدى أشهر وأهم صيغ هيسنبيرغ .

يلعب دليل التفاضل دوراً رئيسياً ومميزاً في معالجة المعادلات التفاضلية الجبرية، ويوجد تعاريف متنوعة للدليل في الأدبيات العلمية ولكن معظمهم يعرفه كالآتي:

تعريف(1) (دليل المعادلة التفاضلية الجبرية)(Vanani & Amintaei, 2011) :

بما أن المعادلة التفاضلية الجبرية هي خليط من معادلات تفاضلية و معادلات جبرية، عندئذ يعرف دليل تفاضل المعادلة التفاضلية الجبرية بأنه أصغر عدد من التفاضلات لـ y و t التي تتطلبها منظومة المعادلات التفاضلية الجبرية من الشكل $F(t, y, y')=0$ لتحويلها إلى منظومة تفاضلية عادية صريحة من الشكل $y'=f(t,y)$.

إن دليل المعادلة التفاضلية الجبرية يقيس درجة الشذوذ (Singularity) في المنظومة وهو يشير بنحو واسع إلى بعض الصعوبات في إيجاد الحلول العددية للمعادلات التفاضلية بالأخص

غير الخطية منها ومن المعلوم أن هذه الصعوبات تزداد كلما ازداد الدليل ارتفاعاً ويقال عن الدليل التفاضلي إنه عالٍ إذا كان أكبر من الواحد(Benhammouda, 2015)

قدم الباحثون العديد من التقنيات العددية لحل مسائل في المعادلات التفاضلية الجيرية ولكن المشكلة تتجلى بضعف أو عدم استقرار الطرائق العددية وتباعد الحل العددي عن الحل الدقيق وبالتالي فشل الطريقة في إيجاد الحل العددي، وتظهر مثل هذه الحالات بالأخص عند حل مسائل غير الخطية وذات دليل أكبر من الواحد.

طور (Celik & Bayram, 2004) في عام 2004 سلسلة تقريبات بادي لحل منظومات تفاضلية جبرية غير الخطية وأختبر طريقته بحل مثال عددي.

قدم (Hosseini, 2006) في عام 2006 طريقة تقريبات أدوميان المعدلة لحل منظومات هايسنبيرغ غير الخطية وأختبر طريقته بحل مثالين عدديين.

طور (Gao & Jiang, 2007) في عام 2007 طريقة تهجين بين تجميع مويجات شرائح تكعيبية وطريقة تكرارية نيوتن المعدلة واختبرت التقنية بحل مثال عددي.

قدم (Mahmoud, 2010) في عام 2010 طريقة التجميع الشرائحية لحل منظومات من المعادلات التفاضلية الجبرية واختبرت بحل بعض الأمثلة العددية.

قدم (Benhammouda, 2015) في عام 2015 تقنية تستخدم حدوديات أدوميان وطريقة تحويل لابلاس لحل مسالة هينسنبيرغ (1) وأختبر تقنيته بحل نموذجين بأدلة تساوي 3، وقدم أيضاً في (Benhammouda, 2018)عام 2018 طريقة تعتمد على متسلسلة القوى وكثيرات حدود أدوميان لإيجاد الحل التحليلي التقريبي وأختبر بحل نموذجين عددين.

استخدم (Ren & Wang, 2017) في عام 2017 تقريبات بادي الكسرية لإيجاد الحل العددي لمنظومات من المعادلات التفاضلية الجبرية واختبر التقنية بحل نموذجين عدديين.

أهمية البحث وأهدافه: Importance of Research and its Aims

تكمن أهمية هذا البحث كونه يتناول دراسة مسألة علمية لها تطبيقات علمية حديثة فيزيائية وكيميائية وهندسية وميكانيكية الخ، ونظراً لأن المسألة ليس لها حلول تحليلية دقيقة لهذا تتجه الدراسات الحديثة إلى تطوير طرائق عددية لتقديم الحلول لمثل هذه المسائل، وخاصة وأن الكثير من

الطرائق العددية تنخفض دقتها أو تفشل في إيجاد حلول عددية مستقرة عندما يتم تطبيقها لحل منظومات غير خطية من المعادلات التفاضلية الجبرية. لهذا نهدف إلى تقديم طريقة عددية مستقرة وعالية التقارب لإيجاد الحلول العددية للمسألة المطروحة.

مواد وطرائق البحث: Methodology

تعتمد طرائق البحث على إنشاء تقريبات بكثيرات حدود تتطلب استخدام بعض المفاهيم الأساسية في التحليل الدالي ونظرية التقريب بالإضافة للحاجة إلى التحليل والجبر الخطي لدراسة الاستقرار والتقارب. ولإجراء الاختبارات والنتائج العددية سنستخدم لغة برمجية سهلة التطبيق عالية المستوى هي لغة البرمجة Mathematica.

النتائج والمناقشة: Results and Discussions

سنقوم بتوصيف طريقة عددية تستخدم كثيرات حدود شرائحية من الدرجه الثامنة، وخمس نقاط تجميعية ودراسة استقراها وتقاربها وتحديد الأخطاء المقتطعة لها.

طريقة التجميع الشرائحية: The Spline Collocation Method

سنقدم فيما يلي صياغة لتقنية عددية وتطبيقها للمنظومة التفاضلية الجبرية غير خطية الآتية:

$$\begin{aligned}
&\frac{du}{dt} = f(t,u,v,w), \\
&\frac{dv}{dt} = g(t,u,v), \qquad t \in [a,b] \\
&0 = q(t,v), \\
&u(a) = u_0,\ v(a) = v_0,\ w(a) = w_0
\end{aligned} \tag{2}$$

تُستخْدم $t_k = a + k\,h,\ k = 0(1)\mathrm{N}$ تجزئة منتظمة للمجال [a,b]، تقسّمه إلى N مجالا جزئياً $\mathrm{I}_k = [t_k, t_{k+1}],\ k = 0(1)N\text{-}1$ وفق خطوة طولها $h = (b-a)/N$.

تُعرِّف الطريقة خمس نقاط تجميع كالآتي:

$$t_{k+z_j} = t_k + z_j h,\ \ j = 1(1)5 \tag{3}$$

في كل مجال جزئي I_k ، ترتبط هذه النقاط بوسطاء التجميع الخمسة الآتية:

$$0 < z_1 < z_2 < z_3 < z_4 < 1\ \ and\ z_5 = 1 \tag{4}$$

نعرف دالة متقطعة في كل مجال جزئي I_k كالآتي:

$$\begin{aligned} S_k(t) &= H_0(\gamma)s_k + H_1(\gamma)s_k^{[1]} + H_2(\gamma)s_k^{[2]} + H_3(\gamma)s_k^{[3]} + H_4(\gamma)\, s_k^{[4]} \\ &+ R_0(\gamma)s_{k+1} + R_1(\gamma)S_{k+1}^{[1]} + R_2(\gamma)s_{k+1}^{[2]} + R_3(\gamma)s_{k+1}^{[3]} + R_4(\gamma)s_{k+1}^{[4]} \ ; \ t \in [t_k, t_{k+1}] \end{aligned} \tag{5}$$

حيث إن:

$$\begin{cases} H_0(\gamma) = (1 - 126\gamma^5 + 420\gamma^6 - 540\gamma^7 + 315\gamma^8 - 70\gamma^9) \\ H_1(\gamma) = (\gamma - 70\gamma^5 - 224\gamma^6 - 280\gamma^7 + 160\gamma^8 - 35\gamma^9) \\ H_2(\gamma) = (\frac{1}{2}\gamma^2 - \frac{35}{2}\gamma^5 + \frac{105}{2}\gamma^6 - 63\gamma^7 + 35\gamma^8 - \frac{15}{2}\gamma^9) \\ H_3(\gamma) = (\frac{1}{6}\gamma^3 - \frac{5}{2}\gamma^5 - \frac{20}{3}\gamma^6 - \frac{15}{2}\gamma^7 + 4\gamma^8 - \frac{5}{6}\gamma^9) \\ H_4(\gamma) = (\frac{1}{24}\gamma^4 - \frac{5}{24}\gamma^5 + \frac{5}{12}\gamma^6 - \frac{5}{12}\gamma^7 + \frac{5}{24}\gamma^8 - \frac{1}{24}\gamma^9) \\ R_0(\gamma) = (126\gamma^5 - 420\gamma^6 + 540\gamma^7 - 315\gamma^8 + 70\gamma^9) \\ R_1(\gamma) = (196\gamma^6 - 56\gamma^5 - 260\gamma^7 + 155\gamma^8 - 35\gamma^9) \\ R_2(\gamma) = (\frac{21}{2}\gamma^5 - \frac{77}{2}\gamma^6 + 53\gamma^7 - \frac{65}{2}\gamma^8 + \frac{15}{2}\gamma^9) \\ R_3(\gamma) = (-\gamma^5 + \frac{23}{6}\gamma^6 - \frac{11}{2}\gamma^7 - \frac{7}{2}\gamma^8 - \frac{5}{6}\gamma^9) \\ R_4(\gamma) = (\frac{1}{24}\gamma^5 - \frac{1}{6}\gamma^6 + \frac{1}{4}\gamma^7 - \frac{1}{6}\gamma^8 + \frac{1}{24}\gamma^9) \end{cases} \tag{5'}$$

و إن: $\gamma = (t - t_k)/h \in [0,1]$ ، وللتبسيط نستخدم الترميزات:

$$\begin{aligned} S_k &= S(t_k), \quad S_k^{[1]} = hS'(t_k), \quad S_k^{[2]} = h^2 S''(t_k), \\ S_k^{[3]} &= h^3 S'''(t_k), \quad S_k^{[4]} = h^4 S^{(4)}(t_k), \qquad k = 0(1)N-1 \end{aligned} \tag{6}$$

وبشكل عام فإن الدالة الشرائحية S(t) تعرف N كثيرة حدود متقطعة $S_k(t)$ من الدرجة التاسعة على الأكثر في المجال [a,b] ، نسميها كثيرة حدود شرائحية تعطى بالشكل:

$$S(t) = \begin{cases} S_0(t), & t \in [t_0, t_1], \\ \vdots \\ S_k(t)\ , & t \in [t_k, t_{k+1}], \\ \vdots \\ S_{N-1}(t), & t \in [t_{N-1}, t_N] \end{cases}$$

وهي تحقق الشروط:

- $S \in C^4[a,b]$
- $S_k^{(m)}(t_k) = S_{k-1}^{(m)}(t_k),\ m = 0,1,\ldots,4,\ k = 1(1)N-1$

إن كثيرة الحدود الشرائحية $S \in C^4[a,b]$، هي دالة ملساء في عقد الوصل بين الشرائح (النقاط الداخلية) $\{t_1,\ldots,t_{n-1}\}$ وهذا ما يجعلنا نتوقع أن تكون الشرائح تقريبات جيدة لدالة حل المسألة.

ويعطى مشتق الدالة (5) بالنسبة لـ t بالشكل:

$$\begin{aligned} hS_k'(t) &= (-630\gamma^4 + 2520\gamma^5 - 3780\gamma^6 + 2520\gamma^7 - 630\gamma^8)S_k + (1 - 350\gamma^4 + 1344\gamma^5 \\ &- 1960\gamma^6 + 1280\gamma^7 - 315\gamma^8)S_k^{[1]} + (\gamma - \tfrac{175}{2}\gamma^4 + 315\gamma^5 - 441\gamma^6 + 280\gamma^7 - \tfrac{135}{2}\gamma^8)S_k^{[2]} + \\ &(\tfrac{1}{2}\gamma^2 - \tfrac{25}{2}\gamma^4 + 40\gamma^5 - \tfrac{105}{2}\gamma^6 + 32\gamma^7 - \tfrac{15}{2}\gamma^8)S_k^{[3]} + (\tfrac{1}{6}\gamma^3 - \tfrac{25}{24}\gamma^4 + \tfrac{5}{2}\gamma^5 - \tfrac{35}{12}\gamma^6 + \\ &\tfrac{5}{3}\gamma^7 - \tfrac{7}{8}\gamma^8)S_k^{[4]} + (630\gamma^4 - 2520\gamma^5 + 3780\gamma^6 - 2520\gamma^7 + 630\gamma^8)S_{k+1} + (1176\gamma^5 - 280\gamma^4 \\ &- 1820\gamma^6 + 1240\gamma^7 - 315\gamma^8)S_{k+1}^{[1]} + (\tfrac{105}{2}\gamma^4 - 231\gamma^5 + 371\gamma^6 - 260\gamma^7 + \tfrac{135}{2}\gamma^8)S_{k+1}^{[2]} + \\ &(-5\gamma^4 + 23\gamma^5 - \tfrac{77}{2}\gamma^6 + 28\gamma^7 - \tfrac{15}{2}\gamma^8)S_{k+1}^{[3]} + (\tfrac{5}{24}\gamma^4 - \gamma^5 + \tfrac{7}{4}\gamma^6 - \tfrac{4}{3}\gamma^7 + \tfrac{3}{8}\gamma^8)S_{k+1}^{[4]} \end{aligned} \tag{7}$$

لنفرض أن $u(t), v(t), w(t)$ هو الحل الدقيق للمنظومة (2) وأن S_u ، S_v ، S_w الحل الشرائحي التقريبي له.

الآن بتطبيق كثيرات الحدود الشرائحية (6)–(7) مع نقاط التجميع(3)–(4) على منظومة المعادلات التفاضلية الجبرية (2)، ينتج لدينا:

$$\begin{aligned} &F_1(C_{k+1,1},\ldots,C_{k+1,15}) = S_u'(t_{k+z_j}) - f(t_{k+z_j}, S_u(t_{k+z_j}), S_v(t_{k+z_j}), S_w(t_{k+z_j})), \\ &F_2(C_{k+1,1},\ldots,C_{k+1,15}) = S_v'(t_{k+z_j}) - g(t_{k+z_j}, S_u(t_{k+z_j}), S_v(t_{k+z_j})), \\ &F_3(C_{k+1,1},\ldots,C_{k+1,15}) = -g(t, S_v(t_{k+z_j})), \qquad j = (1)4,\ \ k = 0(1)N-1 \end{aligned} \tag{8}$$

وهي خاضعة للشروط الابتدائية:

$$S_u^{(m)}(a) = S_{u,0}^{(m)} = u_0^{(m)},\ S_v^{(m)}(a) = S_{v,0}^{(m)} = v_0^{(m)},\ S_w^{(m)}(a) = S_{w,0}^{(m)} = w_0^{(m)},\ (m = 0,1\ldots,4) \tag{9}$$

حيث $t_{k+z_j} \in]t_k, t_{k+1}]$ (j=1,..,5) ،.

يعطى التقريب الشرائحي لدوال الحل $u(t), v(t), w(t)$ على الترتيب:

$$\begin{aligned} S_u(t_{k+z_j}) &= H_0(h z_j)s_{u,k} + H_1(h z_j)s_{u,k}^{[1]} + H_2(h z_j)s_{u,k}^{[2]} + H_3(h z_j)s_{u,k}^{[3]} + H_4(h z_j)s_{u,k}^{[4]} \\ &+ R_0(h z_j)C_{k+1,1} + R_1(h z_j)C_{k+1,2} + R_2(h z_j)C_{k+1,3} + R_3(h z_j)C_{k+1,4} + R_4(h z_j)C_{k+1,5} \end{aligned}$$

$$S_v(t_{k+z_j}) = H_0(h\,z_j)s_{v,k} + H_1(h\,z_j)s_{v,k}^{[1]} + H_2(h\,z_j)s_{v,k}^{[2]} + H_3(h\,z_j)s_{v,k}^{[3]} + H_4(h\,z_j)\,s_{v,k}^{[4]}$$
$$+ R_0(h\,z_j)C_{k+1,6} + R_1(h\,z_j)C_{k+1,7} + R_2(h\,z_j)C_{k+1,8} + R_3(h\,z_j)C_{k+1,9} + R_4(h\,z_j)C_{k+1,10}$$
$$S_w(t_{k+z_j}) = H_0(h\,z_j)s_{w,k} + H_1(h\,z_j)s_{w,k}^{[1]} + H_2(h\,z_j)s_{w,k}^{[2]} + H_3(h\,z_j)s_{w,k}^{[3]} + H_4(h\,z_j)\,s_{w,k}^{[4]}$$
$$+ R_0(h\,z_j)C_{k+1,11} + R_1(h\,z_j)C_{k+1,12} + R_2(h\,z_j)C_{k+1,13} + R_3(h\,z_j)C_{k+1,14} + R_4(h\,z_j)C_{k+1,15}$$

نلاحظ أن $s_{u,k}, s_{u,k}^{[1]},\dots,s_{u,k}^{[4]}, s_{v,k}, s_{v,k}^{[1]},\dots,s_{v,k}^{[4]}, s_{w,k}, s_{w,k}^{[1]},\dots,s_{w,k}^{[4]}$ من أجل k=0 معلومة في المجال الجزئي الأول $[t_0,t_1]$ من شروط البدء انطلاقاً من $t_0 = a$، ونحتاج في الجملة غير الخطية (8) لحساب شعاع المجاهيل :

$$\overline{C}_{k+1} = (C_{k+1,1}, C_{k+1,2}, \dots, C_{k+1,15})^T \qquad (10)$$

وتعويضه في التقريبات $S_w(t_{k+z_j}), S_v(t_{k+z_j}), S_u(t_{k+z_j})$ للحصول على الحل الشرائحي للمسألة عند t_1 والذي سيكون بمثابة شروط بدء لحساب الحل الشرائحي عند t_2 في المجال الجزئي $[t_1,t_2]$ وبالاستمرار تدريجياً يتم التوصل إلى الحل الشرائحي للمسألة على كل المجال $[a,b]=[t_0,t_N]$.

حساب شعاع المجاهيل (Computing coefficients vector)

لنكتب المنظومة غير الخطية (7) بالشكل:

$$F(\overline{C}_{k+1}) = \begin{pmatrix} F_1(C_{k+1,1},\dots,C_{k+1,15}) \\ F_2(C_{k+1,1},\dots,C_{k+1,15}) \\ F_3(C_{k+1,1},\dots,C_{k+1,15}) \end{pmatrix} = 0$$

يُحسبْ شعاع المجاهيل (10) بحل جملة المعادلات غير الخطية الآتية:

$$\overline{C}_{k+1}^{\,i+1} = \overline{C}_{k+1}^{\,i} - [G(\overline{C}_{k+1}^{\,i})]^{-1} F(\overline{C}_{k+1}^{\,i}), \qquad i=0,1,2,\dots;\ k=0,1,\dots,N-1$$

حيث $G(\overline{C}_{k+1})$ هي مصفوفة جاكوبي للدالة F تعطى كالآتي:

$$G(\overline{C}_{k+1}) = \begin{bmatrix} \frac{\partial F_1}{\partial C_{k+1,1}}|_{t_{k+z_1}} & \frac{\partial F_1}{\partial C_{k+1,2}}|_{t_{k+z_1}} & \cdots & \frac{\partial F_1}{\partial C_{k+1,15}}|_{t_{k+z_1}} \\ \frac{\partial F_1}{\partial C_{k+1,1}}|_{t_{k+z_2}} & \frac{\partial F_1}{\partial C_{k+1,2}}|_{t_{k+z_2}} & \cdots & \frac{\partial F_1}{\partial C_{k+1,15}}|_{t_{k+z_2}} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial F_1}{\partial C_{k+1,1}}|_{t_{k+1}} & \frac{\partial F_1}{\partial C_{k+1,2}}|_{t_{k+1}} & \cdots & \frac{\partial F_1}{\partial C_{k+1,15}}|_{t_{k+1}} \\ \frac{\partial F_2}{\partial C_{k+1,1}}|_{t_{k+z_1}} & \frac{\partial F_2}{\partial C_{k+1,2}}|_{t_{k+z_1}} & \cdots & \frac{\partial F_2}{\partial C_{k+1,15}}|_{t_{k+z_1}} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial F_3}{\partial C_{k+1,1}}|_{t_{k+z_1}} & \frac{\partial F_3}{\partial C_{k+1,2}}|_{t_{k+z_1}} & \cdots & \frac{\partial F_3}{\partial C_{k+1,15}}|_{t_{k+z_1}} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial F_3}{\partial C_{k+1,1}}|_{t_{k+1}} & \frac{\partial F_3}{\partial C_{k+1,2}}|_{t_{k+1}} & \cdots & \frac{\partial F_3}{\partial C_{k+1,15}}|_{t_{k+1}} \end{bmatrix}_{15\times 15}$$

الاستقرار المطلق للطريقة : Absolute Stability of the Method

إن دراسة الاستقرار المطلق الخطي يعطي الكثير من المؤشرات عن الطريقة لهذا نأخذ نموذج الاختبار:

$$y'(t) = \lambda y(t), \qquad y(0) = 1$$

حيث $\lambda \in C$. وبتطبيق التقريبات الشرائحية (5)–(6) مع نقاط التجميع (4) في معادلة الاختبار:

$$S'(t_{k+z_j}) = \lambda h S(t_{k+z_j}), \quad j = 1,2,\ldots,5; \quad k = 0,1,\ldots,N-1$$

نحصل على منظومة المعادلات:

$$[630z_j^4-2520z_j^5+3780z_j^6-2520z_j^7+630z_j^8]S_{k+1}+[-280z_j^4+1176z_j^5-1820z_j^6+1240z_j^7-315z_j^8]S_{k+1}^{[1]}+[\tfrac{105}{2}z_j^4-231z_j^5+371z_j^6-260z_j^7+\tfrac{135}{2}z_j^8]S_{k+1}^{[2]}+[-5z_j^4+23z_j^5-\tfrac{77}{2}z_j^6+28z_j^7-\tfrac{15}{2}z_j^8]S_{k+1}^{[3]}+[\tfrac{5}{24}z_j^4-z_j^5+\tfrac{7}{4}z_j^6-\tfrac{4}{3}z_j^7+\tfrac{3}{8}z_j^8]S_{k+1}^{[4]}-[630z_j^4-2520z_j^5+3780z_j^6-2520z_j^7+630z_j^8]S_k+[1-350z_j^4+1344z_j^5-1960z_j^6+1280z_j^7-315z_j^8]S_k^{[1]}+[z_j-\tfrac{175}{2}z_j^4+315z_j^5-441z_j^6+280z_j^7-\tfrac{135}{2}z_j^8]S_k^{[2]}+[\tfrac{1}{2}z_j^2-\tfrac{25}{2}z_j^4+40z_j^5-\tfrac{105}{2}z_j^6+32z_j^7-\tfrac{15}{2}z_j^8]S_k^{[3]}+\left[-\tfrac{25}{24}z_j^4+\tfrac{5}{2}z_j^5-\tfrac{35}{12}z_j^6+\tfrac{5}{3}z_j^7-\tfrac{3}{8}z_j^8+\tfrac{1}{6}z_j^3\right]S_k^{[4]}=$$

$$\begin{aligned}V\Big\{&[126z_j^5-420z_j^6+540z_j^7-315z_j^8+70z_j^9]S_{k+1}\\&+[-56z_j^5+196z_j^6-260z_j^7+155z_j^8-35z_j^9]S_{k+1}^{[1]}\\&+\left[\frac{21}{2}z_j^5-\frac{77}{2}z_j^6+35z_j^7-\frac{65}{2}z_j^8+\frac{15}{2}z_j^9\right]S_{k+1}^{[2]}\\&+\left[-z_j^5+\frac{23}{6}z_j^6-\frac{11}{2}z_j^7+\frac{7}{2}z_j^8-\frac{5}{2}z_j^9\right]S_{k+1}^{[3]}\\&+\left[\frac{1}{24}z_j^5-\frac{1}{4}z_j^6+\frac{1}{4}z_j^7-\frac{1}{6}z_j^8+\frac{1}{24}z_j^9\right]S_{k+1}^{[4]}\\&+[1-126z_j^5+420z_j^6-540z_j^7+315z_j^8-70z_j^9]S_k\\&+[-70z_j^5+224z_j^6-280z_j^7+160z_j^8-35z_j^9+z_j]S_k^{[1]}\\&+\left[\frac{1}{2}z_j^2-\frac{35}{2}z_j^5+\frac{105}{2}z_j^6-63z_j^7+35z_j^8-\frac{15}{2}z_j^9\right]S_k^{[2]}\\&+\left[\frac{1}{6}z_j^3-\frac{5}{2}z_j^5+\frac{20}{3}z_j^6-\frac{15}{2}z_j^7+4z_j^8-\frac{5}{6}z_j^9\right]S_k^{[3]}\\&+\left[\frac{1}{24}z_j^4-\frac{5}{24}z_j^5+\frac{5}{12}z_j^6-\frac{5}{12}z_j^7+\frac{5}{24}z_j^8-\frac{1}{24}z_j^9\right]S_k^{[4]}\Big\}\end{aligned}$$

حيث $V=h\lambda$. وبتجميع المعاملات وكذلك للاختصار سنعوض في المعادلتين:

$S_{k+1}^{[1]}=V\,S_{k+1}$ ، $S_k^{[1]}=V\,S_k$

ينتج لدينا العلاقة التكرارية:

$$M_1(V)\underline{S}_{k+1} = M_2(V)\underline{S}_k \tag{11}$$

حيث:

$M_1(V) = \{\{(-1+z_1)z_1^4(630(-1+z_1)^3 - 70V(-1+z_1)^3(4+z_1) + V^2z_1(-56 + 140z_1 - 120z_1^2 + 35z_1^3)), -\frac{1}{2}(-1+z_1)z_1^4(105 - 21(17+V)z_1 + 7(55+8V)z_1^2 - 5(27+10V)z_1^3 + 15Vz_1^4), \frac{1}{6}(-1+z_1)^2z_1^4(-30+6(13+V)z_1 - (45+11V)z_1^2 + 5Vz_1^3), -\frac{1}{24}(-1+z_1)^3z_1^4(5-(9+V)z_1 + Vz_1^2)\},$

$\{(-1+z_2)z_2^4(630(-1+z_2)^3 - 70V(-1+z_2)^3(4+z_2) + V^2z_2(-56 + 140z_2 - 120z_2^2 + 35z_2^3)), -\frac{1}{2}(-1+z_2)z_2^4(105 - 21(17+V)z_2 + 7(55+8V)z_2^2 - 5(27+10V)z_2^3 + 15Vz_2^4), \frac{1}{6}(-1+z_2)^2z_2^4(-30+6(13+V)z_2 - (45+11V)z_2^2 + 5Vz_2^3), -\frac{1}{24}(-1+z_2)^3z_2^4(5-(9+V)z_2 + Vz_2^2)\},$

$\{(-1+z_3)z_3^4(630(-1+z_3)^3 - 70V(-1+z_3)^3(4+z_3) + V^2z_3(-56 + 140z_3 - 120z_3^2 + 35z_3^3)), -\frac{1}{2}(-1+z_3)z_3^4(105 - 21(17+V)z_3 + 7(55+8V)z_3^2 - 5(27+10V)z_3^3 + 15Vz_3^4), \frac{1}{6}(-1+z_3)^2z_3^4(-30+6(13+V)z_3 - (45+11V)z_3^2 + 5Vz_3^3), -\frac{1}{24}(-1+z_3)^3z_3^4(5-(9+V)z_3 + Vz_3^2)\},$

$\{(-1+z_4)z_4^4(630(-1+z_4)^3 - 70V(-1+z_4)^3(4+z_4) + V^2z_4(-56 + 140z_4 - 120z_4^2 + 35z_4^3)), -\frac{1}{2}(-1+z_4)z_4^4(105 - 21(17+V)z_4 + 7(55+8V)z_4^2 - 5(27+10V)z_4^3 + 15Vz_4^4), \frac{1}{6}(-1+z_4)^2z_4^4(-30+6(13+V)z_4 - (45+11V)z_4^2 + 5Vz_4^3), -\frac{1}{24}(-1+z_2)^3z_2^4(5-(9+V)z_2 + Vz_2^2)\}\}$

,

$$\mathbf{M}_2(V) = \{\{-(-1+z_1)^4 z_1(-630z_1^3 + 70V(-5+z_1)z_1^3 + V^2(-1-4z_1-10z_1^2-20z_1^3+35z_1^4)), -\frac{1}{2}(-1+z_1)^4 z_1(2-(-8+V)z_1 - 4(-5+V)z_1^2 - 5(27+2V)z_1^3 + 15Vz_1^4), -\frac{1}{6}(-1+z_1)^4 z_1^2(3-(-12+V)z_1 - (45+4V)z_1^2 + 5Vz_1^3), -\frac{1}{24}(-1+z_1)^4 z_1^3(4-(9+V)z_1 + Vz_1^2)\},$$

$$\{-(-1+z_2)^4 z_2(-630z_2^3 + 70V(-5+z_2)z_2^3 + V^2(-1-4z_2-10z_2^2-20z_2^3+35z_2^4)), -\frac{1}{2}(-1+z_2)^4 z_2(2-(-8+V)z_2 - 4(-5+V)z_2^2 - 5(27+2V)z_2^3 + 15Vz_2^4), -\frac{1}{6}(-1+z_2)^4 z_2^2(3-(-12+V)z_2 - (45+4V)z_2^2 + 5Vz_2^3), -\frac{1}{24}(-1+z_2)^4 z_2^3(4-(9+V)z_2 + Vz_2^2)\}$$

,

$$\{-(-1+z_3)^4 z_3(-630z_3^3 + 70V(-5+z_3)z_3^3 + V^2(-1-4z_3-10z_3^2-20z_3^3+35z_3^4)), -\frac{1}{2}(-1+z_3)^4 z_3(2-(-8+V)z_3 - 4(-5+V)z_3^2 - 5(27+2V)z_3^3 + 15Vz_3^4), -\frac{1}{6}(-1+z_3)^4 z_3^2(3-(-12+V)z_3 - (45+4V)z_3^2 + 5Vz_3^3), -\frac{1}{24}(-1+z_3)^4 z_3^3(4-(9+V)z_3 + Vz_3^2)\}$$

,

$$\{-(-1+z_4)^4 z_4(-630z_4^3 + 70V(-5+z_4)z_4^3 + V^2(-1-4z_4-10z_4^2-20z_4^3+35z_4^4)), -\frac{1}{2}(-1+z_4)^4 z_4(2-(-8+V)z_4 - 4(-5+V)z_4^2 - 5(27+2V)z_4^3 + 15Vz_4^4), -\frac{1}{6}(-1+z_4)^4 z_4^2(3-(-12+V)z_4 - (45+4V)z_4^2 + 5Vz_4^3), -\frac{1}{24}(-1+z_4)^4 z_4^3(4-(9+V)z_4 + Vz_4^2)\}\}$$

تعريف (Mahmoud, 2010): تكون طريقة البحث المعرفة بالمنظومة التكرارية (11) مستقرة مطلقا (absolute stable) إذا وجدت $V = h\lambda$ تحقق المتراجحة

$$G(V) = ||\mathbf{M}_1^{-1}(V)\mathbf{M}_2(V)|| < 1$$

وهذا يكافئ أن تكون القيم المميزة $\xi_1(V), \xi_2(V), \xi_3(V), \xi_4(V)$ للمسألة المميزة المعممة الآتية:

$$\xi M_1(V)\underline{X} = M_2(V)\underline{X}$$

تقع جميعها داخل قرص الواحدة في المستوي العقدي، يعني إذا كان:

$$|\xi_1|, |\xi_2|, |\xi_3|, |\xi_4| < 1$$

وتعرف منطقة الاستقرار المطلق للطريقة المقترحة بمجموعة النقاط:

$$\Omega = \{h\lambda \in C \ | G(V) < 1\}$$

ندرس السلوك المقارب للطريقة عندما $V \longrightarrow \infty$ حيث تعطى المعادلة الخاصة لمسألة القيمة المميزة كالآتي:

$$\lim_{V\to\infty} V^{-4}\, Det(\xi M_1(V) - M_2(V)) =$$

$\{\{-z_1 + 14(5+4\xi)z_1^5 - 28(8+7\xi)z_1^6 + 20(14+13\xi)z_1^7 - 5(32+31\xi)z_1^8 + 35(1+\xi)z_1^9, -\frac{1}{2}(-1+z_1)^2 z_1^2(1+2z_1+3z_1^2+(-31+21\xi)z_1^3 - 5(-8+7\xi)z_1^4 + 15(-1+\xi)z_1^5), \frac{1}{6}(-1+z_1)^3 z_1^3(1+3z_1-3(3+2\xi)z_1^2+5(1+\xi)z_1^3), -\frac{1}{24}(-1+z_1)^4 z_1^4(1+(-1+\xi)z_1)\},$

$\{-z_2 + 14(5+4\xi)z_2^5 - 28(8+7\xi)z_2^6 + 20(14+13\xi)z_2^7 - 5(32+31\xi)z_2^8 + 35(1+\xi)z_2^9, -\frac{1}{2}(-1+z_2)^2 z_2^2(1+2z_2+3z_2^2+(-31+21\xi)z_2^3 - 5(-8+7\xi)z_2^4 + 15(-1+\xi)z_2^5), \frac{1}{6}(-1+z_2)^3 z_2^3(1+3z_2-3(3+2\xi)z_2^2+5(1+\xi)z_2^3), -\frac{1}{24}(-1+z_2)^4 z_2^4(1+(-1+\xi)z_2)$

,

$\{-z_3 + 14(5+4\xi)z_3^5 - 28(8+7\xi)z_3^6 + 20(14+13\xi)z_3^7 - 5(32+31\xi)z_3^8 + 35(1+\xi)z_3^9, -\frac{1}{2}(-1+z_3)^2 z_3^2(1+2z_3+3z_3^2+(-31+21\xi)z_3^3 - 5(-8+7\xi)z_3^4 + 15(-1+\xi)z_3^5), \frac{1}{6}(-1+z_3)^3 z_3^3(1+3z_3-3(3+2\xi)z_3^2+5(1+\xi)z_3^3), -\frac{1}{24}(-1+z_3)^4 z_3^4(1+(-1+\xi)z_3)\}$

,

$\{-z_4 + 14(5+4\xi)z_4^5 - 28(8+7\xi)z_4^6 + 20(14+13\xi)z_4^7 - 5(32+31\xi)z_4^8 + 35(1+\xi)z_4^9, -\frac{1}{2}(-1+z_4)^2 z_4^2(1+2z_4+3z_4^2+(-31+21\xi)z_4^3 - 5(-8+7\xi)z_4^4 + 15(-1+\xi)z_4^5), \frac{1}{6}(-1+z_4)^3 z_4^3(1+3z_4-3(3+2\xi)z_4^2+5(1+\xi)z_4^3), -\frac{1}{24}(-1+z_4)^4 z_4^4(1+(-1+\xi)z_4)\}\}$

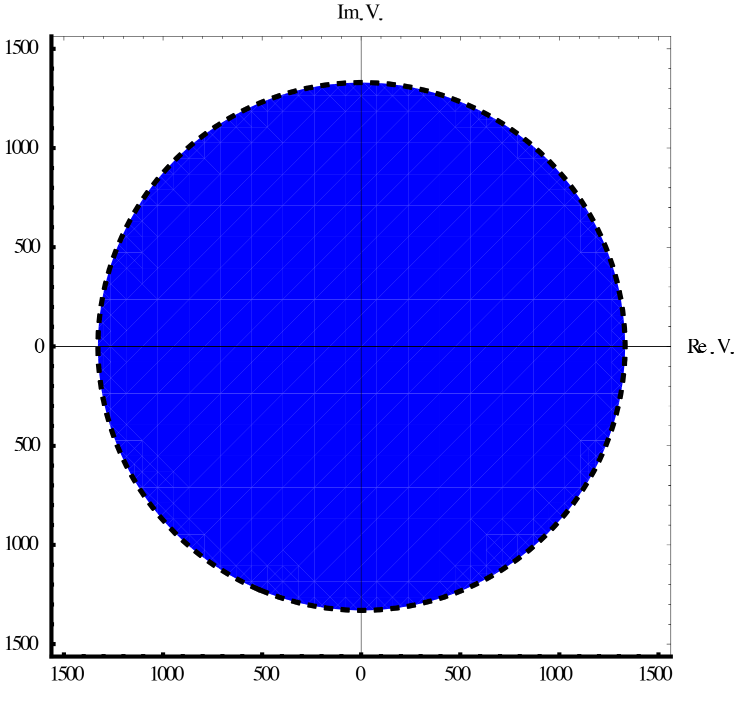
باستخدام برنامج Mathematica وباختيار إحدى القيم المعيارية لوسطاء التجميع:

$$z_1 = 0.86\,;\, z_2 = 0.90;\; z_3 = 0.940;\; z_4 = 0.99;$$

نحصل على القيم المميزة الآتية:

$$\xi_1 = -0.9657698, \xi_2 = -0.00208183, \xi_3 = -0.00000125, \xi_4 = -7.354 \times 10^{-12}$$

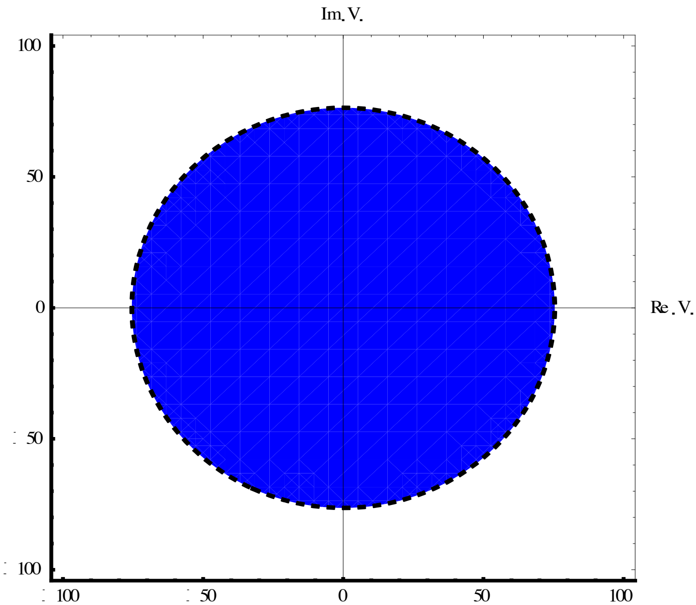
وجميعها أصغر تماما من الواحد بالقيمة المطلقة، وبالتالي تقع جميعها داخل قرص الواحدة إذن فالطريقة مستقرة بحسب التعريف (Mahmoud, 2010). نرسم باستخدام Mathematica في الشكل (1) منطقة الاستقرار المطلق للوسطاء التجميعية المذكورة أعلاه: وهي المنطقة المظللة ضمن الدائرة، ومن الواضح أن الطريقة ترسم مساحات كبيرة جداً من الاستقرار المطلق وتتسع هذه المساحات كلما ازدادت وسطاء التجميع باتجاه الطرف الأيمن للمجال [0,1].



الشكل(1): منطقة الاستقرار المطلق لأجل وسطاء التجميع

$$z_1 = 0.86; z_2 = 0.90; z_3 = 0.940; z_4 = 0.99;$$

ونرسم أيضاً في الشكل (2) منطقة الاستقرار المطلق لأجل وسطاء تجميع موزعة على أبعاد متساوية، وهي المنطقة المظللة ضمن الدائرة، ومن الواضح أن المساحة صغيرة جداً بالقياس للمساحة الأولى.



الشكل(2): منطقة الاستقرار المطلق لأجل وسطاء تجميع موزعة على أبعاد متساوية في كل مجال شرائحي

$$z_1 = 0.2\,; z_2 = 0.4;\ z_3 = 0.6;\ z_4 = 0.8;$$

خطأ الاقتطاع للطريقة: Truncation Error

نحسب خطأ الاقتطاع بتطبيق الطريقة للمعادلة غير الخطية الآتية $y' = f(t,y),\ y(a) = y_0$

$$S'(t_{k+z_j}) = hf(t_{k+z_j}, S(t_{k+z_j})),\ \ j = 1,2,\dots,4;\ \ k = 0,1,\dots,N-1$$

وبالتالي ينتج لدينا:

$$A\,\overline{S}_{k+1} + B\,\overline{S}_k = h\,H\,\overline{F}_{k+1}$$

حيث نستخدم الترميزات:

$$\overline{S}_{k+1} = (S_{k+1}, S_{k+1}^{[2]}, S_{k+1}^{[3]}, S_{k+1}^{[4]})^T,\quad \overline{F}_{k+1} = (f_k, f_{k+z_1}, f_{k+z_2}, f_{k+z_3}, f_{k+z_4}, f_{k+1})^T$$

$S_k^{[1]} = hf_k$، $S_{k+1}^{[1]} = hf_{k+1}$، $f_{k+z_j} = f(t_{k+z_j}, S_{k+z_j})$، وبأخذ نقاط التجميع الموزعة بالتساوي كونها الحالة الأسوأ للطريقة: $z_1 = 0.2\,;\, z_2 = 0.4;\, z_3 = 0.6;\, z_4 = 0.8$ ، وبفرض أن $y(t) \in C^{10}$ هو الحل الدقيق للمسألة غير الخطية واستخدام منشور تايلور حول t_k ، يعطى عندئذ خطأ الاقتطاع المحلي عند t_{k+1} للطريقة:

$$\tau_{k+1} = \overline{Y}_{k+1} + A^{-1}B\overline{Y}_k - hA^{-1}\,H\,\overline{Y'}_{k+1}$$

$$= h^{10} y_k^{(10)} \{-\frac{47}{190512000000}, \frac{1}{9450000}, \frac{173}{56700000}, \frac{673}{12600000}\}^T$$

ومنه $\|\tau_{k+1}\| = \frac{673}{12600000} h^{10} y_k^{(10)} \equiv O(h^{10})$ ويكون الخطأ المقتطع على كامل المجال بعد N خطوة:

$$T_{k+1} = N.O(h^{10}) \equiv O(h^9)$$

حيث:

$$A = \begin{bmatrix} \frac{32256}{78125} & \frac{2396}{78125} & -\frac{216}{78125} & \frac{128}{1171875} \\ \frac{163296}{78125} & \frac{9096}{78125} & -\frac{144}{15625} & \frac{126}{390625} \\ \frac{163296}{78125} & \frac{486}{78125} & \frac{162}{78125} & -\frac{54}{390625} \\ \frac{32256}{78125} & -\frac{10624}{78125} & \frac{768}{78125} & -\frac{352}{1171875} \end{bmatrix}, B$$

$$=\begin{bmatrix} -\frac{32256}{78125} & \frac{10624}{78125} & \frac{768}{78125} & \frac{352}{1171875} \\ -\frac{163296}{78125} & -\frac{486}{78125} & \frac{162}{78125} & \frac{54}{390625} \\ -\frac{163296}{78125} & -\frac{9096}{78125} & -\frac{144}{15625} & -\frac{126}{390625} \\ -\frac{32256}{78125} & -\frac{2396}{78125} & -\frac{216}{78125} & -\frac{128}{1171875} \end{bmatrix}$$

$$H=\begin{bmatrix} -\frac{59392}{78125} & 1 & 0 & 0 & 0 & \frac{13523}{78125} \\ \frac{26163}{78125} & 0 & 1 & 0 & 0 & \frac{59008}{78125} \\ \frac{59008}{78125} & 0 & 0 & 1 & 0 & \frac{26163}{78125} \\ \frac{13523}{78125} & 0 & 0 & 0 & 1 & -\frac{59392}{78125} \end{bmatrix} . \ A^{-1}$$

$$=\begin{bmatrix} -\frac{10625}{6048} & \frac{41875}{48384} & -\frac{625}{5832} & \frac{263125}{774144} \\ \frac{3125}{4} & -\frac{3125}{12} & \frac{3125}{27} & -\frac{3125}{64} \\ \frac{246875}{12} & -\frac{53125}{8} & \frac{446875}{162} & -\frac{353125}{384} \\ \frac{634375}{2} & -\frac{1571875}{16} & \frac{1018750}{27} & -\frac{2778125}{256} \end{bmatrix}$$

نتيجـة: نسـتنتج تعريـف التناسـق(consistent) (Mahmoud, 2010) أن الطريقـة الشـرائحية المطبقة لأجل المسألة غير الخطية تكون متناسقة من الرتبة التاسعة.

اختبارات عددية: Numerical Experiment

يتم اختبار فعالية الطريقة المقترحة بحل عدة مسائل نموذجية لها حلول تحليلية للتمكّن من حساب الأخطاء في الحل الشرائحي للطريقة وكذلك لتوضيح النتائج النظرية التي تم التوصل إليها.

المسألة(1): لنأخذ منظومة هايسنبيرغ التفاضلية الجبرية بدليل-3 الآتية (Benhammouda, 2015) :

$$u_1' = 2v_1 \quad , u_2' = 2v_2$$
$$v_1' = -2v_1 + \exp(u_2) + w + \varphi_1(t) \ ,$$
$$v_2' = 2v_2 + \exp(u_1) + w + \varphi_2(t) \ ,$$
$$0 = u_1 + u_2 - \varphi_3(t) \quad , \quad t \in [0,1) \, ,$$

حيث

$$\varphi_1(t) = -\frac{2t^4 + 2t^3 + 1}{2(1+t)^2}; \ \varphi_2(t) = \frac{-2t^4 + 2t^3 - 1}{2(1-t)^2}; \ \varphi_3(t) = \ln(1 - t^2)$$

مع الحل التحليلي: $u_1(t)=Ln(1+t)$, $u_2(t)=Ln(1-t)$، $v_1(t) = \frac{1}{2(1+t)}$, $v_2(t) = -\frac{1}{2(1-t)}$.

ندرج في الجدول (1) الأخطاء في الحل الشرائحي للمسألة(1). نرسم في الأشكال(3)-(10) على الترتيب الحل الشرائحي مع الحل التحليلي والأخطاء في الحل الشرائحي للمسألة (1) بخطوة h=0.06125.

استخدام Benhammouda في [2] حدوديات أدوميان وطريقة التحويل التفاضلية وحصل على الحل التحليلي التقريبي للمسألة:

$u_1(t)=t-1/2\ t^2+1/3\ t^3-1/2\ t^4+1/5\ t^5-1/6\ t^6$

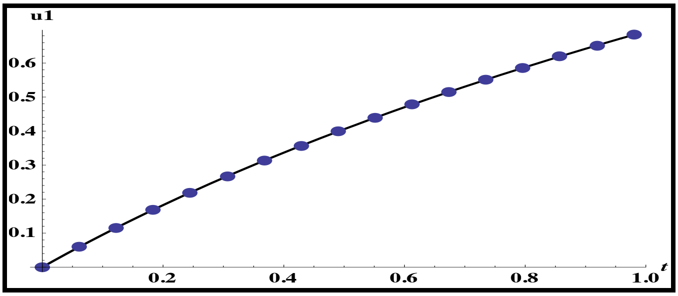
$u_2(t)=-t-1/2\ t^2-1/3\ t^3-1/2\ t^4-1/5\ t^5-1/6\ t^6$

$v_1(t)=1/2-1/2t+1/2\ t^2-1/2\ t^3+1/2\ t^4-1/2\ t^5$

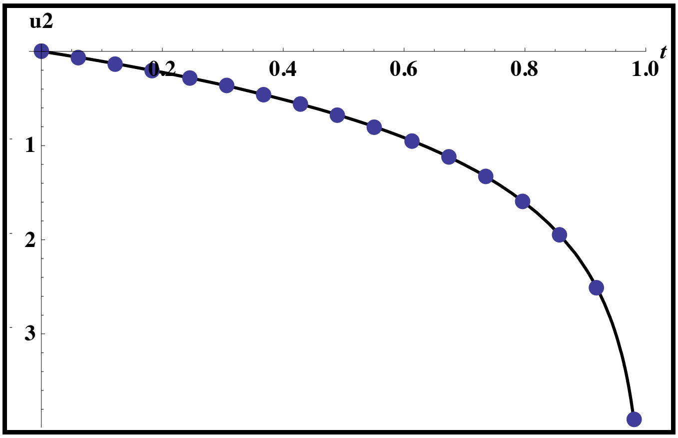
$v_2(t)=-1/2-1/2t-1/2\ t^2-1/2\ t^3-1/2\ t^4-1/2\ t^5$

الجدول(1) الأخطاء الحل الشرائحي بطريقة البحث في حل المسألة (1)

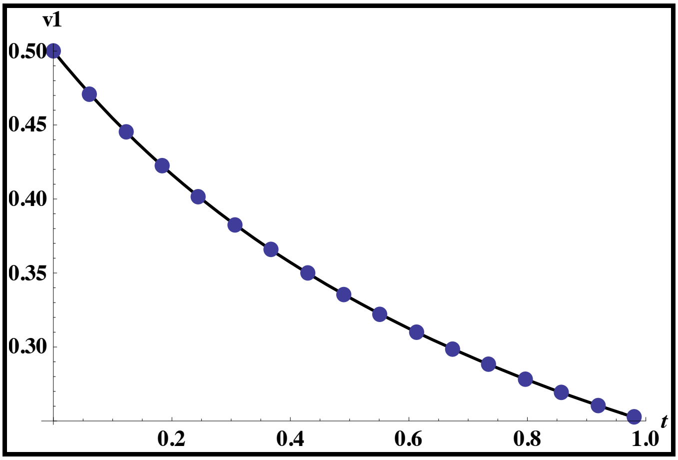
t	$z_1 = 0.86$; $z_2 = 0.90$; $z_3 = 0.94$; $z_4 = 0.99$;			
	Error=S-u_1	**Error=S-u_2**	**Error=S-v_1**	**Error=S-v_2**
0.06125	-1.22945901E-13	1.63590726E-13	-2.0898414E-13	2.65278324E-13
0.1225	-1.88022968E-13	2.3422339E-13	-2.9050928E-13	3.62591838E-13
0.18375	-3.23294550E-13	4.07370614E-13	-5.4995192E-13	6.94169224E-13
0.245	-4.25189987E-13	5.35242437E-13	-6.4889022E-13	8.16899187E-13
0.30625	-5.01929869E-13	6.31837051E-13	-6.6335020E-13	8.34756972E-13
0.3675	-5.6844593E-13	7.15528024E-13	-6.3950784E-13	8.04513161E-13
0.42875	-6.3519569E-13	7.99513897-13	-6.2593134E-13	7.86986616E-13
0.49	-7.0653942E-13	8.8917845E-13	-6.4239263E-13	8.06463889E-13
0.55125	-7.9383729E-13	9.9851424E-13	-7.4496825E-13	9.31772338E-13
0.6125	-9.232777E-13	1.1605581E-12	-1.0670109E-12	1.32714832E-12
0.67375	-1.05382811E-12	1.3261886E-12	-1.2151180E-12	1.52277559E-12
0.735	-1.2175617E-12	1.5326497E-12	-1.5453821E-12	1.94536158E-12
0.79625	1.44508294E-12	1.8187137E-12	-2.1369092E-12	2.68149715E-12
0.8575	-1.76193106E-12	2.2177191E-12	-3.2855042E-12	4.12075119E-12
0.91875	-2.30130021E-12	2.8949536E-12	-6.5224012E-12	8.11333625E-12
0.98	-3.4983613E-12	4.4041759E-12	-1.9617238E-11	2.46966398E-11



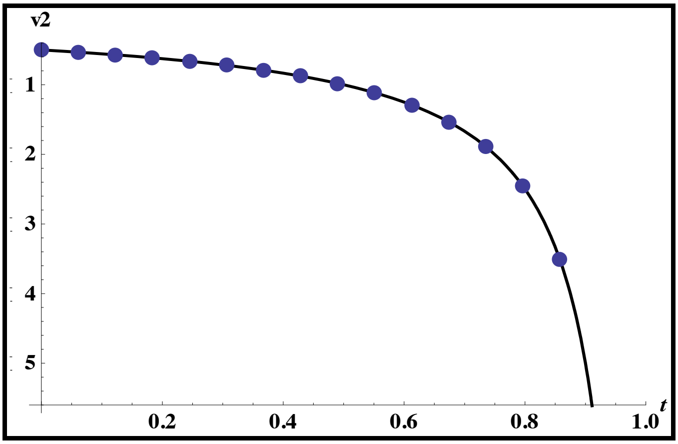
الشكل(3) الحل الشرائحي مع الحل التحليلي u_1 للمسألة (1) بخطوة h=0.06125.



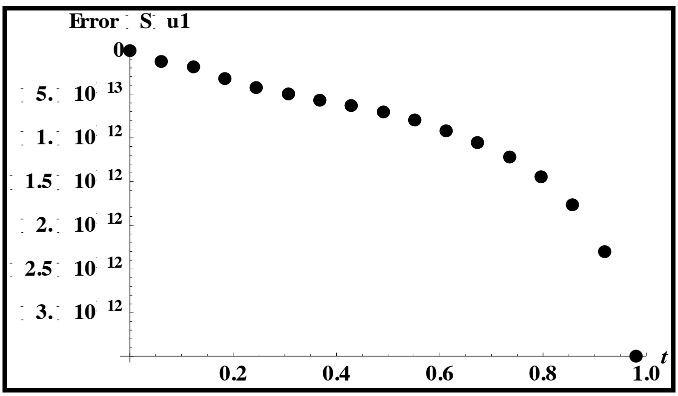
الشكل(4) الحل الشرائحي مع الحل التحليلي u_2 للمسألة (1) بخطوة h=0.06125.



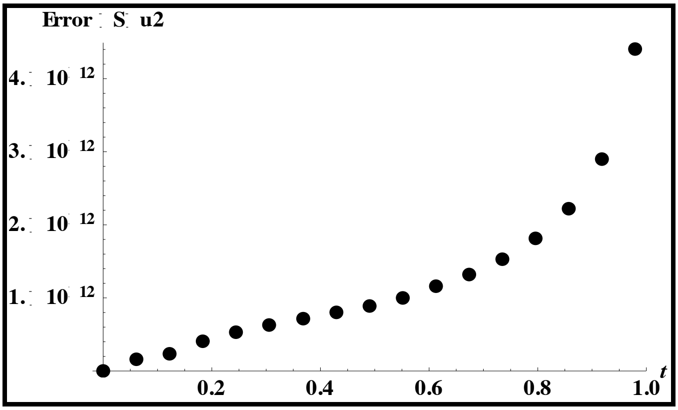
الشكل(5) الحل الشرائحي مع الحل التحليلي v_1 للمسألة (1) بخطوة h=0.06125.



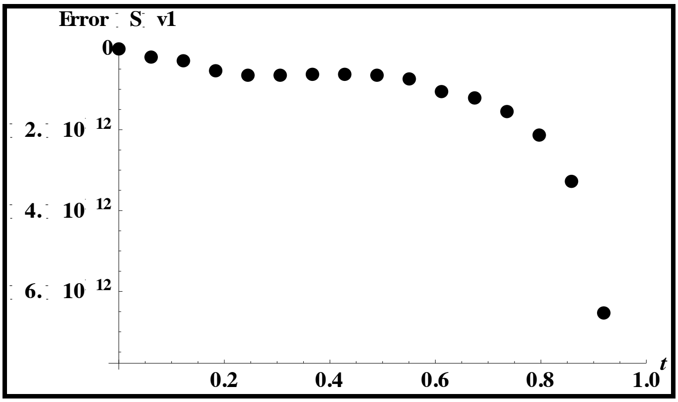
الشكل(6) الحل الشرائحي مع الحل التحليلي v_2 للمسألة (1) بخطوة h=0.06125.



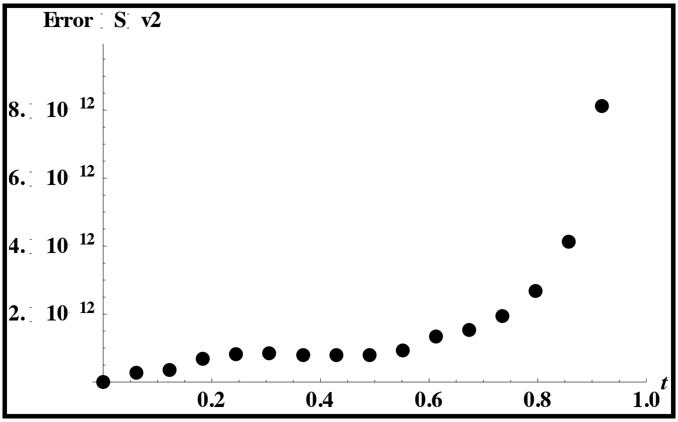
الشكل(7) الخطأ في الحل الشرائحي لـ u_1 للمسألة (1) بخطوة h=0.06125.



الشكل(8): الخطأ في الحل الشرائحي لـ u_2 للمسألة (1) بخطوة h=0.06125.



الشكل(9): الخطأ في الحل الشرائحي لـ v_1 للمسألة (1) بخطوة h=0.06125.



الشكل(10) الخطأ في الحل الشرائحي لـ v_2 للمسألة (1) بخطوة h=0.06125.

المسألة(2): (Marz & Tischendorf, 1994): منظومة هايسنبيرغ بدليل -2:

$$y' + \sin(arc\cos y) + w^2 - y^{-2} + 1 = 0\,,$$

$$z' + w = 0\,, \qquad t \in [0.1, 1.5]$$

$$z - Ln(y) = 0 \quad ,$$

تخضع للشروط الابتدائية:

$$y(0) = 1,\ z(0) = 0,\ w(0) = 0$$

الحل التحليلي:

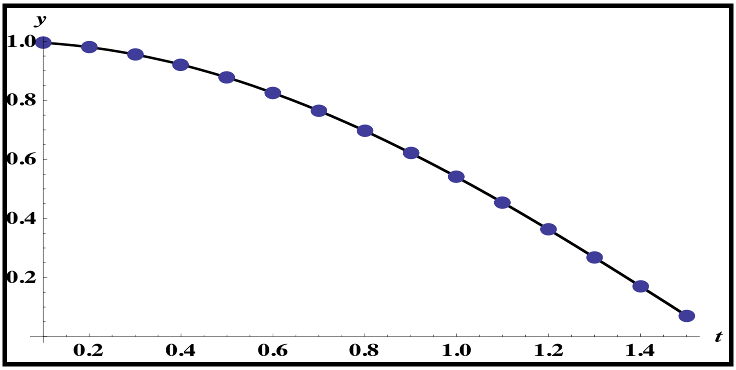
$$.\,,\ z(t) = Ln[\cos(t)]\,,\ y(t) = \cos(t)\ \ w(t) = \tan(t)$$

استخدم (Marz & Tischendorf, 1994) في صيغ التفاضلات التراجعية وطرائق رانج-كوتا لحل المسألة2، وكذلك تم حلها باستخدام طريقتنا وسجلت الأخطاء المطلقة في الحل العددي لكلتا الطريقتين في الجدول(2).

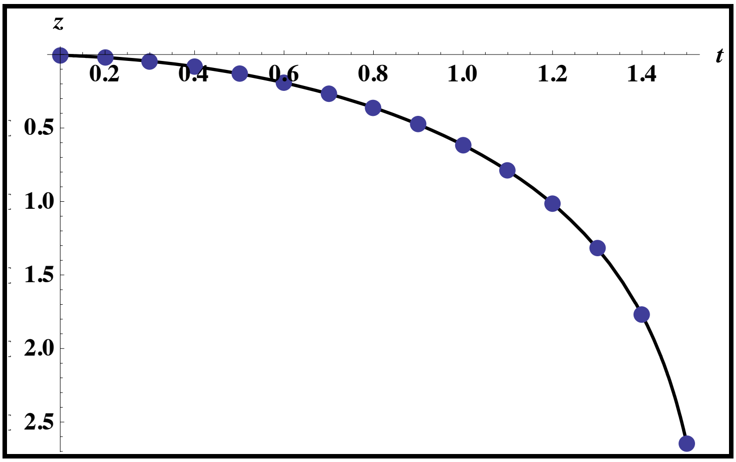
نرسم في الأشكال(11)-(16) على الترتيب الحل الشرائحي مع الحل التحليلي بالإضافة إلى الأخطاء في الحل الشرائحي للمسألة (2) بخطوة h=0.1 . وبمقارنة نتائج طريقتنا مع نتائج صيغة التفاضلات التراجعية وطريقة رانج-كوتا (Marz & Tischendorf, 1994) في المجال [0.6,1.5] نجد أن طريقتنا أكثر دقة.

الجدول(2) مقارنة الأخطاء المطلقة بطريقة البحث مع طريقة في Marz & Tischendorf, (1994) للمسألة (2)

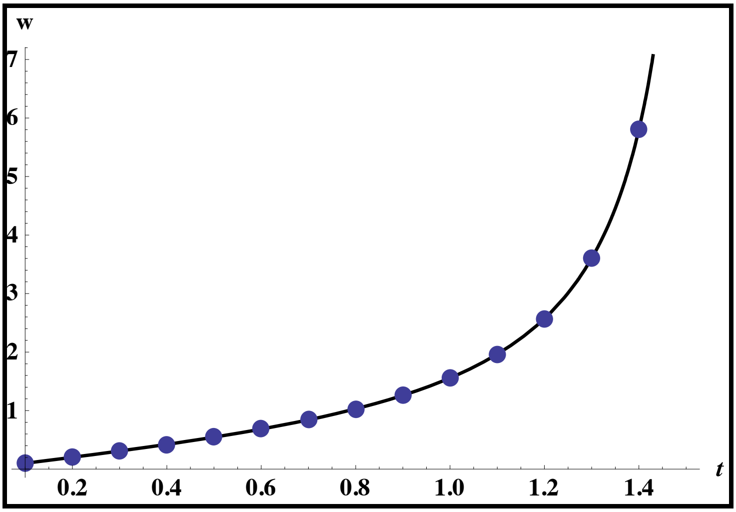
	صيغة التفاضلات التراجعية وطريقة رانج-كوتا[8]			طريقتنا الشرائحية $z_1=0.86,\ z_2=0.9;\ z_3=0.94;\ z_4=0.99$		
	δy_1	δy_2	δy_3	δy_1	δy_2	δy_3
0.6	0.8933E-11	0.109 E-10	0.120 E-08	8.525959E-14	3.26673 E-13	2.21676 E-13
0.7	0.4033E-09	0.5273 E-09	0.7393 E-09	9.724691E-14	4.0204 E-13	2.58017 E-13
0.8	0.729E-09	0.105 E-08	0.2023 E-08	1.082755E-13	4.91455 E-13	3.1095 E-13
0.9	0.940E-09	0.151E-08	0.5053 E-08	1.182353E-13	6.01496 E-13	3.90574 E-13
1.0	0.105E-08	0.1943 E-08	0.2683 E-08	1.270178E-13	7.43417 E-13	5.17097 E-13
1.1	0.115E-08	0.2533 E-08	0.5033 E-08	1.345229E-13	9.3785 E-13	7.33666 E-13
1.2	0.121E-08	0.3353 E-08	0.8443 E-08	1.406899E-13	1.22786 E-12	1.14968 E-12
1.3	0.122E-08	0.4573 E-08	0.1763 E-07	1.454344E-13	1.71932 E-12	2.10943 E-12
1.4	0.110E-08	0.6483 E-08	0.3853 E-07	1.487463E-13	2.76759 E-12	5.2254 E-12
1.5	0.5603E-09	0.7913 E-08	0.112 E-06	1.506101E-13	6.73368 E-12	3.01815 E-11



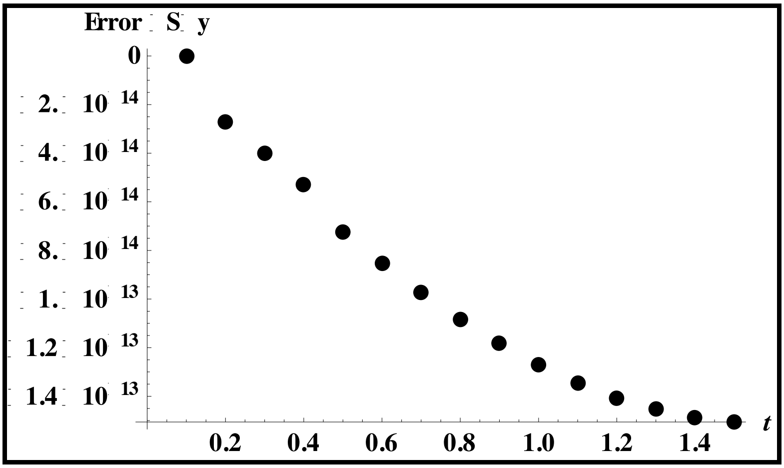
الشكل(11) الحل الشرائحي ●●●● مع الحل التحليلي ـــــ لـ y للمسألة (2) بخطوة h=0.1 .



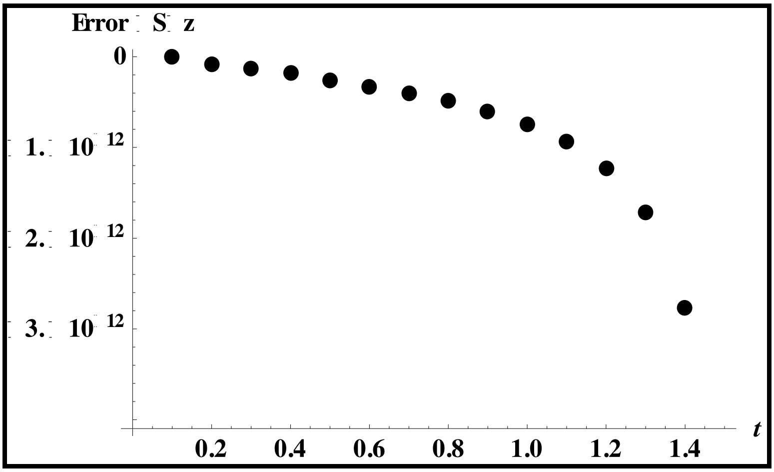
الشكل(12) الحل الشرائحي ●●●● مع الحل التحليلي ـــــ لـ z للمسألة (2) بخطوة h=0.1 .



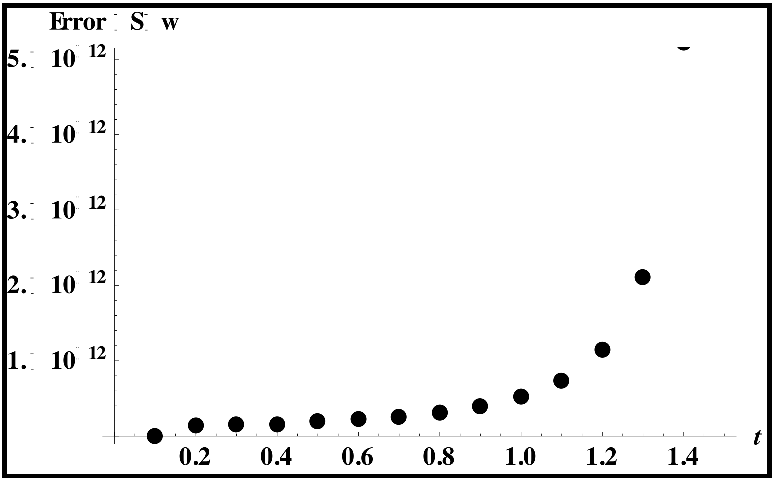
الشكل(13) الحل الشرائحي ●●●● مع الحل التحليلي ــــــ لـ w للمسألة (2) بخطوة h=0.1 .



الشكل(14) الخطأ في الحل الشرائحي لـ y للمسألة (2) بخطوة h=0.1 .



الشكل(15) الخطأ في الحل الشرائحي لـ z للمسألة (2) بخطوة h=0.1 .



الشكل(16) الخطأ في الحل الشرائحي لـ w للمسألة (2) بخطوة h=0.1 .

<u>المسألة(3):</u> منظومة هايسينبيرغ [6-7]:

$$y' = t\, z^2 + w + g_1(t)\,,$$
$$z' = t \exp(y) + t \;\; w + g_2(t)\,, \quad t \in [0, 4]$$
$$0 = y + t\, z + g_3(t) \;\; ,$$

تخضع للشروط الابتدائية:

$$y(0) = z(0) = w(0) = 0$$

حيث تعطى الدوال $g_1(t), g_2(t), g_3(t)$ بحيث يتحقق الحل التحليلي:

$$. \, , \;\; z = t/(1+t)\,, \;\; y = \log(1+t) \;\; w = t/(1+t)$$

ندرج في الجدول (3) نتائج الأخطاء المطلقة في الحل الشرائحي لطريقتنا، وندون في الجدول(4) نتائج الأخطاء المطلقة لطريقة أدميان المعدلة(Hosseini, 2006) وطريقة التجميع الشرائحي في (Mahmoud, 2010). ونرسم في الأشكال(17)–(22) الحل الشرائحي مع الحل التحليلي بالإضافة إلى الخطأ المطلق في الحل الشرائحي للمسألة (3) بخطوة h=0.2. وبمقارنة نتائج طريقتنا مع نتائج الطريقتين (Hosseini, 2006; Mahoud, 2010) نجد أن طريقتنا أكثر دقة.

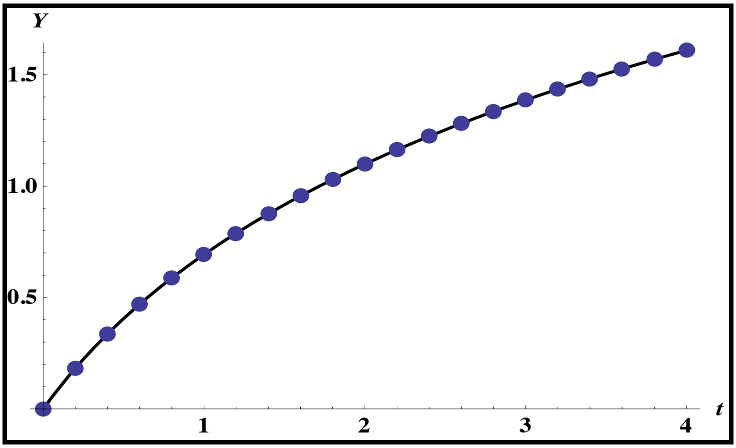
الجدول(3) الأخطاء المطلقة باستخدام طريقتنا الشرائحية للمسألة (3) في المجال [0,4]

t	**z_1=0.86, z_2=0.9; z_3=0.94; z_4=0.99, h=0.2**		
	Error=|S-y|	**Error=|S-z|**	**Error=|S-w|**
0.2	2.3325313E-12	1.16626625E-11	1.18379639E-11
0.4	4.3148262E-12	1.07870601E-11	1.05750463E-11
0.6	5.2415516E-12	8.73590644E-12	7.11877778E-12
0.8	5.79838399E-12	7.24796334E-12	3.49885120E-12
1.0	4.651712348E-12	4.65171234E-12	2.71449529E-15
1.4	2.32640573E-12	1.66171520E-12	2.21118678E-12

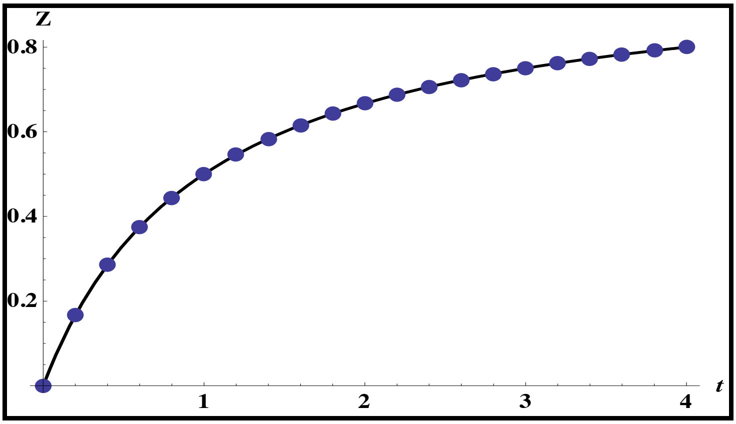
t	z_1=0.86, z_2=0.9; z_3=0.94; z_4=0.99, h=0.2		
	Error=|S-y|	Error=|S-z|	Error=|S-w|
1..8	6.249667450E-13	3.47200046E-13	1.03271835E-12
2.0	8.1998852152E-13	4.09994260E-13	1.72269976E-12
2.4	4.805045250E-13	2.00217620E-13	1.29136701E-12
2.8	4.894085137E-13	1.74793512E-13	1.60389479E-12
3.0	5.0048853950E-13	1.66822111E-13	1.76392234E-12
3.4	6.350253656E-13	1.86772819E-13	2.54680720E-12
3.8	7.999823026E-13	2.10531592E-13	3.58566509E-12
4.0	8.665068662E-13	2.16637818E-13	4.1119552E-12

الجدول(4) الأخطاء المطلقة للمسألة (3) في المجال [0,1]

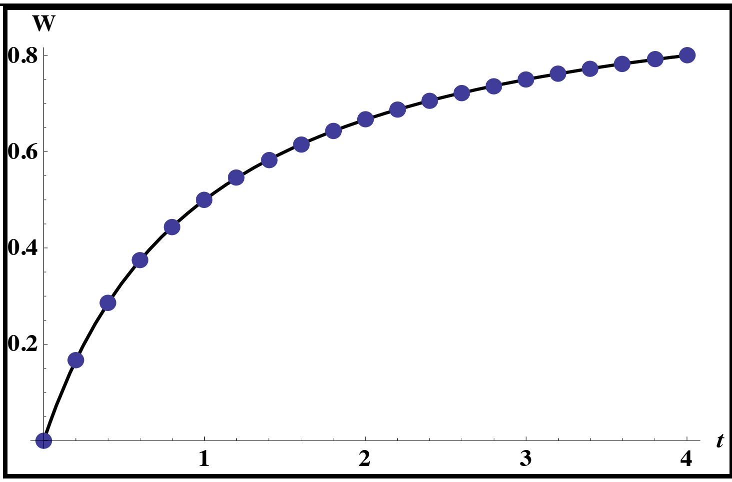
t	Adomian decomposition method [6]			Quintic C^2- Spline Collocation Methods for c_1=0.5, c_2=0.9998 [7]		
	Error=|S-y|	Error=|S-z|	Error=|S-w|	Error=|S-y|	Error=|S-z|	Error=|S-w|
0.2	4.63777E-7	1.16056E-7	8.92432E-6	2.06748E-10	1.03374E-9	1.01819E-9
0.4	2.40711E-4	1.06358E-4	4.25255E-3	4.82894E-10	1.20723E-9	1.12924E-9
0.6	9.34963E-3	5.59329E-3	1.44694E-1	6.48861E-10	1.08143E-9	8.14168E-10
0.8	1.25531E-1	9.18675E-2	1.58743	6.76113E-10	8.45141E-10	3.43036E-10
1.0	9.41377E-1	8.00027E-1	8.62456	5.93930E-10	5.93930E-10	6.03585E-11



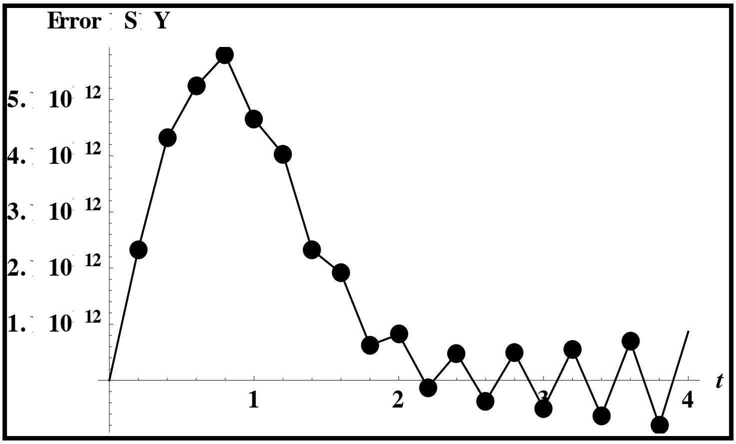
الشكل(17) الحل الشرائحي ●●●● مع الحل التحليلي ـــــ لـ y للمسألة (3) بخطوة h=0.2 .



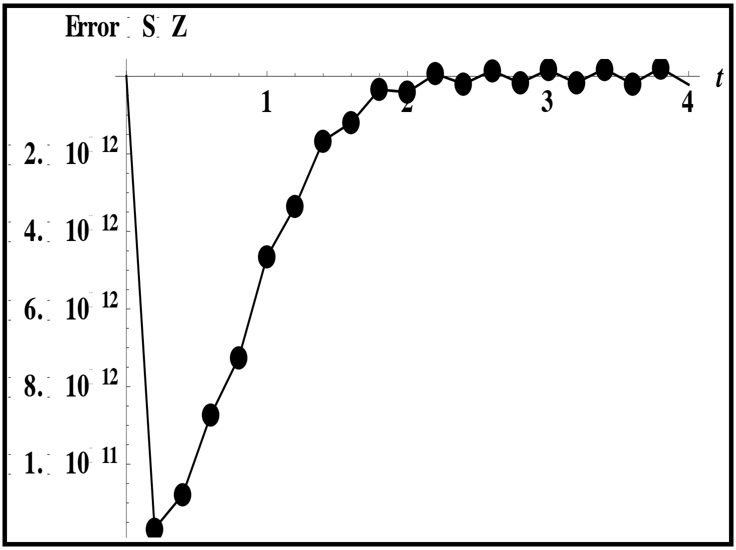
الشكل(18) الحل الشرائحي ●●●● مع الحل التحليلي ـــــ لـ z للمسألة (3) بخطوة h=0.2 .



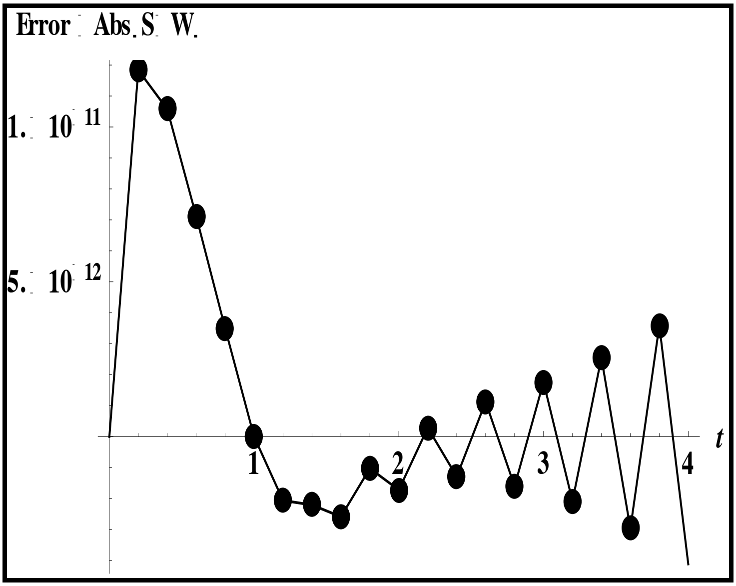
الشكل(19) الحل الشرائحي ●●●● مع الحل التحليلي ــــــ لـ w للمسألة (3) بخطوة h=0.2 .



الشكل(20): الخطأ في الحل الشرائحي لـ y للمسألة (3) بخطوة h=0.2 .



الشكل(21) الخطأ في الحل الشرائحي لـ z للمسألة (3) بخطوة h=0.2 .



الشكل(21) الخطأ في الحل الشرائحي لـ w للمسألة (3) بخطوة h=0.2 .

الاستنتاجات والتوصيات: Conclusions and Recommendations

تم تطوير طريقة تجميع شرائحية بنجاح للحل العددي لمنظومات المعادلات التفاضلية الجبرية غير الخطية. بينت الدراسة أن الطريقة المقترحة مستقرة ومتناسقة ومتقاربة من الرتبة التاسعة.

تم اختبار فعالية ودقة الطريقة بحل ثلاث مسائل محلولة بطرائق أخرى مختلفة في المراجع Hosseini, 2006; Mahmoud, 2010; Marz & Tischendorf, 1994; Ren & (Wang, 2017)

تشير النتائج المدرجة في الجداول(1)–(3) من خلال المقارنات إلى أن طريقتنا أكثر دقة من طريقة صيغ التفاضلية التراجعية المعممة (Marz & Tischendorf, 1994) ، طريقة تقريبات بادي في (Gao & Jibag, 2007) ، طريقة أدوميان المعدلة(Hosseini, 2006) ، طريقة شرائحية بثلاث نقاط تجميع (Mahmoud, 2010) . كذلك تبين الأشكال (1)–(21) أن طريقتنا المقترحة تستطيع تقديم حل شرائحي يتطابق إلى حد كبير مع الحل الدقيق.

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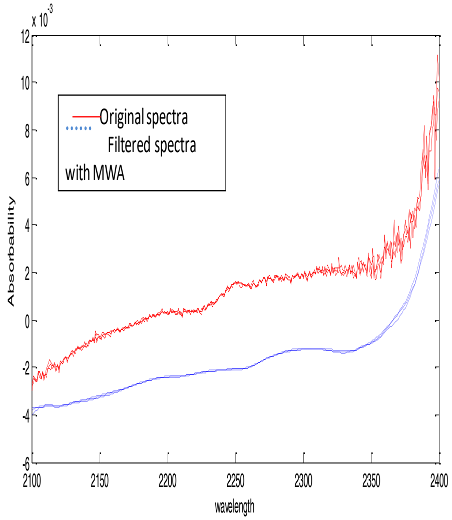
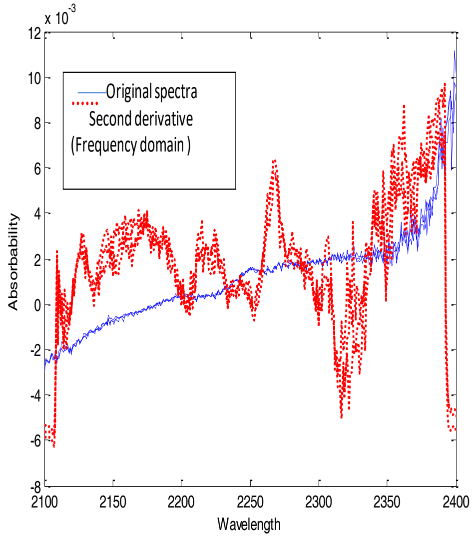
6. Conclusions

This work investigated the effect of different preprocessing techniques on the prediction ability of the ICR model of Glucose concentration. Spectral pre-processing techniques were used to remove the baseline variations and high frequency noise components. The optimization process is done with no prior information available regarding the spectra. The results show an improvement of the capability of proposed models to predict the glucose concentration from aqueous solution with high clinical accuracy. The BPF filter gives the minimum SEP with the high correlation coefficient R^2.

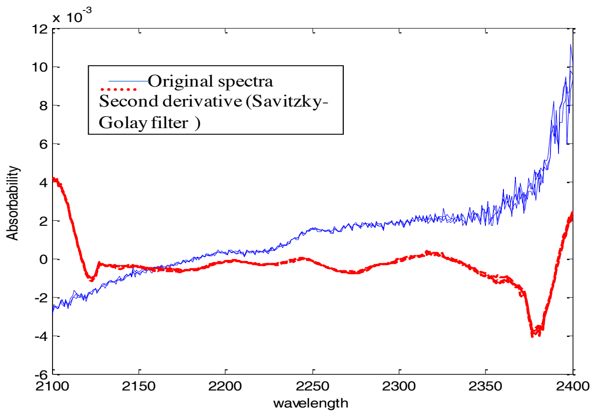
Each one of the proposed techniques has its relative advantages and limitations. Thus, work can be carried out to find the improvement in the performance by combining them in the future with the ICR model in the qualitative and quantitative analysis of the NIR spectra. It is important to select the parameters of the calibration models accurately in order to control the instrumental and temperature variations which will enhance the performance of any calibration model.



(c)



(d)

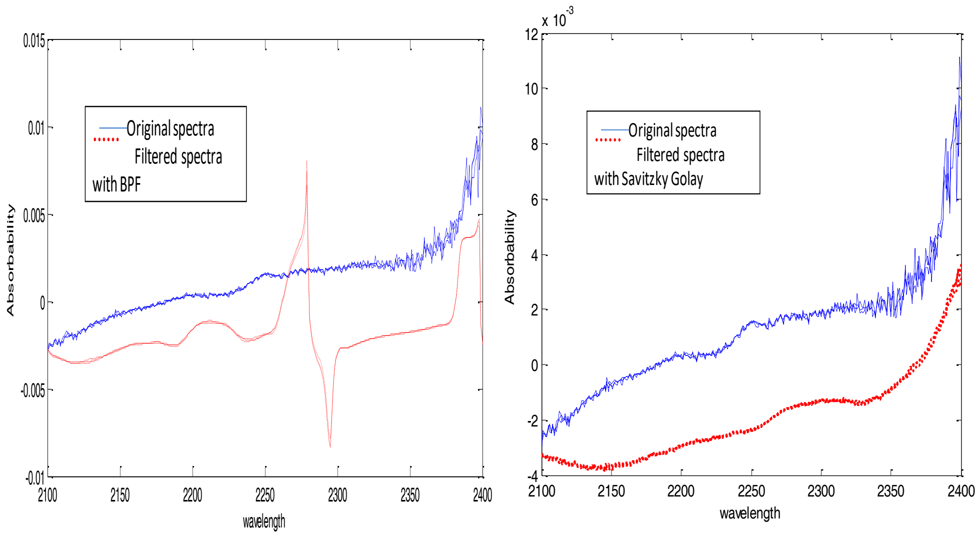


(e)

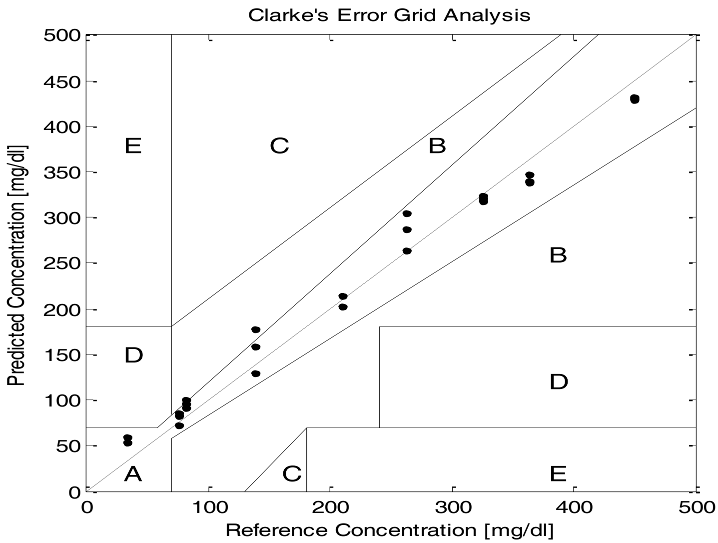
Figure (4) Illustration of the effect of using the preprocessing methods: (a) MWA (b) Savitzky Golay filter (c) BPF filter (d) second derivative (e) second derivative based on Savitzky-Golay filter on the replicate absorbance spectra of the sample that was prepared with glucose concentration=179 mg/dL,

spectra so the glucose absorption bands at wave numbers 4400 cm^{-1}, 4300 cm^{-1}, and 4700 cm^{-1} are clearly observable. Moreover, figure (4) shows that the difference between the replicate spectra is reduced to a very small value compared to raw spectra, and this confirms the fact that the proposed models are capable of suppressing most of the baseline variations.

The second derivative based on Savitzky- Golay filter produces a SEP of 14.61 while using the second derivative based on frequency domain produces a SEP of 16.56. On the other hand, the computation and the optimization process of the second derivative based on the frequency domain is easier compared to Savitzky- Golay filter.



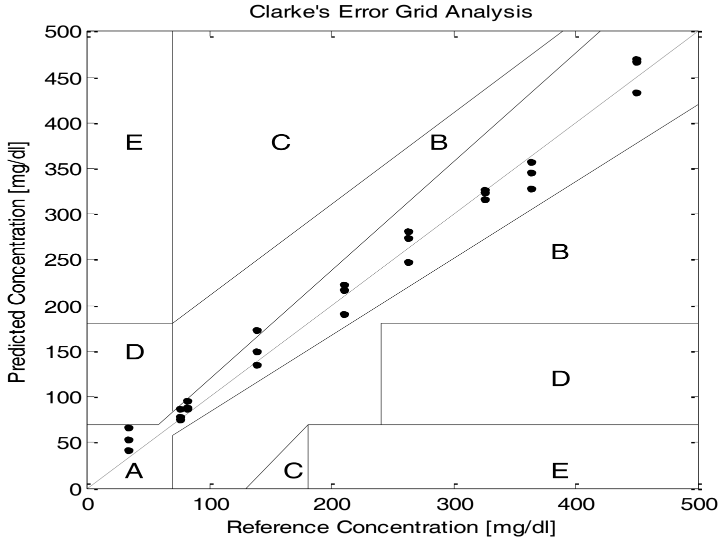
(a) (b)

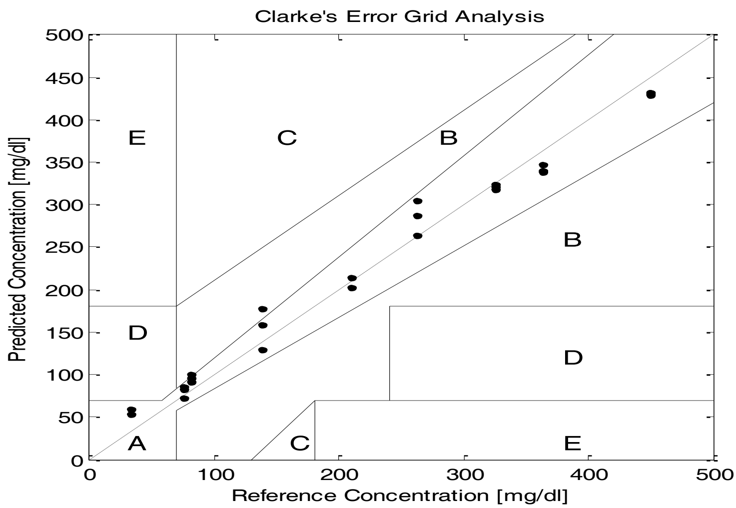


(g)

Figure 3 The Clarke plot of predicted glucose concentration versus the actual concentration of the testing data that results from the optimal models of (a) ICR (b) ICR -MWA (c) ICR - Savitzky- Golay filter (d) ICR -BPF filter (e) ICR - second derivative and MWA (f) ICR -second derivative and Golay filter (g) ICR -second derivative based on Savitzky- Golay filter.

The replicate original spectra of the of the sample that was prepared with glucose concentration = 179 mg/dL before and after preprocessing methods and mean centering were plotted in figure 4. Figures (4 a-b) reveal that the MWA and Savitzky–Golay filter only smooth the raw spectra without any change in their profiles, while the second derivative and BPF filter change the appearance profile of the raw spectra as shown in figures (4 c-e). Using the second derivative and BPF filter enhance the resolution of the resultant


Clarke's Error Grid Analysis
Predicted Concentration [mg/dl]
Reference Concentration [mg/dl]
E
C
B
B
D
D
A
C
E
0
50
100
150
200
250
300
350
400
450
500
0
100
200
300
400
500


Clarke's Error Grid Analysis
Predicted Concentration [mg/dl]
Reference Concentration [mg/dl]
E
C
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D
D
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0
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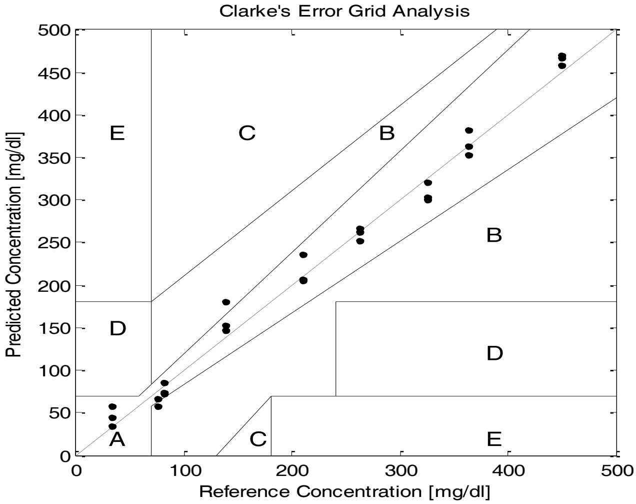
300
400
500

(e) (f)


Clarke's Error Grid Analysis
Predicted Concentration [mg/dl]
Reference Concentration [mg/dl]
0
100
200
300
400
500
0
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150
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250
300
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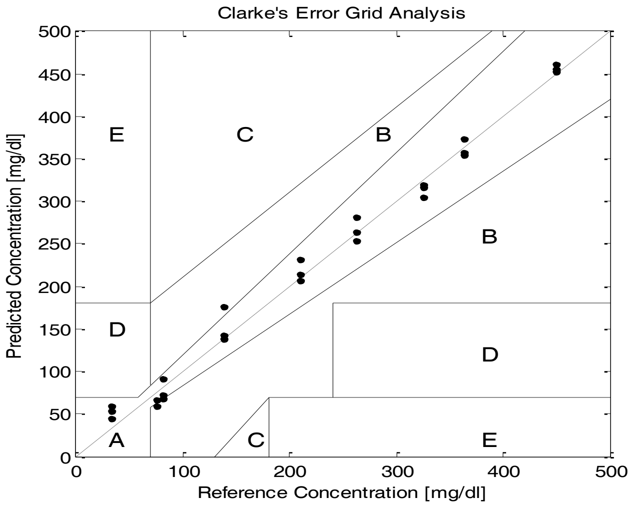
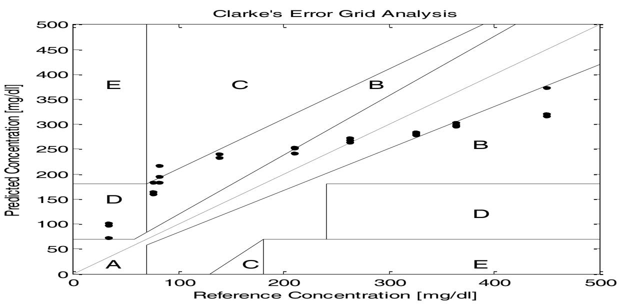
400
450
500
A
B
B
C
C
D
D
E
E

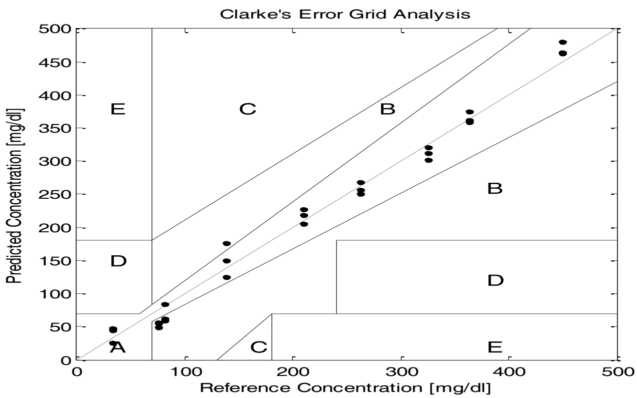

Clarke's Error Grid Analysis
Predicted Concentration [mg/dl]
Reference Concentration [mg/dl]
0
100
200
300
400
500
0
50
100
150
200
250
300
350
400
450
500
A
B
B
C
C
D
D
E
E

(c) (d)

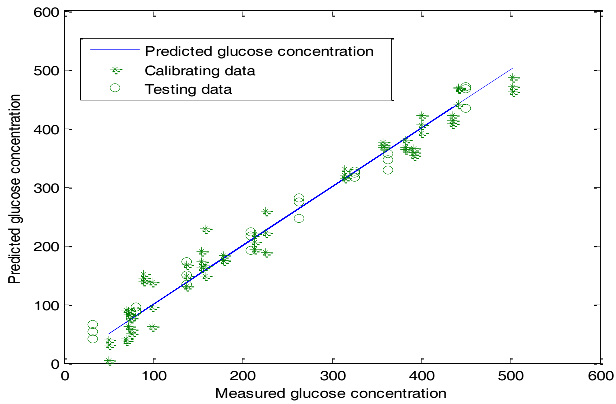
all the proposed models in this work as shown in figure 3. Figure (4a) shows that most of the predicted values of concentration for the ICR model are in region B and D, which are not clinically accepted.

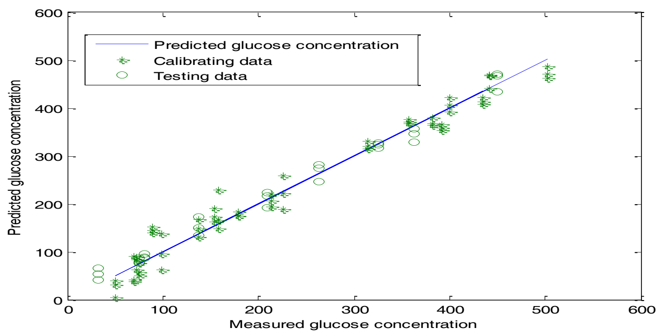
Figures (4 b-g) display the Clarke plots for the optimum ICR model combined with the proposed preprocessing methods in this work. These figures illustrate that all of the predicted glucose concentrations of the testing samples are in region A of Clarke plot, which indicates that the model is medically accurate. It shows that the prediction ability of the proposed model is consistent for low and high concentration levels. They also demonstrate the ability of the proposed model to suppress most of the variations between the replicate spectra of the same sample.





(a) (b)

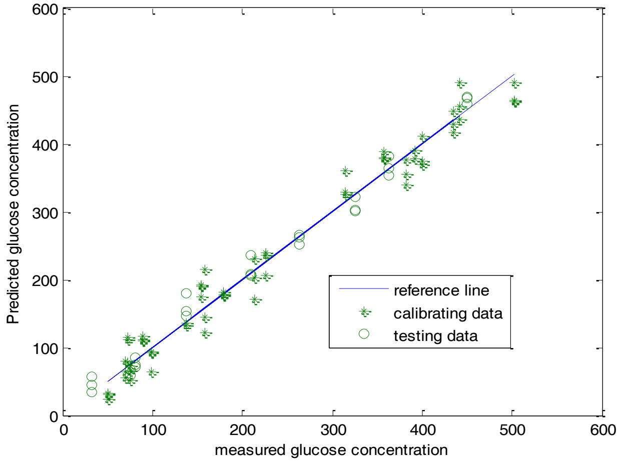


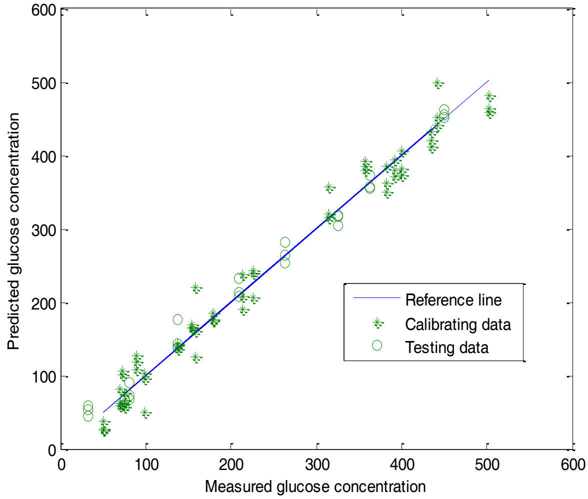


(e) (f)

Figure 2 The predicted glucose concentration versus the actual concentration of the test and training data resulted from the optimal ICR model (a) that employs 17 factors (b) combined with the MWA (c) combined with the Savitzky- Golay filter (d) combined with the BPF filter (e) combined with the second derivative and MWA (f) combined with the second derivative and Golay filter.

The predicted glucose concentration based on the recommendation of the American Diabetes Association, should be within ±15% of the reference value in order to be clinically accepted (Shaw et al. 2006). In order to clarify these requirements and to show the negative impact of resultant scattering on the predicted concentration of glucose the Clarke error grid is plotted for

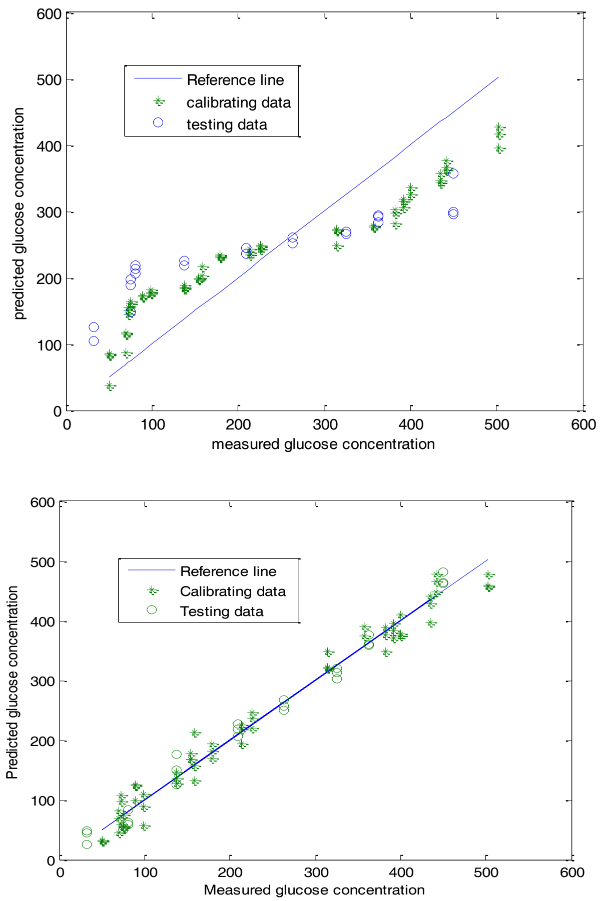

Predicted glucose concentration
measured glucose concentration
0
100
200
300
400
500
600
reference line
calibrating data
testing data


Predicted glucose concentration
Measured glucose concentration
0
100
200
300
400
500
600
Reference line
Calibrating data
Testing data

(c) (d)

derivative and MWA, and ICR combined with the second derivative and Golay filter.

Table 1 and figure 2 show that the best preprocessing method is the BPF filter where the SEP of the ICR model is decreased to 14.07, and correlation coefficients is increased from 0.842 to 0.9898. The ICR model combined with the second derivative and Savitzky Golay filter is the second best preprocessing method. using the MWA filter produces a good SEP and at the same it has low computation complexity and it is easy to implement compared to the other studied techniques.



(a) (b)

Table (1) Summary of optimal model results

No.	Model	SEP	R^2	MMPE	No. of ICA factors	Optimum parameters
1	ICR	79.78	0.842	66.13	17	-
2	ICR-MWA	16.47	0.9876	12.76	18	MWA length=12
3	ICR-Golay	16.08	0.9868	11.188	19	Order of poly.=3, window length=39
4	ICR-BPF	14.07	0.9898	12.56	17	Center freq.=0.0181 BW=0.01
5	ICR-2nd derivative based on freq. domain and MWA	16.56	0.9875	12.99	16	MWA length=9
6	ICR-2^{nd} derivative based on freq. domain and Golay	18.89	0.9884	15.11	19	Order of poly.=3, window length=39
7	ICR-2^{nd} derivative based on Golay filter	14.61	0.9893	8.879	17	Order of poly.=4, window length=55

Figure 2 shows the predicted glucose concentration versus the reference glucose concentration of the training and testing data for the optimal ICR, ICR combined with the MWA, ICR combined with Savitzky-Golay filter , ICR combined with the BPF filter, ICR combined with the second solution. Urea and triacetin are used to model the urea and triglycerides in blood, respectively. The glucose concentration of the prepared samples ranged from 20 to 500 mg/dL. The concentrations of the Glucose were selected to be higher than its physiological range in blood. The samples were placed on infrared quartz cuvette with a fixed path length of 1 nm. Three spectra were collected for each sample without removing the sample from the spectrometer in a double beam mode. The collected data spanned the spectral region from 2000 nm to 2500 nm (4000-5000 cm^{-1}) with a spectra resolution of 1nm. The collected spectra were divided randomly into two sets, each set spanned the whole range of concentration. The first set contains the three replicate spectra of 20 samples and was used to build the calibration model. The second set was used in the prediction phase to test the calibration model and contains the triplicate spectra of 10 samples.

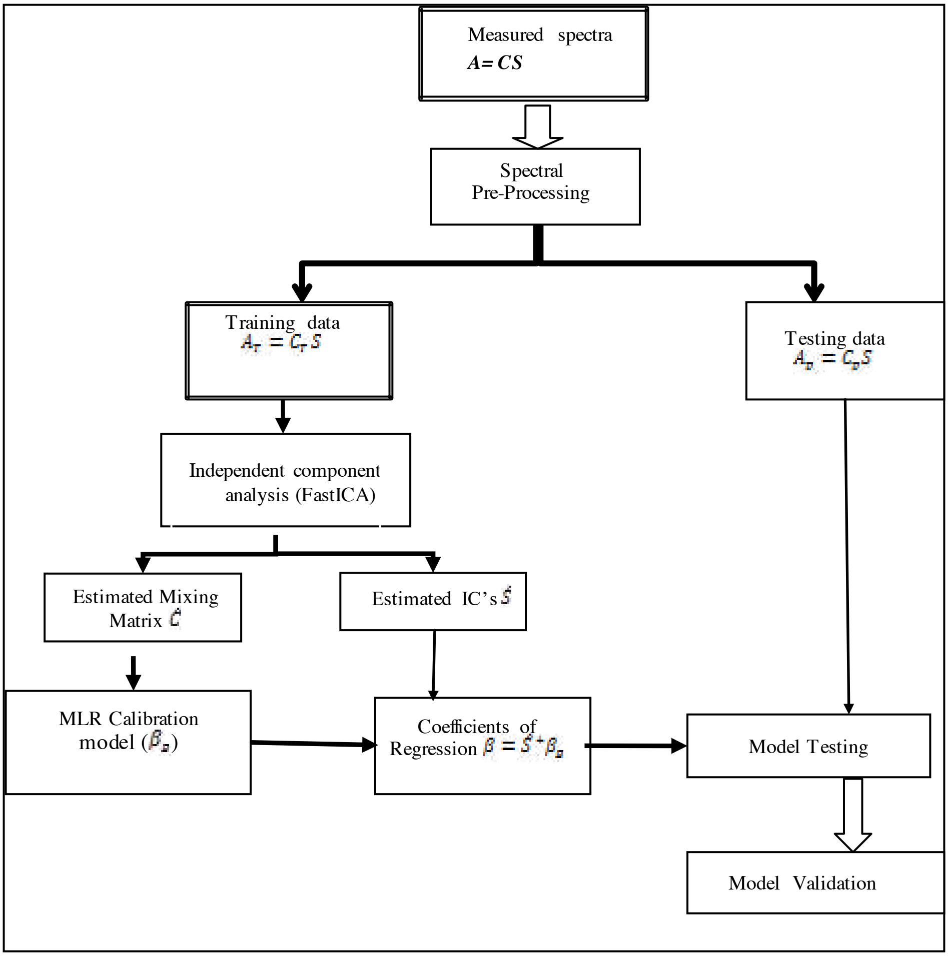
5. Results and Discussion

Various ICR calibration models were developed by combining different preprocessing techniques with the ICR regression model. The SEP, the MMPE, R^2 and the Clarke plot were used to evaluate the capability of the ICR model to predict the Glucose concentration from the processed spectra.

The grid search optimization method is used to select the optimum parameters of the proposed methods.

The obtained optimal models for the ICR model combined with different preprocessing methods are listed in Table 1. It shows that the SEP of the ICR model without any preprocessing method was 79.78 with 17 ICA factors. The table shows that all of the used preprocessing methods in this work improve the perdition ability and accuracy of the ICR model and this is also verified in figure 2.

Figure (1) The ICR Model Combined with Preprocessing Technique



4. Experimental Data

The spectra were collected with a Fourier transform spectrophotometer (spectrophotometer cary 5000 version 1.09), in which a total of 90 NIR spectra were collected for a 30 mixtures of a simulated biological matrix prepared by dissolving glucose, urea and triacetin in a phosphate buffer method (MWPLSF) and the simple difference method (Chau et al. 2004), which computes the derivative in frequency domain (Kauppinen et al. 1981, Bush 1974, Zhang et al. 2002, Horlick 1973).

The order of the derivative and the SNR of the original spectra are the two factors that controls the resolution enhancement rate of the absorbance spectra. Applying the derivative increases the high frequency components and thus degrades the signal to noise ratio of the raw spectra. To improve the SNR of the differentiated spectra, smoothing of the raw spectra should be done prior to the derivative. Several methods of smoothing filters can be used to reduce the effects of random noise (Lam et al. 1981). In this work the second derivative is computed in the frequency domain and combined with the MWA and the Savitzky-Golay filters (Savitzky, 1964).

The n^{th} derivative based on the frequency domain is computed by multiplying the Fourier transform of the spectrum by a complex linear ramp $(j\omega)^n$, and then, the Inverse Fast Fourier Transform (IFFT) of the multiplier output is computed (Horlick 1973, Wabomba et al. 2003, Frenich et al. 1986, Sauke et al. 2005). Computing the derivative in the frequency domain is direct, fast, simple, and does not require complex tables.

The whole process of prediction of the ICR method combined with the preprocessing methods is shown in figure 1.

filters have the advantage that the output is measured by a finite sum of the input values without any feedback of past or future outputs. This makes the implementation and construction of the filter simpler and more stable.

In the MWA filter, a window of size 2t+1 is defined. The smoothed points s_i^* of the 1×m raw spectrum are defined by the following expression:

$$s_i^* = \frac{1}{2t+1}\sum_{-t}^{t} s_{i+j} \qquad (8)$$

Where s_i^* is the ith smoothed point, s_{i+j}^* is the raw spectrum points, i = t+1, t+2,…,m-t-1 and j = -t,…,0,…t. Then, the window is moved by one point to calculate the smoothed point i+1. Each time the window moves by one point until the original spectrum is scanned and smoothed. The MWA is unable to smooth the first and last t points of the raw spectrum. The effect of using the MWA on the quality of the raw spectra is strongly related to the window size.

The Savitzky-Golay filter is used widely in smoothing processes (Chau et al. 2004). It is used to eliminate the high frequency components of noise without distorting the spectrum features like the peaks, relative amplitudes and width. It weighs the moving average filter output, at the same time it regresses the output against local polynomial with order k. The Savitzky-Golay filter has to optimize the polynomial order and the window size so that the original spectra are smoothed well.

Derivative applies mathematical functions to reduce the scattering effects and to enhance the resolution of the spectra. It is also applied for removing baseline effects and enhancing spectral differences. The first derivative enhances the resolution and determines the peaks while the second derivative removes the constant and linear background, it enhances the sharp bands, reduces the overlapping, eliminates the baseline variation (Chen et al. 2001) and produces inverse peaks at the original peaks or shoulders (Kauppinen et al. 1981, Bush 1974).

Several methods can be used to compute the derivative of the NIR spectroscopy such as the Moving Window Polynomial Least Squares Fitting frequency domain (Arnold et al. 2005 b, Small et al. 1993) and time domain as well (Ham et al. 1997, Al-Mbaideen et al. 2010). In time domain filtering, Chebyshev or Butterworth filter are used. Time domain filtering process is obtained by convoluting the measured spectra with the unit impulse response function of the required filter.

BP filtering process is based on the frequency domain. It is achieved by multiplying the Fast Fourier transformation of the measured spectra by a truncation function (window) with desirable characteristics. Then, the inverse Fast Fourier transform is computed to reconstruct the signal to its original absorbance spectra.

Time domain filtering can be used for the on-line filtering process and has better computational efficiency compared to the frequency domain filtering. However the construction and optimization of the frequency domain filter is simpler and easier as compared to the time domain filtering. The design and optimization of the BPF filter parameters should be combined with the PLS regression model, as the nature of the high and low frequency noise are not known. The Grid Search Optimization method was used to select the optimal parameters of the filter (Arnold et al. 2005 b, Small et al. 1993).

Smoothing process is also used to improve the signal-to-noise (SNR) ratio of the raw spectra by eliminating the influence of the high-frequency components of the raw spectrum (Burns et al. 2008). It is considered as a type of low pass filters and computed in time domain by convolving the measured spectra with the selected smoothing function (Ando, 2005). Various methods have been developed and introduced to smooth the spectra, such as the moving window average smoothing filter (MWA) and the Savitzky-Golay filter which will be used in this paper.

MWA filter is used to reduce the random noise while keeping the sharp step response at the same time. It computes the weighted average of the adjacent points of the input signal to produce each point in the output signal. The MWA Filter is a type of the finite impulse response (FIR) filters. FIR pseudo-inverse of the estimated independent components from the ICA model. The matrix $\hat{S}^{+}\beta_{g}$ can be indicated as β. The regression coefficients β then can be used to predict the unknown concentration at once from the spectra without the requirement of decomposing the testing spectra using ICA.

$$C_{gnew} = (A_{new} - \bar{A})\beta + \bar{C}_{g} \quad (7)$$

The regression coefficient matrix β in the last two equations shows the contribution of each IC's to the concentration of all constituents made by the rows of β.

Practically, ICR algorithm uses only statistically independent sources to extract the ICs from the mixtures. ICA deals with noise-free data, while the collected spectra are distorted with high-frequency noise and baseline variations. The chemical and physical interaction between the components and the ambient factors can correlate the sources. These restrictions prevent the ICA method from extracting information related to the analyte of interest accurately. Thus, the quality of the raw spectra must be improved before applying the ICA algorithm.

3. Spectral Data Pre-Processing

To improve the accuracy, reliability and prediction ability of the ICR model, different preprocessing techniques are used. These techniques are used to overcome the influence of irrelevant information such as baseline variation and noise.

In this work several preprocessing techniques are used, including Moving average filter, Savitzky- Golay filter, BPF and Second derivative. All the collected spectra were firstly pretreated using mean centering and variance scaling methods prior to applying the preprocessing methods.

BPF is widely used in chemometrics as preprocessing techniques to remove the high-frequency components of noise and baseline variations that effect the NIR spectra (Smith, 2003). BPF filtering can be established in the

Where, W is the demixing matrix. If the extraction process of the independent components of $\hat{S}$ was made correctly, the demixing matrix W will be the reciprocal (inverse) of the mixing matrix C and their product is a generalized permutation matrix.

2. Independent Component Regression (ICR)

ICR combines MLR with ICA and can be used to estimate glucose concentrations from NIR spectra (Puntonet et al. 2004). The mixing matrix and IC's are predicted using ICA. The estimated mixing matrix $\hat{C}$ will, in most, represent the relative concentration level of each component in the mixtures but not their accurate concentration $C_g \propto \hat{C}$ (Chen et al. 2001). That is due to the high overlapping of NIR spectra, baseline variation and the noise in the collected spectra. The MLR calibration model is then generated by regression the estimated mixing matrix $\hat{C}$ against the concentration of the glucose of the training data (Chen et al. 2001, Smith 2003). Thus, the estimated concentration of glucose will be predicted.

$$C_g = \hat{C}\beta \qquad (4)$$

Where: $\hat{C} = W^+$ is the pseudo-inverse of the demixing matrix W. and C_g is the concentration of glucose. The coefficients of regression β can be estimated using the least square method (Geladi et al. 1986). The coefficients of regression β_g that relates the glucose concentration of the training data to the mixing matrix is defined as

$$\beta_g = (\hat{C}'\hat{C})^{-1}\hat{C}'C_g \qquad (5)$$

The coefficients of regression β_g is then used to predict the glucose concentration of the testing data C_{gnew} as

$$C_{gnew} = (A_{new} - \bar{A})\hat{S}^+\beta_g + \bar{C}_g \qquad (6)$$

Where: $\bar{A}$: is the column average of the training spectra. $\bar{C}g$: is the average value of the glucose concentration of the training data and $\hat{S}^+$: is the prior knowledge of the mixture. The function of ICA is to determine the source signals S based only on the information about the mixtures (Hyvarinen et al. 2001, Hyvärinen et al.2000). The noise-free ICA model can be given as (Puntonet et al. 2004)

$$\mathbf{A} = \mathbf{CS} \qquad (1)$$

Where: $A \in \mathbb{R}^{n \times L}$, $C \in \mathbb{R}^{n \times m}$, $S \in \mathbb{R}^{m \times L}$, L is the number of samples, n is the number of mixtures and m is the number of analytes in each mixture. Based on Beer-Lambert's Law, the spectroscopy of the i^{th} mixture can be defined as

$$A_i = C_{i1}S_1 + C_{i2}S_2 + \cdots + C_{im}S_m \qquad (2)$$

Where: A_i: is the NIR spectrum of the i^{th} mixture, i = 1, 2, $\cdots$ n, for n mixtures. C_{ij}: is the concentration of j^{th} component in the i^{th} mixture, j = 1, 2,$\cdots$ m. m is the number of components in each mixture and S_j: is the pure individual spectra for each component.

The ICA model assumes that the collected spectra should be the linear combination of the pure spectrum of the analytes that composed the mixtures. This assumption is satisfied by modeling the collected spectra by the linear region of the Beer's Lambert law. Additionally, the ICA model assumes that the number of collected spectra n should be at least equal to the number of sources L.

The ability of the ICA model to separate the pure spectra of the analytes is based on two assumptions, namely, the spectroscopy of the pure components should be non-Gaussian and statistically independent (Puntonet et al. 2004, Oja et al. 2002).

The most important goal of the ICA algorithm (Puntonet et al. 2004, Oja et al. 2002) is to estimate both of the unknown mixing matrix C and the pure individual spectra $\hat{S}$ from the observed spectra of the mixtures with no-prior information about the mixture. $\hat{S}$ can be given as:

$$\hat{S} = WA \qquad (3)$$

To extract the information about the analyte of interest, the multivariate methods generate a calibration model to find the relationship between the response (absorbance spectra) and the predictors (concentration of the analyte). This calibration model verifies the relation between the absorbance spectra and the concentration of the analyte of interest and then it is used to predict the response of new variables (Amerov et al. 2004, Burmeister et al. 1999, Arnold et al. 2005, Chen et al. 2004, Ham et al. 1997, Cingo et al. 2000).

Previous studies in this field show that the NIR spectroscopy combined with the multivariate regression methods provide good results in the ability of detection of Glucose concentration (Kasahara et. al. 2018). However, due to irrelevant information that corrupt the collected spectra, the accuracy and ability of the prediction model is negatively affected (Geladi et al. 1986, Haaland et al. 1988). Therefore, the preprocessing techniques are used to improve the quality of the raw spectra. Several preprocessing techniques are of common use in literature such as smoothing, filtering, derivative, Standard Normal Variate Transformation (SNV), Multiplicative Scatter Correction (MSC),etc.. However, the difficulty in selecting the appropriate preprocessing method still exists since there is no sufficient or/and irrelevant information that affects the raw spectra (Hyvarinen et al. 2001).

The objective of this work is to investigate the effect of using different preprocessing methods on the prediction ability of the ICR model. ICR has got a great attention as multivariate method in the analysis of the NIR spectroscopy . ICR model is developed based on the independent component analysis (ICA) which is a High Order Statistic (HOS) method. ICR combines ICA with the Multiple Linear Regression (MLR). ICA is a free noise model, therefore, its application in chemometrics is a big challenge for the interested researchers.

1. Independent Component Analysis (ICA)

ICA is a type of Blind Source Separation (BSS) based on a high order statistic (HOS). it separates source signals from their mixtures without a

Introduction:

Near-infrared (NIR) spectroscopy has received a lot of attention in the few past years. It is widely used in biomedical chemistry, environmental analysis and many other fields. NIR spectroscopy has got a great attention in the noninvasive detection of Glucose in blood (Ranaware et. al. 2017). It uses the electromagnetic radiation in the wavelength range of 2.5µm -0.78 µm (4000-12800 cm^{-1}) (Amerov et al. 2004, Burmeister et. al. 1999, Arnold et. al. 2005 a).

The main concept of the noninvasive detection of Glucose using NIR Spectroscopy is to pass a band of NIR radiation through vascular region of body (could be the index finger or the earlobe) to excite vibrations in the constituent molecules and then extract the glucose concentration in the blood from the resulting spectral information, which must be collected with high signal-to-noise ratio (SNR) so that the glucose information is distinguished accurately (Arnold, 1996). Using NIR Spectroscopy, each component of the blood can be determined by its unique response to the NIR radiation that can be defined by the wavelength range, the number of peaks and their positions, and the profile of the spectrum (Han et. al. 2017).

Practically, the isolation of glucose spectra is quite difficult due to several reasons such as; the high overlapping of the spectra of the blood components, the baseline variations resulted from the ambient and instrument variations, and the low concentration of glucose in the blood. Therefore, signal processing techniques must be developed to extract the glucose concentration accurately (Amerov et al. 2004, Burmeister et al. 1999, Arnold et al. 2005, Chen et al. 2004, Ham et al. 1997, Cingo et al. 2000).

Most of the recent studies use multivariate techniques for their ability to analyze large data-sets (Thomas et. al. 1990). These techniques are used in chemometrics to extract the concentration of the analyte from the measured spectra of the samples. Multivariate Regression techniques are used to solve the qualitative or quantitative problems of the measurements of chemical data.

تحسين دقة التنبؤ لنموذج معايرة الانحدار المستقل للمكونات من أجل التحليل الكمي للتحليل الطيفي للأشعة القريبة من تحت الحمراء

آمنة المبيضين

منى الصعوب

ملخص

لقد أظهر الانحدار المستقل للمكونات (ICR) قدرة عالية وواعدة كطريقة سريعة وغير مدمرة في الكشف غير البضاعي للجلوكوز في الدم باستخدام التحليل الطيفي للأشعة تحت الحمراء (NIR). تم في هذا البحث دراسة تأثير العديد من طرق المعالجة المسبقة على نموذج معايرة المكونات المستقلة (ICR) وتحليلها بما في ذلك مرشح متوسط نافذة النقل (MWA)، مرشح سافيتسكي كولي ومرشح تمرير النطاق (BPF) والمشتقة الثانية جنبا إلى جنب مع MWA ومرشح سافيتسكي كولي والمشتقة الثانية على أساس مرشح سافيتسكي كولي. تظهر النتائج تحسنًا واضحًا في قدرة نموذج ICR على التنبؤ بتركيز الجلوكوز في المحاليل المائية. بشكل عام، أعطى مرشح BPF والمشتقة الثانية القائم على مرشح سافيتسكي كولي نتائج أفضل من طرق المعالجة المسبقة الأخرى. الخطأ القياسي للتنبؤ (SEP)، معاملات الارتباط r^2 وخطأ الجذر الوسطي للتنبؤ (MMPE) لـ BPF-ICR هي 14.07، 0.9898 و 12.56 على التوالي.

Improving the Prediction Accuracy of the Independent Component Regression Calibration Model for the Quantitative Analysis of the Near Infrared Spectroscopy

Amneh Al-Mubedeen *

Muna Al-Suoob

Abstract

Independent Component Regression (ICR) has shown promise as a rapid and non-destructive regression method in the noninvasive detection of Glucose using Near-infrared spectroscopy (NIR). In this work, the effect of several preprocessing methods on the independent component calibration model (ICR) was investigated and analyzed including the Moving Window Average filter (MWA), Savitzky Golay filter, Band pass filter (BPF), Second derivative combined with the MWA and Savitzky Golay filter and second derivative based on Savitzky Golay filter. The results show a clear improvement in the capability of ICR model to predict the glucose concentration from aqueous solutions. In general, the BPF filter and second derivative based on Savitzky Golay filter gave better results than the other preprocessing methods. The standard Error of prediction (SEP), correlation coefficients r^2 and root mean square error of prediction (MMPE) for the BPF-ICR are 14.07, 0.9898 and 12.56, respectively.

Keywords: Near-infrared spectroscopy (NIR), Independent Component Regression (ICR), Moving Average filter, Noninvasive, Glucose.

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programs. Finally, further research needed to highlight a clear picture about future readiness to manage any disaster event.

5. Conclusion

The main conclusion of this study is that nursing students be enrolled in a disaster management program were aware of the potential risks of disasters in the community. However, they demonstrated a perception deficit in the area of disaster nursing management. The inclusion of a disaster nursing practical component is urgently needed. Other nursing programs such as postgraduate degrees also need more specialty courses with adequate practical parts. However, according to the university's rules, it is important to note that adding a new part to the curricula requires a four-year wait before it can be added to the study plan, and a long accreditation and approval process is also involved. It is hoped that this study could provide essential data to be used for health programs in Jordan in order to assess the preparedness level of students or future employees. Also, this study has implications related to research on further disaster course development and evaluation of current courses in order to meet the global demand for disaster preparedness. However, further research is needed to provide direction in prioritizing curricula for both undergraduate and postgraduate nursing students. This study showed that the nursing faculty curriculum at mutah university, Jordan includes only a theoretical or non-practical part. However, given the current turbulent global situation, particularly in the Middle East (including Jordan), it appears that there is a need to include a practical component in their future curricula. A significant difference was noted in the disaster perception mean test scores before and after implementation of the educational program ($p < 0.001$). Also, a significant difference was found between the intervention and control groups.

Our results showed that nursing students after the intervention had more positive attitudes toward disaster management, where they were more familiar with local emergency response, triage principles, and the use of equipment, but they were less prepared to engage in a disaster course compared to the control group. This result is consistent with the results of Schmidt et al (2011) regarding the assumption of a caregiver role during a disaster event but not a triage or other managerial role. For any disaster event, our participants reported that they know who to contact, which is consistent with Al Khalaileh et al. (2012), who reported that half of the respondents were aware of the community contacts during disaster events.

We could conclude that the inadequacy of the current educational curriculum plans in both undergraduate and postgraduate levels could be the main reason for nurses' inadequate knowledge and attitudes related to disaster events, but this could be modified to fulfill this need. A simulation intervention targeted to undergraduate students is needed with robust demonstration part in future research to develop appropriate educational and training programs in nursing disaster management. We recommend that health stakeholders in Jordan particularly hospital managers could play an essential role in maintaining and updating nurses' perceptions and attitudes through ongoing training and in-service education in disaster management.

4.1 Limitations

This quasi-experimental study evaluated the effectiveness of educational program on undergraduate nursing students' perception about disaster management. The result does not reflect the other students' opinions such as first year under graduate and post graduate students and non-respondents. Another limitation of this study is the one- time shot survey in one setting which may not reflect opinion change over the time of the students study as time series studies and other national university student who has nursing

However, an integrative review done by Chaffee (2009) revealed that a lack of willingness on the part of healthcare providers to participate in disaster response was associated with concerns about personal safety measures.

Despite the participants, after the intervention, perceived themselves as better prepared for disaster management compared to before intervention, they had more concerns about the need for further practice in disaster response. Our intervention lack of robust demonstration part, and participants viewed integrating a demonstration part could fill full this need and concerns. Before 2011, there were no Jordanian programs or courses, and only few programs in the Western and Asian universities that involved nurses to assist during disaster events (Yin et al., 2011, Al Khalaileh et al., 2012). Nowadays, despite disaster and emergency courses already available in nursing faculties in many of surrounding countries to Jordan that give students the chance to acquire fundamental theoretical information, but are still lacking of demonstrating in the practical part (Baack and Alfred, 2013). Thus, a disaster course in the curricula of undergraduate and postgraduate nursing programs that includes a practical part would assist future nurses in gaining knowledge and skills that could increase their awareness and prepare them for any future disaster event (Schmidt et al., 2011, Markenson and Reilly, 2011, Baack and Alfred, 2013).

Al Khalaileh and colleagues (2012) recommended incorporating disaster management into nursing curricula in Jordanian nursing programs to improve nurses disaster preparedness. Despite the WHO (2009) recommended in that disaster nursing courses should be part of all nursing curricula (WHO & International Council of Nurses, 2009), a descriptive survey of Australian undergraduate nursing curricula (Usher and Mayner, 2011) showed that only few schools in Australia had disaster courses in their curricula, and they only had a theoretical component. Furthermore, a recent study by Öztekin et al. (2016) showed that nurses were unable to respond to many disaster events and were not aware of their workplace emergency disaster plan and did not think they could execute it. Moreover, a study among 1348 American university students showed that they were not well-prepared for disaster management(Schmidt et al., 2011).

perceived disaster training is more necessary to be provided to all healthcare providers compared to in the control group (3.77 vs. 2.74, P =0.018). Students were asked if it is necessary to have a nursing disaster plan in place, and 3.72 (1.02) agreed. However, some students thought that there is no need to know about disaster plans (3.01, SD = 1.09), because they perceived that disaster management is not an essential nursing role (3.08, SD = 1.15).

4. Discussion

Based on the above results and the integration of the results of other previous studies in the field of disaster nursing for healthcare students and professionals, teaching disaster courses to undergraduate (and in the future, postgraduate) nursing students is effective. A positive response was achieved from our sample of 183 nursing students. Implementing disaster educational program have major effects on participants perceptions and attitudes towards disaster. Implementation of such program among wider range of students such as postgraduate students is recommended as a next step.

The results demonstrated that the disaster course could be offered to postgraduate nursing students and even as an educational course for working nurses to increase their competency in this area. This result is consistent with a Chinese study that used the ICN framework (Chan et al., 2010). Generally, participants in this study reported that they were aware of the potential risks in the community, which is consistent with Turkish / Japanese nursing students study who identified examples such as earthquakes and typhoons/hurricanes as potential risks in the area (Öztekin et al., 2015, Öztekin et al., 2016). After the program, participants were more willing and interested to participate as a team during a disaster, which was highlighted in our results and was supported by the results of Chan et al. (2010) whose respondents were willing to act as helpers in disaster event.

I consider myself prepared for the management of disasters	3.29 (1.16)	2.80 (1.22)	0.021
Disaster management is not essential nursing role	3.11 (1.05)	3.08 (1.15)	0.82
Local disaster plans required continues updating	3.45 (1.18)	3.02 (1.23)	0.04
I think it is necessary to have a nursing disaster plan in place	3.72 (1.02)	3.01(1.09)	0.01
Drills should be conducted regularly in nursing faculty	3.19 (1.01)	2. 90 (1.15)	0.04
I'm competent to participate as a team member of disaster management	3.56 (1.01)	3.12 (0.99)	0.032
Willing to participate in continuing education	3.38 (1.08)	3.08 (0.88)	0.01
Training about disaster is necessary for all health care providers	3.77 (1.06)	2. 74 (1.01)	0.018
I feel confident recognizing different need for disaster victim	3.62 (1.06)	3.02 (1.04)	0.021
I have acquired basic knowledge to identify possible disaster threat in my local community	3.11 (1.06)	2.81 (1.01)	0.030
Total Score	49.72 (11.03)	40.02 (9.75)	0.001

In terms of item analysis (Table 4), the students of intervention group became more willing to participate in continuing education about disasters (3.18, SD = 1.08), and they perceived themselves as more competent in teamwork (3.56, SD = 1.01). They felt that confident they could recognize the different needs of disaster victims (3.22, SD = 1.06). In addition, students of intervention group were more interested in future training and

(52.1%) knew the types and phases of disasters, compared to 36.5% of the control group (p = 0.010). The result also showed that 53% of the students knew the disaster plan of their faculty, compared to 34.9% of the control group (p = 0.059). More than half of the intervention group (57.6%) showed that they knew the recommended supplies for disaster events, compared to 35.9% of the control group (p = 0.008). The results of the study also revealed that 64.7% of the nursing students knew who to contact during a disaster event, compared to 50.8% of the control group (p = 0.079).

3.2 Students' attitudes toward disasters

Table 3 presents students' attitude toward disaster management, the total mean score for attitude among intervention group was significantly higher compare to control group after the education program (36.00 vs. 49.72, P = 0.001). In addition to, paired t-test showed significant improvements in students' attitude toward disaster between the pre and posttest (49.72 vs. 40.02, P=0.001) (Table 4).

Table (4) Comparison in participants' attitudes between the study groups

Item	Intervention group Mean (SD)	Control group Mean (SD)	P-Value
I have the required skills for to participate in disaster situations	3.32 (1.11)	3.00 (1.34)	0.001
I do not need to know about disaster plans	3.37 (1.08)	2.97 (1.17)	0.001

Attitude toward disaster management					
Pretest	119	36.00	8.96	11.17	0.001
Post test	119	49.72	11.03		

Chi- squire test was conducted to examine the differences in individual items between the intervention and control groups (Table 2). A significant difference was noticed between the intervention and control groups in most items of perception of disaster preparedness. For example, among the intervention group, 78% were aware of the potential risks in the community compared to 60.91% in control group, (p = 0.033). Also, there was a significant difference in disaster preparation strategies (63% vs. 31.3%, p = 0.001). Significantly high percent of intervention group (68.1%) understood nurses' roles in perception of disaster management compared to lower percentage (25.4%) in control group. Furthermore, the results showed that 63.6% were familiar with local disaster preparation strategies, compared to 40.6% in the control group (63.6% vs. 40.6%, p = 0.008). More than half of students considered themselves prepared for disaster management (67.5% vs. 42.9%, p = 0.001). The same significant result was noticed with students who were familiar with local emergency response (66.1% vs. 41.3%, p = 0.001).

Familiarity with accepted triage principles and know-how regarding personal protective equipment use were exactly the same for the intervention group (66.7%), while for the control group the values were 41.3% (p = 0.001) and 43.8% (p = 0.010), respectively. More than half of the intervention group (59.5%) said that they were familiar with the social and spiritual needs of disaster victims, compared to 34.4% of the control group (p = 0.004).

The data also reflected that less than half of the intervention group (39%) said that they have a personal disaster plan, compared to 31.3% of the control group (p = 0.131). More than half of the intervention group

Item	Intervention group 119 (65%)	Control group 64 (35%)	P= value
Know types and phases of disaster	52.1%	36.5%	0.010
What the disaster plans are at your faculty	53%	34.9%	0.059
Recommended supplies at disaster event	57.6%	35.9%	0.008
Who to contact during the disaster event	64.7%	50.8%	0.079
Practiced disaster drills (mock exercise) at faculty	50.8%	26.6%	0.003
Familiar with Evacuation principles	52.5%	31.3%	0.004
Total Score Mean (SD)	13.83 (4.66)	7.43 (3.37)	0.001

Also, a significant improvement in level of disaster preparedness between the pre and post test, among intervention group, was revealed (6.95 vs. 13.83, P= 0.001) (Table 3).

Table (3) The change in perceived disaster management and preparedness before and after attending the course

Item	N	Mean	SD	t	P-Value
Disaster preparedness perception					
Pretest	119	6.95	3.01	5.90	0.001
Post test	119	13.83	4.66		

Table (2) A Comparison in perceived disaster management and preparedness between the study groups

Item	Intervention group 119 (65%)	Control group 64 (35%)	P= value
Familiar with potential risks in my community	78.2%	60.91%	0.033
Familiar with local disaster preparation strategies	63%	31.3%	0.001
Understand nurses role in disaster management	68.1%	25.4%	0.001
Familiar with local policies of emergency and disaster management	63.6%	40.6%	0.008
Consider myself prepared for disasters management	67.5%	42.9%	0.001
Familiar with the local emergency response	66.1%	41.3%	0.001
Familiar with accepted triage principles	66.7%	40.6%	0.001
Know how to use personal protective equipment	66.7%	43.8%	0.010
Familiar with social and spiritual needs of disaster victims	59.5%	34.4%	0.004
Do you have a personal disaster plan	39%	31.3%	0.131

Table (1) Comparison of participants' characteristics in both groups (N= 183)

	Intervention group (n= 119)	Control group (n=64)	P - value
Age mean (SD)	20.8 (1.5)	20.6 (1.9)	0.752*
Gender:			
Male	28 (23.6%)	22 (34.4%)	0.065#
Female	91 (76.4%)	42 (65.6%)	
Previous disaster course	4 (3.36%)	2 (3.125%)	0.086 #
Academic Years:			
Second year	42 (35.6%)	29 (46%)	0.055#
Third year	34 (28.7%)	24 (38.1%)	
Fourth year	43 (36.4%)	11 15.9%)	

* = P-value of Independent t-test, #= P-value of Chi square

3.1 Perception of disaster preparedness

At baseline, the total score of disaster preparedness for both study groups was quite similar, with no significant differences ($P > 0.05$). After completing the disaster program, both groups completed the questionnaire for the second time, independent t-test showed significant differences between the intervention and control group in the total mean score of perception of disaster preparedness (M=13.83 vs. 7.43, P= 0.001) (Table 2).

2.8 Data Analysis

Standard descriptive statistics including frequencies and percentages were used to describe the characteristics of the sample and the level of disaster management perception and attitudes among nursing students. To examine the effect of the educational program on nursing students' perception and attitudes about disaster management, two main comparisons were conducted. To examine the differences between control and intervention groups unvaried analysis was conducted, independent t test, and ANOVA used. Between groups, a comparison was performed using independent t-tests to assess the difference between students who had or had not attended the program (intervention vs. control group). A within-group comparison was performed using paired t-tests to examine the change in perception level of disaster management and preparedness before and after attending the program. A p value of < 0.05 was considered significant in all statistical tests. The tests were conducted using IBM Statistical Package for the Social Sciences (SPSS, version 21) (IBM Corp., 2012).

3. Results

The questionnaire was completed by 183 nursing students out of 194 students (giving a response rate of 94%). Most students (n= 112, 61%) were in their third academic year with an average age of 20.8 (SD =1.5) (Table 1). The majority of students were female 133 (72.7 %). A total of 119 students (65%) were enrolled in the intervention group and 64 (35%) were in the control group. There were no significant differences between the study groups based on their demographical data (Table 1).

Disaster planning and emergency preparedness; resources and policies of emergency and disaster utilization; principles of disaster nursing and care for patients with trauma; and principles of evacuation, first aid, and triage were included in this course to ensure the emotional, social, and spiritual needs of those affected by a disaster would be met. Definitions of disaster types and phases, disaster management phases, nurses' role in disasters, and Jordanian policies and regulations regarding disasters were also covered. The program was developed by a team of nursing academics with expertise in emergency care and community health. The International Council of Nurses (ICN, 2009) Framework of Disaster Nursing Competencies was the standard framework used in developing the educational program. The person who provided the educational program was not involved in the data collection process.

2.7 Ethical considerations

The study was approved by the Mutah University Ethics Committee. The questionnaires were distributed in classrooms after the trainer and principle investigators had left the room. The students were informed that their participation was completely voluntary, and that their consent was required to participate in the study. In addition, the participants were informed verbally and in writing that: 1) their answers to the questionnaire were kept completely anonymous; 2) there were no apparent risks from participating or negative consequences affected their course marks if they chose not to participate in the study; 3) all research data were stored securely on a researcher's computer or in a locked file box for one year and then destroyed; and 4) the aggregate data results were used for publication in professional journals or reported at professional conferences.

The researchers approached students who were eligible for study during their attendance of lectures during the second semester. Students who were willing to take part and were registered for the disaster course module were considered for the intervention group, and students who were not registered for the disaster course were assigned to the control group. Students who accepted to participate in both groups were asked to sign a consent form and complete the disaster perception questionnaire (considered as pretest baseline). To reduce response bias, participants were asked to drop the completed questionnaire with the consent form into assigned data collection boxes. The researchers were not the instructors of the course, and that the instructors did not know who participated and who did not. After completing the disaster program, 12 weeks after the pre-test had been completed, both study groups participants were asked to complete the post-test questionnaire, which had the same items as the pre-test. To match the pre and post test questionnaire, each participant at pretest was assigned an ID that was used to identify the participants at post test. The participants dropped the completed questionnaire into the assigned boxes, just as with the pre-test.

2.6 Disaster education program

The disaster educational program was conducted over 12 weeks for 3 hours a week. It is a research-based course design program conducted in the faculty of nursing over two days classroom lectures using power point data show and open oral discussion. It aimed to give nursing students an opportunity to acquire the knowledge, and principles required to manage a wide variety of natural and manmade disasters and major incidents, including natural disasters, acts of terrorism, and acts of war, with a strong emphasis on the role of nurses during a time of disaster.

Two main outcomes were evaluated in this study: nursing students' perception and attitudes toward disaster preparedness. Nursing students' knowledge and attitudes were evaluated using a structured self-administered questionnaire that was developed specifically for this study based on previous literature (Al Khalaileh et al., 2012, Chan et al., 2010, Schmidt et al., 2011) . The questionnaire had two sections: the first evaluated students' perceptions of disaster preparedness and included 16 items and were scored as "Yes" = 1 or "No" = 0. A score of 1 is given for each Yes answer, and score of zero is given for question answered no. Total scores range from zero to 16; higher scores indicate a higher perception of disaster preparedness. The second section evaluated students' attitudes toward nursing disaster management. This section contains 12 items with scores ranging from 1 ("strongly disagree") to 5 ("strongly agree"). Total score range from 12 to 60, with higher score indicating favorable attitude of disaster management.

To ensure the clarity of the content of the questionnaire and suitability, the items of the questionnaire was reviewed by a panel of researchers who were specialized in emergency and disaster nursing and academic staff specialized in the field. Culture sensitivity and internal reliability of the questionnaire was tested in a pilot study of 10 students. The final version of the questionnaire was modified based on the feedback from the panel and pilot study. The average content validity index for the knowledge items was ranged from 0.73 to 0.87 and the content validity index for the attitude items was ranged from 0.78 to 0.89.

The Cornbach's alpha for the total score for perception was $\alpha = 0.76$ and 0.83 for the attitudes for the pretest questionnaire and for the post test questionnaire was $\alpha = 0.84$ for the perception and 0.87 for the attitudes.

2.5 Data collection procedure

educational program on nursing students' perception and attitudes towards disaster preparedness and management.

2. Methods

2.1 Design

A non-randomized control group (quasi-experimental) design was utilized to evaluate the effects of an educational program on nurses' perception and attitudes towards disaster management and preparedness. Both pre- and post-intervention measurements as well as non-randomly selected groups were used in this study.

2.2 Setting

The study was conducted in the Faculty of Nursing ("xxx") during the second semester of academic year 2014/2015.

2.3 Sampling

A convenience sample of undergraduate nursing students was approached to participate in the study. Students were initially informed about the study by a poster posted in the nursing faculty. In addition, a brief description of the study purpose was provided by the primary investigator to all students in the lecturing rooms during the break time. Students were considered for participation in the study if they were in at least their second academic year, had not taken a disaster and emergency nursing course module previously, and were willing to participate.

2.4 Measurement

investigation and educational efforts to help theses nurses improve their perception, knowledge, and skills (Al Khalaileh et al., 2012).

This problem is also available among nursing students. For example, a recent Saudian study investigated nurses' knowledge, attitudes, and perceptions regarding disasters and emergency management (Ibrahim, 2014). The researchers approached 252 Saudi nurses; who had lack knowledge and practical skills at an acceptable level, and had little familiarity with disaster management. The researchers recommended that nurses be provided with clearly titled educational and training programs regarding disaster and emergency management. Another Saudi study assessed a sample of 396 military and civilian nurses' perceptions about their knowledge of disaster management. The results showed that their knowledge was moderate and they perceived themselves as unprepared for disaster management (Al-Thobaity et al., 2015).

Schmidt and colleagues (2011) explored 1,348 American nursing students' perceptions of personal and program awareness about disasters. The results showed that nursing students were generally not well prepared for disasters; therefore, the researchers concluded that all students should receive disaster preparedness education as a part of their nursing program. In line with this study, Fung et al. (2009) found that 75% of post-graduate nursing students in Hong Kong were not well prepared for a disaster. Veenema (2013) stated that baccalaureate programs should help nurses to understand their role and participation in a disaster emergency, and preparedness needs to include awareness of environmental risk factors that could affect them and their patients.

Therefore, it is important to identify Jordanian undergraduate nursing students' perceptions of disaster management to provide culturally and socially sensitive information in order to fulfill the Jordanian MOH's disaster management plan. This study sought to evaluate the impact of an

657,000 refugees have been hosted by Jordan as a result of the Syrian revolution (Ghazal, 2017).

The Jordanian Ministry of Health (JMOH, 2012) developed a Jordanian national plan for disaster management. The purpose of this plan is to manage disasters that may occur in different parts of the country. Also, due to the increased frequency of disasters worldwide, the WHO and other global health organizations highlighted the need to expand educational programs on disaster management (National Student Nurses' Association 2011, American Red Cross, 2011). Similarly, several Jordanian studies have recommended that nurses should have educational training in disaster management (Al Khalaileh et al., 2012, Al Khalaileh et al., 2010) . In addition, several international studies and organizations have stressed the need for educational preparation for disasters as a part of basic nursing programs (World Health Organization and International Council of Nurses, 2009, World Health Organization, 2013a).

Nurses are the largest group of health taskforces, and they are considered the first respondents to any natural or manmade disaster. They need to be equipped with the required knowledge and training, and they should be aware of the importance of their role during different stages of a disaster (Mitchell et al., 2012). They should also have positive attitudes toward participation in disaster management as a part of their role and responsibility to their community (Baack and Alfred, 2013).

In the Jordanian context, there is a scarcity of studies that examined the level of disaster preparedness and knowledge of registered nurses. Al-Khalaileh and colleagues (2012) assessed the perception of 474 registered nurses regarding their knowledge of disaster management. The results showed that 65% of the nurses described their current disaster preparation as weak. Also, an unanticipated finding was that 69% of the registered nurses had not received any education about disasters at the undergraduate level. Lastly, the authors recommended further

1. Introduction

A disaster is a natural or manmade event that causes a level of destruction or emotional trauma exceeding the abilities of those affected to respond to without community assistance (World Health Organization, 2013a). There are three main types of disasters: natural disasters such as earthquakes, manmade disasters such as nuclear accidents or acts of terrorism, and hybrids (e.g., bioterrorism) (Veenema, 2009). When disaster strikes, the demand for nurses is much greater than that for other healthcare professionals (Nekooei Moghaddam et al., 2014). Nurses are considered the major professional respondents when a disaster occurs; hence, they need to respond promptly and effectively. Preparing nurses to respond to disasters is essential in reducing loss of life or future health problems. Several studies have explored nurses' experiences and knowledge of disaster management, revealing inadequate training and preparation to respond to a disaster (World Health Organization and International Council of Nurses, 2009, WHO & International Council of Nurses, 2009, Fung et al., 2009), as well as the need for at least a minimum level of disaster nursing training and knowledge (Nekooei Moghaddam et al., 2014). To date, minimum knowledge is available about essential nursing perception and attitudes required to respond at a disaster site. Further, Zinsli and Smythe (2009) have shown that not enough attention is paid to nurses' preparation for disaster management

Although awareness of disaster management has been increasing among health professionals, the concept is relatively new to many nurses in Jordan. Jordan has been fairly safe from natural disasters. The risk of war in the Eastern Mediterranean, however, has left the country in an unstable condition. In 2000, the invasion of Iraq forced around 10,000 refugees to enter Jordan within few months, and this put enormous pressure on Jordanian hospitals (UNHCR, 2017). Recently, more than

مفاهيم وسلوك طلاب التمريض في إدارة الكوارث: دراسة شبه تجريبية

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محمد دار عواد

ملخص

الخلفية الأدبية: إن الحالة العالمية المضطربة الراهنة، ولا سيما في الشرق الأوسط، توجه الانتباه إلى إدارة الكوارث والتأهب لها.

الطريقة: تم استخدام تصميم شبه تجريبي بين 183 طالب تمريض. وتلقت مجموعة التدخل برنامجا تعليميا مدته 12 أسبوعاً. تم تقييم تصورات المشاركين ومواقفهم فيما يتعلق بإدارة الكوارث والتأهب لها قبل وبعد البرنامج بالنسبة للمجموعتين.

النتائج: لوحظ وجود فرق كبير في تصور الكارثة في درجات قيمة المتوسط الحسابي قبل وبعد تنفيذ برنامج التعليم (M = 13.83، SD = 4.66 مقابل M = 6.95، SD = 3.01؛ p = 0.001). كما وجد فرق معنوي في متوسط الدرجة الكلية لإدارة الكوارث والتأهب بين التدخل (M = 13.83، SD = 4.66) ومجموعات السيطرة (M = 7.43، SD = 3.37؛ p = 0.011).

الاستنتاجات: كان طلاب التمريض المسجلين في الكلية على بينة من المخاطر المحتملة لأي كارثة ممكن ان تحدث في المجتمع. ومع ذلك، فإنها أظهرت فقط المعرفة المعتدلة والمهارات الحركية في مجال إدارة تمريض الكوارث. ويمكن زيادة هذا مع المزيد من التدريب التمريضي العملي لتحسين نوعية خريجي التمريض الذين سيعملون في بيئات سريرية مختلفة.

الكلمات الدالة: طلاب التمريض؛ ادارة الكوارث؛ برنامج تعليمي؛ التأهب للكوارث؛ سلوك الطلاب

Nursing Students' Perception and Attitudes in Disaster Management: A Quasi-Experiments Study

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Sultan Musleh

Muhammad Darawad

Abstract

Background: The current tumultuous global situation, particularly in the Middle East, is drawing attention to disaster management and preparedness.

Methods: A quasi-experimental design was used among 183 nursing students. The intervention group received a 12-week educational program. Participants' perception and attitudes regarding disaster management and preparedness were evaluated before and after the program for both groups.

Results: A significant difference was noted in the disaster perception mean test scores before and after implementation of the education program (M = 13.83, SD = 4.66 vs. M = 6.95, SD = 3.01; $p = 0.001$). Also, a significant difference was found in mean total score for disaster management and preparedness between the intervention (M = 13.83, SD = 4.66) and control groups (M = 7.43, SD = 3.37; $p = 0.011$).

Conclusions: Nursing students enrolled in the faculty were aware of the potential risks of a disaster in the community. However, they only demonstrated moderate knowledge and perception in the area of disaster nursing management. This could be increased with more disaster nursing practical training to improve the quality of nursing graduates who will work in clinical settings.

Keywords: Nursing students; Disaster management; Educational program; Disaster preparedness; Students' attitude.

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R is the gas constant (J/mol.K).

T is the absolute temperature (K).

x is the membrane active layer thickness.

xstep is the step-size.

X_d is the effective membrane charge density (mol/m^3).

z_i is the valence of ion (i).

γ_i is the activity coefficient of ion (i) in the membrane.

γ_i° is the activity of ion (i) in the bulk solution.

ϕ is the steric partitioning term.

λ is the stokes radius of component (i) to pore radius ratio.

Ψ is the electrical potential (V).

$\Delta\Psi_D$ is the Donnan potential (V).

known for its limitation and for being more descriptive than predictive, and in-order to overcome these limitations experimental parameters were used. The chosen ions were Na^{1+}, Mg^{2+}, Cl^{1-} and SO_4^{2-} ions. The model was solved for two different feed concentrations, which were 10 and 100 mol/m^3. The membrane active layer thickness was assumed to be equal to 20.0E-6 m, which was obtained from experimental work. For each concentration value, the model was solved for different volume flux values that ranged between 1.0E-7 to 9.0E-6 $m^3/m^2.s$. More work need to be done in-order to improve this method such understanding the physics of solutions and the properties of ions because they have great effect on the nanofiltration separation process.

Nomenclature

c_i is the concentration in the membrane (mol/m^3), the initial solute concentration inside themembrane - at the feed/membrane interface.

C_i is the ion concentration in the solution (mol/m^3).

$C_{i,p}$ is the concentration of ion (i) in the permeate (mol/m^3).

$C_{i,f}$ is the concentration of ion (i) in the feed (mol/m^3).

$D_{i,\infty}$ is the bulk diffusivity (m^2/s).

$D_{i,p}$ is the hindered diffusivity (m^2/s).

F is Faraday constant (C/mol).

j_i is the flux of ion (i) based on the membrane area ($mol/m^2.s$).

J_v is the volume flux based on the membrane area ($m^3/m^2.s$).

$K_{i,c}$ is the hindrance factor for convection inside the membrane.

$K_{i,d}$ is the hindrance factor for diffusion.

node is the number of steps.

r_i is the ion radius.

r_p is the membrane pore radius.

result, anions would pass through the membrane active layer and cations would be rejected. The membrane effective charge supports the higher rejection of anions than the rejection of cations for NaCl solution, Na_2SO_4 solution, $MgCl_2$ solution, $MgSO_4$ solution, and $MgSO_4$ and $MgCl_2$ solution (Afonso and Pinho, 2000).

Except for NaCl and Na_2SO_4 solution, the rejection of Cl^{1-} was higher than the rejection of Na^{1+}. And for Na_2SO_4 and $MgCl_2$ solution the rejections of Cl^{1-} and SO_4^{2-} were Na^{1+} and Mg^{2+}. And for NaCl and $MgSO_4$ solution, the rejection of SO_4^{2-} was higher than Na^{1+}, Cl^{1-}, and Mg^{2+}. The rejection of ions from NaCl and $MgSO_4$ solution, and Na_2SO_4 and $MgCl_2$ solution, is supported by the concentration of ions inside the membrane active layer.

Furthermore, the concentration of the ions inside the membrane active layer decreased as the volumetric flux based on membrane area (J_v) increased (Meer et al., 1996; Song et al., 2011; Song et al., 2013), which supports the increase in the ions rejection as the volumetric flux based (J_v) increases. The previous is true except for NaCl and $MgSO_4$ solution, and Na_2SO_4 and $MgCl_2$ solution.

In the case of mixed solution of NaCl and $MgSO_4$, the concentrations of Mg^{2+}, Na^{1+}, and Cl^{1-} ions inside the membrane active layer increased as it moved from the feed side to the outlet side, while the concentration of SO_4^{2-} inside the membrane active layer decreased as it moved from the feed side to the outlet side.

In the case of mixed solution of Na_2SO_4 and $MgCl_2$, the concentrations of Mg^{2+} and Na^{1+} ions inside the membrane active layer increased as it moved from the feed side to the outlet side, while the concentration of Cl^{1-} and SO_4^{2-} inside the membrane active layer decreased as it moved from the feed side to the outlet side.

Conclusion:

The calculation method for the Nernst-Planck equation was described. The extended Nernst-Planck equation was solved using Euler mathematical method. FORTRAN programme was used to solve the model. This model is boundary conditions that were used, where the rejection increased as the volumetric flux based on membrane area (J_v) increased. Moreover when applying the volumetric flux based on membrane area (J_v) that were used in Bowen et. al. work (Bowen et al., 1998-a; Bowen et al., 1998-b), similar results were obtained with the model that was used in this work.

In the case of mixed salts solution (NaCl and $MgSO_4$), the rejection of SO_4^{2-} increased as the permeate volume flux based on the membrane area (J_v) increased. On the other hand, the rejection of Na^{1+}, Cl^{1-}, and Mg^{2+} decreased as the permeate volume flux based on the membrane area (J_v) increased.

In the case of mixed salts solution (Na_2SO_4 and $MgCl_2$), the rejection of Cl^{1-} and SO_4^{2-} increased as the permeate volume flux based on the membrane area (J_v) increased. On the other hand, the rejection of Na^{1+} and Mg^{2+} decreased as the permeate volume flux based on the membrane area (J_v) increased.

In the case of NaCl solution and Na_2SO_4 solution, the rejection of Na^{1+} was higher than the rejection of Cl^{1-} and SO_4^{2-}. For $MgCl_2$ solution and $MgSO_4$ solution the rejection of Mg^{2+} was higher than the rejection of Cl^{1-} and SO_4^{2-}. For NaCl and Na_2SO_4 solution, the rejection of ions took the following trend $Cl^{1-} > Na^{1+} > SO_4^{2-}$. For $MgSO_4$ and $MgCl_2$ solution, the rejection of ions took the following trend $Mg^{2+} > SO_4^{2-} > Cl^{1-}$. For NaCl and $MgSO_4$ solution, the rejection of ions took the following trend $SO_4^{2-} > Na^{1+} > Cl^{1-} > Mg^{2+}$. For Na_2SO_4 and $MgCl_2$ solution, the rejection of ions took the following trend $Cl^{1-} > SO_4^{2-} > Na^{1+} > Mg^{2+}$ (Bandini, 2005, pp. 75-86).

The rejection behaviour is related to the membrane effective charge, where the membrane effective charge (X_d) was used as a condition to integrate equation (3) to obtain the electrical potential gradient. In addition, the electrical potential gradient was used to integrate the Nernst-Planck equation to obtain the ions concentration inside the membrane and the permeate solution (see equations 4, 5 and 6) (Fievet et al., 2002).

The membrane effective charge was assumed to be negative. Thus repulsion between the membrane charge and anions would occur while attraction between the membrane charge and cations would occur. As a

For Na_2SO_4 and $MgCl_2$ 10 and 100 mol/m^3 solutions, the rejection of ions took the following trend Cl^{1-} > SO_4^{2-} > Na^{1+} > Mg^{2+}. The rejection of Cl^{1-} and SO_4^{2-} had positive values, while the rejection of Na^{1+} and Mg^{2+} had negative values (Figure 17). The concentrations of Na^{1+} and Mg^{2+} ions inside the membrane active layer increased as it moved from the feed side to the outlet side; while the concentration of Cl^{1-} and SO_4^{2-} inside the membrane active layer decreased as it moved from the feed side to the outlet side.

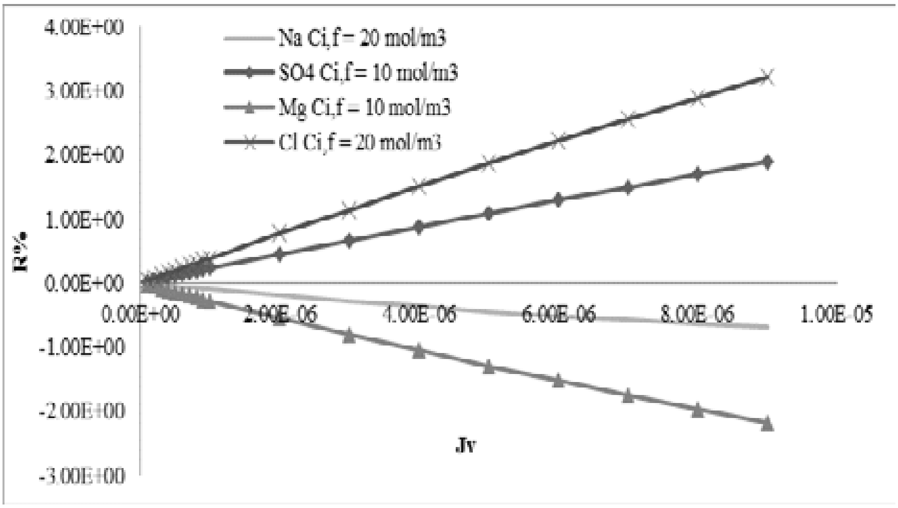

Figure 17. R% of Mg^{2+}, Na^{1+}, SO_4^{2-} and Cl^{1-} versus J_v ($m^3/m^2.s$).

Discussion

The ions rejection increased as the permeate volume flux based on the membrane area (J_v) increased, for NaCl solution, Na_2SO_4 solution, $MgCl_2$ solution, $MgSO_4$ solution, NaCl and Na_2SO_4 solution, and $MgCl_2$ and $MgSO_4$ solution. These results are related to the trans-membrane pressure (TMP), where the theory suggests that the ions rejection would increase as the TMP increases (Peeters et al., 1998; Fievet et al., 2002; Wadley et al., 1995; Song et al., 2011; Song et al., 2013). Similar results were obtained by Bowen et. al. (Bowen et al., 1998-a; Bowen et al., 1998-b) over the

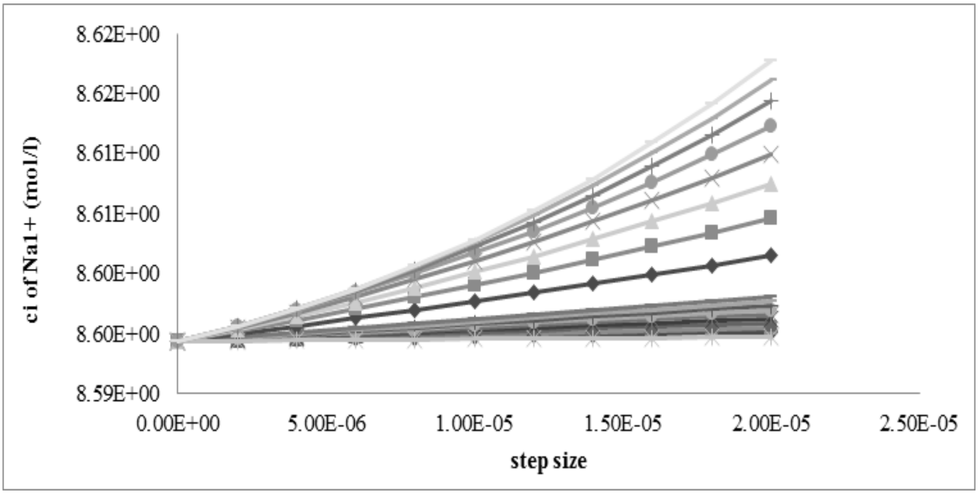

Figure 15. The concentration of Na^{1+} inside the membrane active layer versus step size.

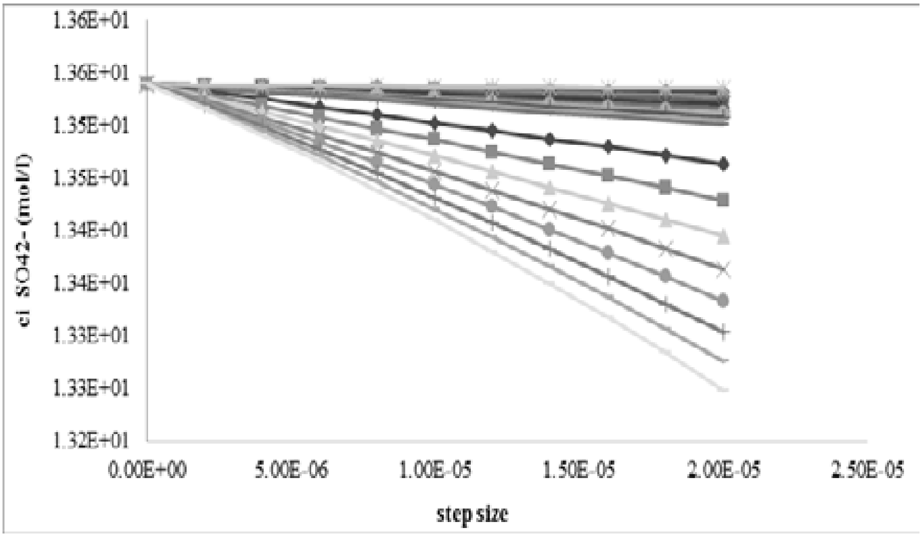

Figure 16. The concentration of SO_4^{2-} inside the membrane active layer versus step size.

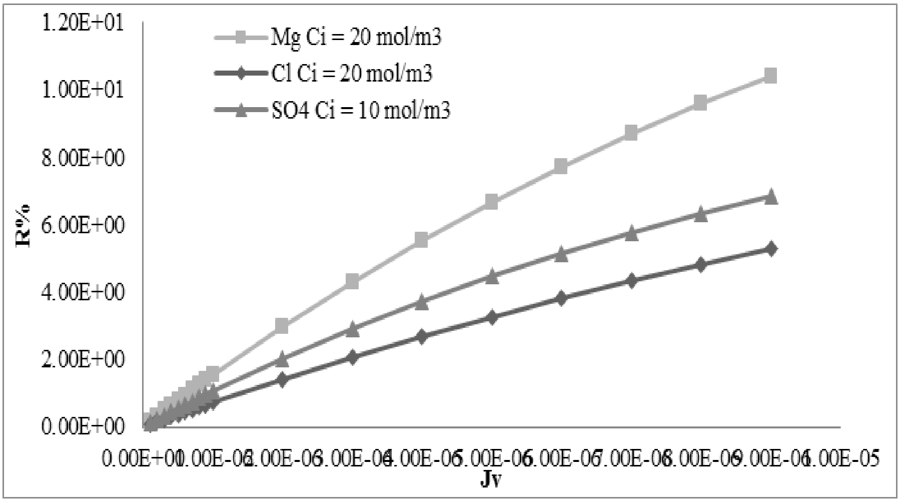

Figure 13-b. R% of Mg^{2+}, Cl^{1-} and SO_4^{2-} versus J_v ($m^3/m^2.s$).

For NaCl and $MgSO_4$ 10 and 100 mol/m^3 solutions, the rejection of SO_4^{2-} was higher than the rejection of Na^{1+}, Cl^{1-}, and Mg^{2+} (Figure 14). The concentration of SO_4^{2-} inside the membrane active layer decreased as it moved from the feed side to the outlet side, while the concentrations of Mg^{2+}, Na^{1+}, and Cl^{1-} ions inside the membrane active layer increased as it moved from the feed side to the outlet side.

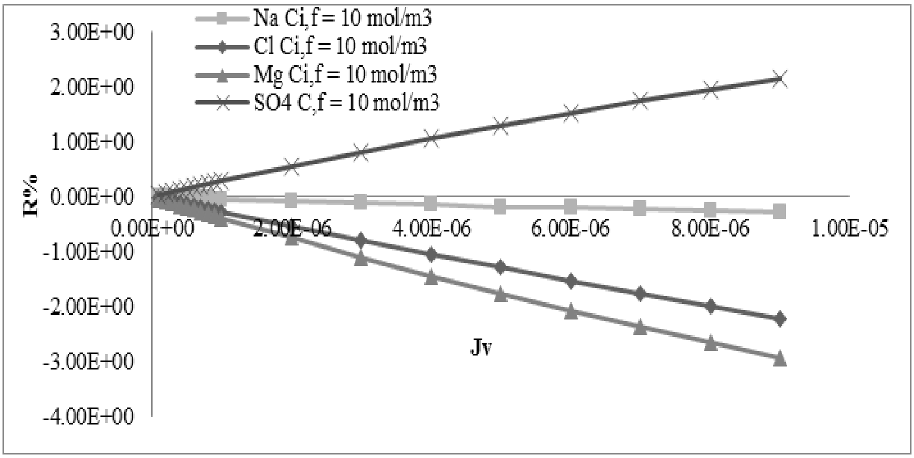

Figure 14. R% of Mg^{2+}, Na^{1+}, SO_4^{2-} and Cl^{1-} versus J_v ($m^3/m^2.s$).

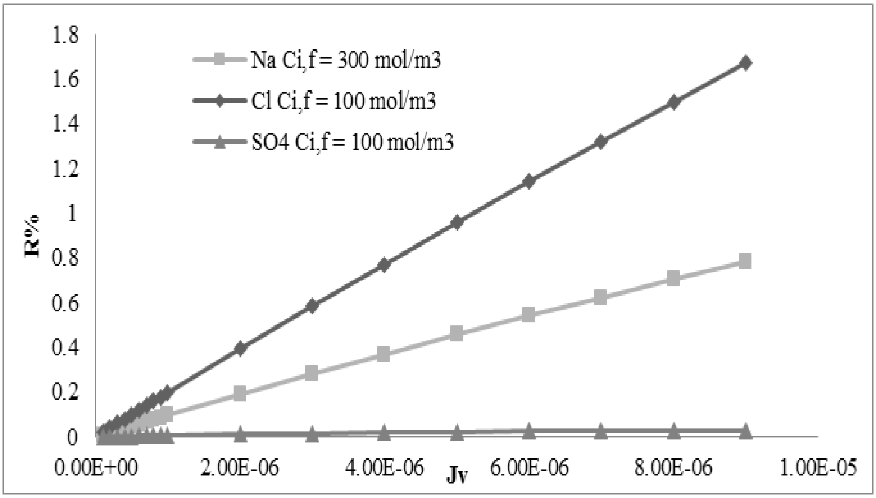

Figure 12-b. R% of Na^{1+}, Cl^{1-} and SO_4^{2-} versus J_v ($m^3/m^2.s$).

For $MgSO_4$ and $MgCl_2$ 10 and 100 mol/m^3 solutions, the rejection of Mg^{2+} was higher than the rejection of Cl^{1-}, and SO_4^{2-}, (Figure 13). The rejection of SO_4^{2+} was higher than the rejection of Cl^{1-}. The concentrations of Mg^{2+}, Cl^{1-} and SO_4^{2-} ions inside the membrane active layer decreased as it moved from the feed side to the outlet side.

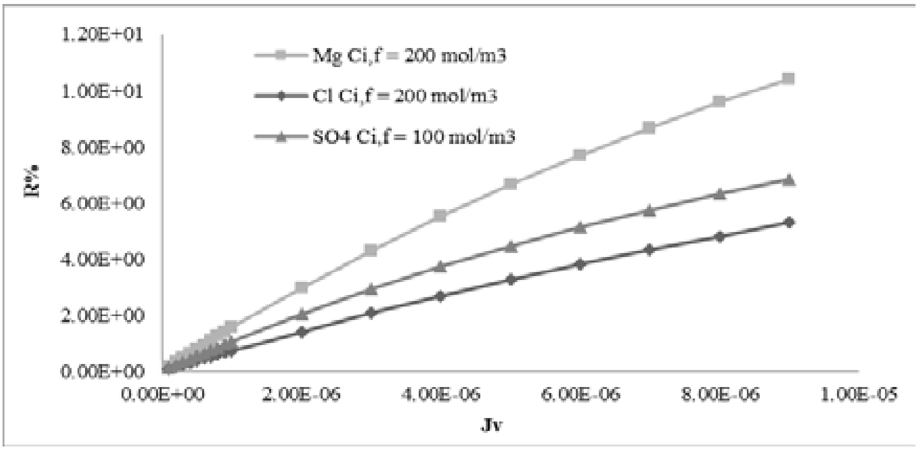

Figure 13-a. R% of Mg^{2+}, Cl^{1-} and SO_4^{2-} versus J_v ($m^3/m^2.s$).

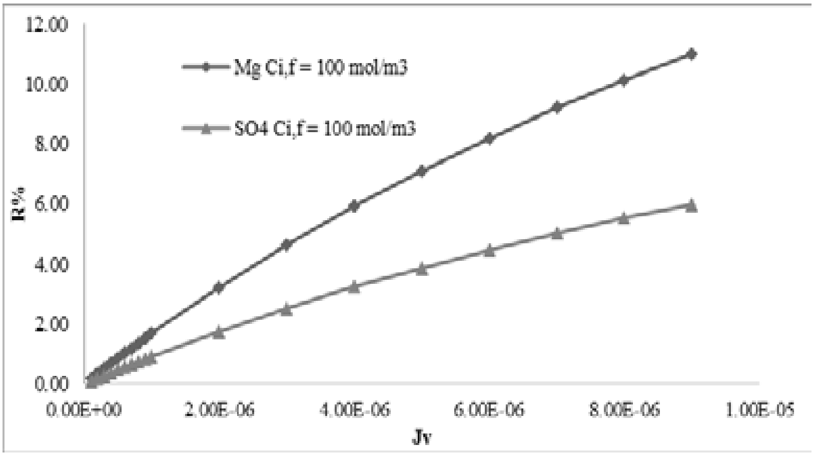

Figure 11-b. R% of Mg^{2+} and SO_4^{2-} versus J_v (100 $m^3/m^2.s$).

For NaCl and Na_2SO_4 10 and 100 mol/m^3 solutions, the rejection of Cl^{1-} was higher than the rejection of Na^{1+} and SO_4^{2+}, (Figure 12). The rejection of Na^{1+} was higher than the rejection of SO_4^{2-}. The concentrations of Na^{1+}, Cl^{1-} and SO_4^{2-} ions inside the membrane active layer decreased as it moved from the feed side to the outlet side.

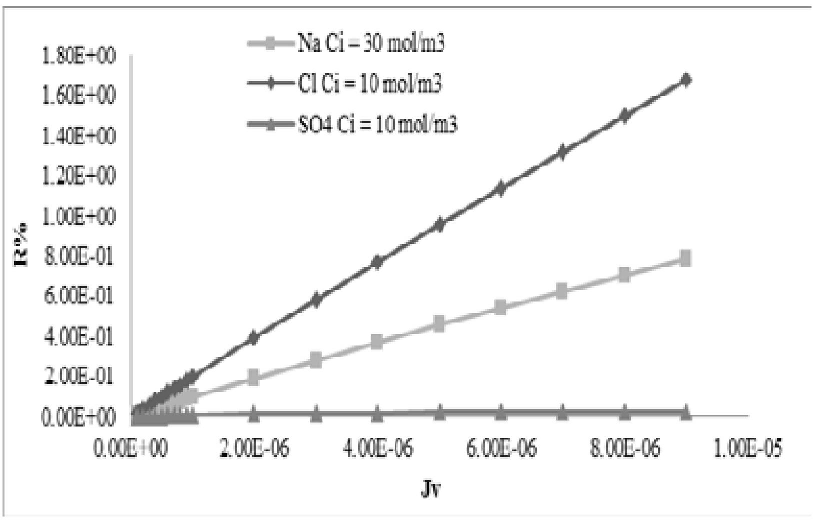

Figure 12-a. R% of Na^{1+}, Cl^{1-} and SO_4^{2-} versus J_v ($m^3/m^2.s$).

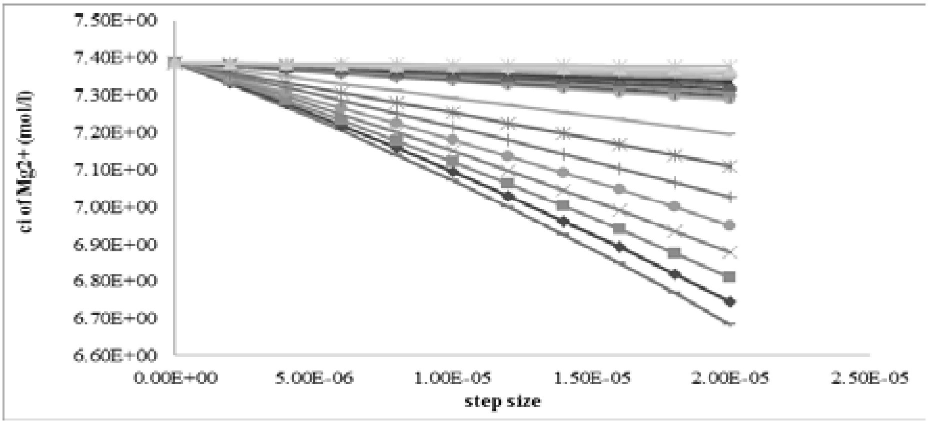

Figure 10. The concentration of Mg^{2+} inside the membrane active layer versus step size.

For $MgSO_4$ 10 and 100 mol/m^3 solutions, the rejection of Mg^{2+} was higher than the rejection of SO_4^{2-}, (Figure 11). The rejections of Mg^{2+} and SO_4^{2-} from 10 and 100 mol/m^3 solutions were almost similar. The rejection of Mg^{2+} was higher than the rejection of SO_4^{2-}. The concentrations of Mg^{2+}, and SO_4^{2-} ions inside the membrane active layer decreased as it moved from the feed side to the outlet side.

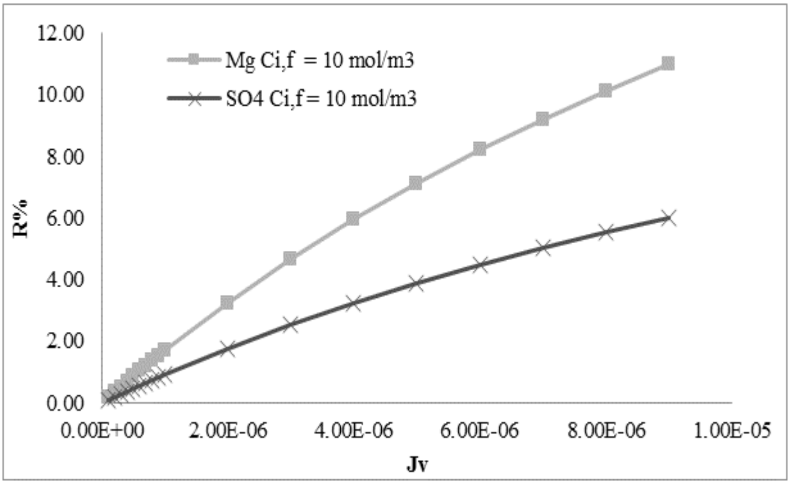

Figure 11-a. R% of Mg^{2+} and SO_4^{2-} versus J_v (10 m^3/m^2.s).

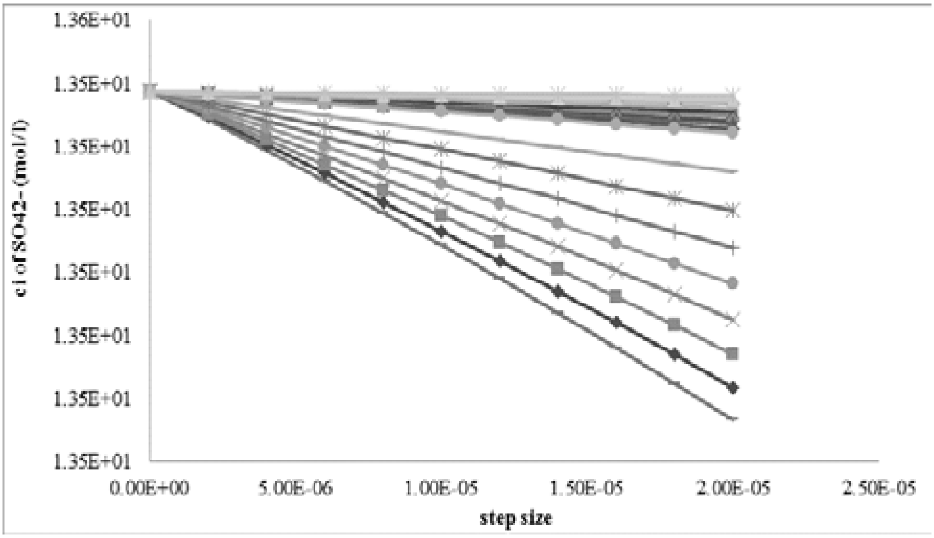

Figure 8. The concentration of SO42- inside the membrane active layer versus step size.

For $MgCl_2$ 10 and 100 mol/m^3 solutions, the rejection of Mg^{2+} was higher than the rejection of Cl^{1-}, (Figure 9). The concentrations of Mg^{2+}, and Cl^{1-} ions inside the membrane active layer decreased as it moved from the feed side to the outlet side.

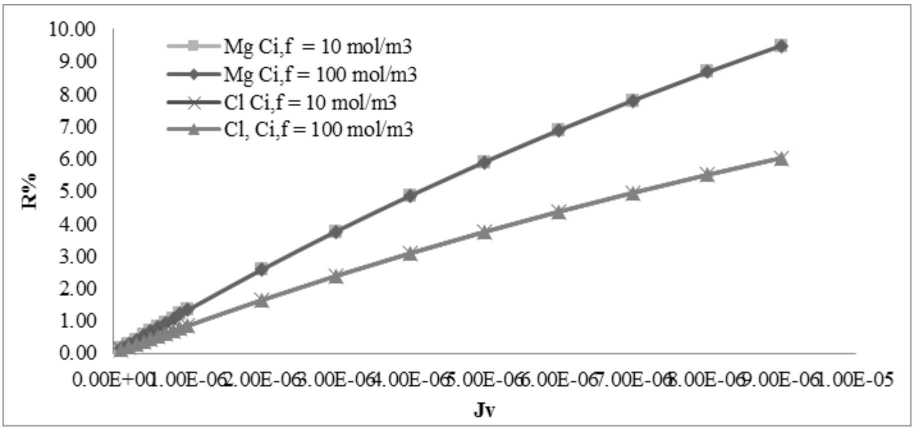

Figure 9. R% of Mg^{2+} and Cl^{1-} versus J_v ($m^3/m^2/s$).

For Na_2SO_4 10 and 100 mol/m^3 solutions, the rejection of Na^{1+} was higher than the rejection of SO_4^{1-} (Figures 6 and 7). The concentrations of Na^{1+}, and SO_4^{2-} ions inside the membrane active layer decreased as it moved from the feed side to the outlet side.

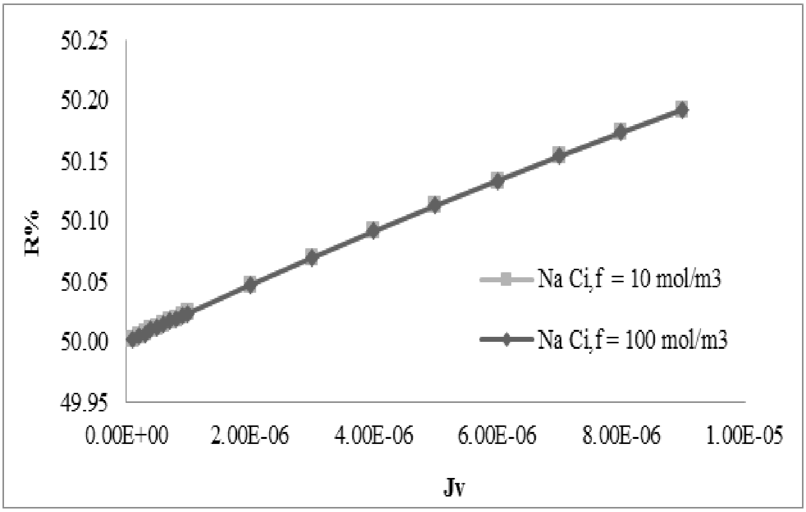

Figure 6. R% of Na^{1+} versus J_v ($m^3/m^2.s$).

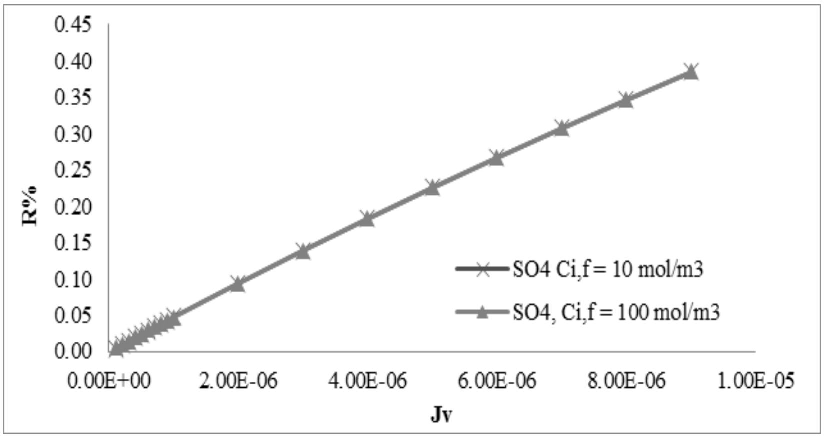

Figure 7. R% of SO_4^{2-} versus J_v ($m^3/m^2.s$).

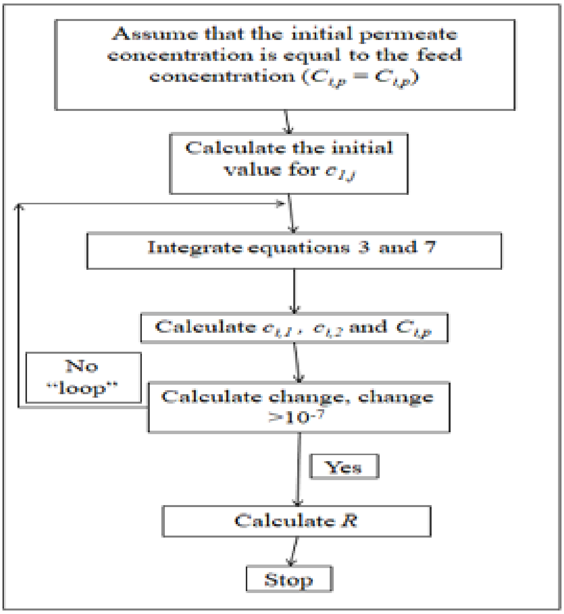

Figure 4. Euler numerical method steps.

Results

For both concentration values - 10 and 100 mol/m^3 - it was noticed that the rejection of ions increased as the volumetric flux based on membrane area (J_v) increased. For NaCl 10 and 100 mol/m^3 solutions, the rejection of Na^{1+} was higher than the rejection of Cl^{1-} (Figure 5). The concentrations of Na^{1+}, and Cl^{1-} ions inside the membrane active layer decreased as moving from the feed side to the outlet side.

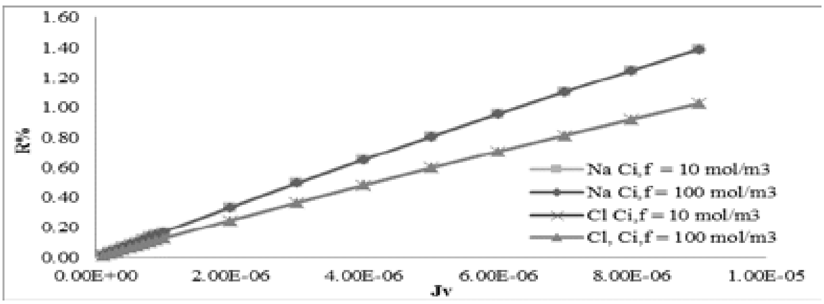

Figure 5. Rejection of Na^{1+} and Cl^{1-} versus J_v ($m^3/m^2.s$).

$$\frac{c_{i,N+1} - c_{i,N}}{\Delta x} = \frac{J_v}{D_{i,p}}\left(K_{i,c} c_{i,N} - C_{i,p}\right) - \frac{z_i c_{i,N}}{RT} F \frac{d\Psi}{dx} \qquad (24)$$

Equation (15) was used to calculate the concentration inside the membrane. Then equation (7) was used to calculate the potential gradient (dΨ/dx), where it was substituted into equation (15) to calculate a new value for the solute concentration inside the membrane. After that, the step-size was assumed to be equal to the membrane active layer thickness over the number of steps (Hajarat, 2010), where the number of steps was equal to 200, as in the following equation

$$(25) \qquad size\ of\ step = \frac{x}{number\ of\ steps}$$

where x is the membrane active layer thickness. The ion concentration inside the membrane active layer changes from $c_{i,1}$ at the feed-solution interface side to $c_{i,200}$ at the permeate-solution interface side. The final concentration inside the membrane was used to calculate the permeate concentration by substituting its value into equation (9). The solute concentration in the permeate is given as

$$C_{i,p} = \frac{c_i}{\exp\left(-\frac{z_i F}{RT}\Delta\Psi_D\right)} \qquad (26)$$

where $C_{i,p}$ is the solute concentration in the permeate solution. The rejection of ions was calculated using equation (10), where the rejection percentage is

$$(27) \qquad R\% = \left(1 - \frac{c_{i,p}}{c_{i,f}}\right) \times 100\%$$

The programme would keep running until the difference between the initial and final permeate concentration would be greater than 1.0^{-7}. If the difference between the initial and final permeate concentration is less than 1.0^{-7}, this would indicate that separation did not occur.

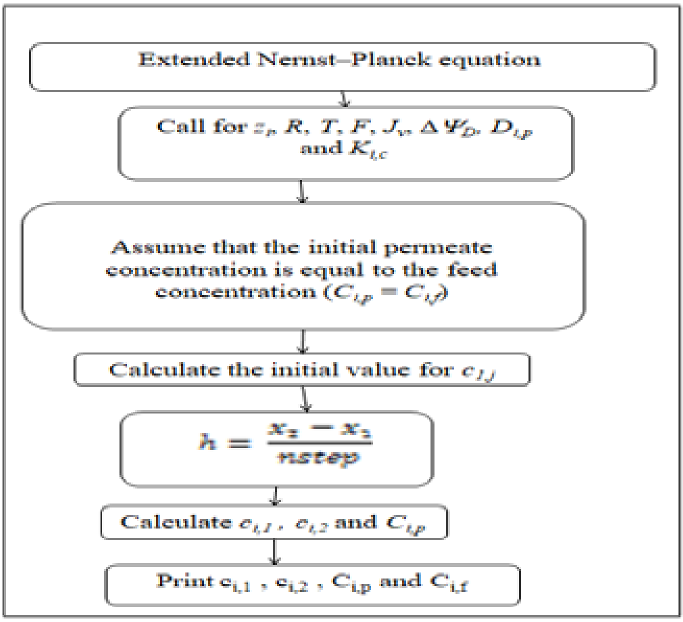

Figure 3. Fortran programme chart.

1.1 Euler's numerical method

At the beginning, the initial permeate concentration ($C_{i,p}$) was assumed to be equal to the feed concentration ($C_{i,f}$) to be able to calculate the initial value of the concentration inside the membrane (c_i), (Schäfer et al., 2005; Hajarat, 2010) (Figure 4). Then equation (9) was rearranged as follows

$$c_i = C_{i,f} \exp\left(-\frac{z_i F}{RT} \Delta\Psi_D \right) \qquad (23)$$

where $C_{i,f}$ is the solute concentration in the feed solution. Equation (14) was used to determine the initial solute concentration inside the membrane (c_i) - at the feed/membrane interface - by using the solute feed concentration. Then equation (3) was written according to Euler's method as follows for the value of the permeate concentration ($C_{i,p}$). As a result, it was assumed that the initial permeate concentration ($C_{i,p}$) was equal to the feed concentration ($C_{i,f}$) which implies that rejection does not take place.

The hindered diffusivity ($D_{i,p}$), the hindrance factor for convection ($K_{i,c}$), and the hindrance factor for diffusion ($K_{i,d}$) were obtained as follows (Labbez et al., 2003; Gao et al., 2007; Bórquez, and Ferrer, 2016; Bowen et al., 1997)

$$D_{i,p} = K_{i,d} D_{i,\infty} \quad (19)$$

$$K_{i,d} = -1.705\lambda + 0.946 \quad (20)$$

$$K_{i,c} = -0.301\lambda + 1.022 \quad (21)$$

where $D_{i,\infty}$ is the bulk diffusivity (m^2/s), and λ is the stokes radius of component (i) to pore radius ratio. The Donnan potential ($\Delta\Psi_D$) was obtained from equation (9) (Labbez et al., 2003; Geraldes and Alves, 2008). The stokes radius of component is obtained from the following equation (Morão et al., 2008)

$$\lambda = r_i / r_p \quad (22)$$

where r_i is the ion radius, and r_p is the membrane pore radius. The thickness of the membrane active layer was considered as the membrane thickness because it is the main part of the membrane where ions separation occurs. In addition, the pore radius of the support layer is larger than the ions radius thus the ions would pass easily through the support layer; as a result, the support layer thickness can be neglected. The solution was assumed to be dilute, as a result the activity coefficient, to be accounted for inside the membrane by the effective membrane charge density, would be equal to unity.

Numerical Calculation Methodology

Nernst-Planck equation was solved by using Euler mathematical method, and the solution was obtained using FORTRAN program, (Figure 3). The program was run for different feed concentrations and permeates flux (volume flux based on the membrane area). The model was solved for NaCl, $MgCl_2$ and Na_2SO_4 solutions at two different feed concentrations, which were 10 and 100 mol/m^3 (Hajarat, 2010). For each concentration value, the model was solved for different volume flux values that ranged between 1.0×10^{-7} to 9.0×10^{-6} $m^3/m^2.s$. The changes in these parameters values were done to observe their effect on the membrane rejection. The membrane active layer thickness was assumed to be equal to 20.0×10^{-6} m (Hajarat, 2010). The concentration, membrane thickness, and volume flux values were obtained from previous experimental work that was done for nanofiltration process (Hajarat, 2010).

Equations (3), (7) and (9) were used to describe ion permeation through nanofiltration membrane. Equations (3) and (7) were integrated across the membrane active layer thickness, where the internal solute concentrations ($c_{i,1}$) is related to the bulk feed concentration ($C_{i,f}$) at the feed/membrane interface and the internal solute concentration ($c_{i,N}$) is related to the permeate concentration ($C_{i,p}$) at the membrane/permeate interface through equation (9).

The feed concentration ($C_{i,f}$) was substituted in Equation (9) in order to calculate the initial concentration inside the membrane ($c_{i,1}$), followed by the integration of equations (3) and (7). Then the estimate of the permeate concentration ($C_{i,p}$) was calculated by applying the estimate of ($c_{i,N}$) into equation (9). Then the ion rejection was calculated using equation (10). Euler mathematical method was used to integrate equations (3) and (7). The permeation of ions through the membrane active layer is illustrated in Figure 1.

A value for $d\Psi/dx$ is needed in-order to integrate equation (3), thus a value of the permeate concentration ($C_{i,p}$) is needed. Consequently, it is reasoning to solve the model in an iterative function using an initial guess

Where K is the hydrodynamic drag coefficient and λ is the stokes radius of component (i) to pore radius ration. The hydrodynamic drag coefficients (K) and (G) are given as follows (Bowen and Mohammad, 1998; Bowen and Mukhtar, 1996)

$$K^{-1}(\lambda_i, 0) = 1.0 - 2.30\lambda_i + 1.154\lambda_i^2 + 0.224\lambda_i^3 \qquad (16\text{-a})$$

$$G(\lambda_i, 0) = 1.0 + 0.054\lambda_i - 0.988\lambda_i^2 + 0.441\lambda_i^3 \qquad (16\text{-b})$$

Substituting equations 11, 12, 13, 14, 15, 16-a and 16-b into equations 3 and 7 gives the following

$$\frac{dc_i}{dx} = \frac{J_v}{\left(1.0 - 2.30\lambda_i + 1.154\lambda_i^2 + 0.224\lambda_i^3\right)D_{i,\infty}}\left(\left(2-(1-\lambda_i)^2\right)\left(1.0 + 0.054\lambda_i - 0.988\lambda_i^2 + 0.441\lambda_i^3\right)c_i - C_{i,p}\right) - \frac{z_i c_i}{RT}F\frac{d\Psi}{dx}$$

(17)

$$\frac{d\Psi}{dx} = \frac{\sum_{i=1}^{n}\frac{z_i J_v}{\left(1.0 - 2.30\lambda_i + 1.154\lambda_i^2 + 0.224\lambda_i^3\right)D_{i,\infty}}\left(\left(2-(1-\lambda_i)^2\right)\left(1.0 + 0.054\lambda_i - 0.988\lambda_i^2 + 0.441\lambda_i^3\right)c_i - C_{i,p}\right)}{\frac{F}{RT}\sum_{i=1}^{n} z_i^2 c_i}$$

(18)

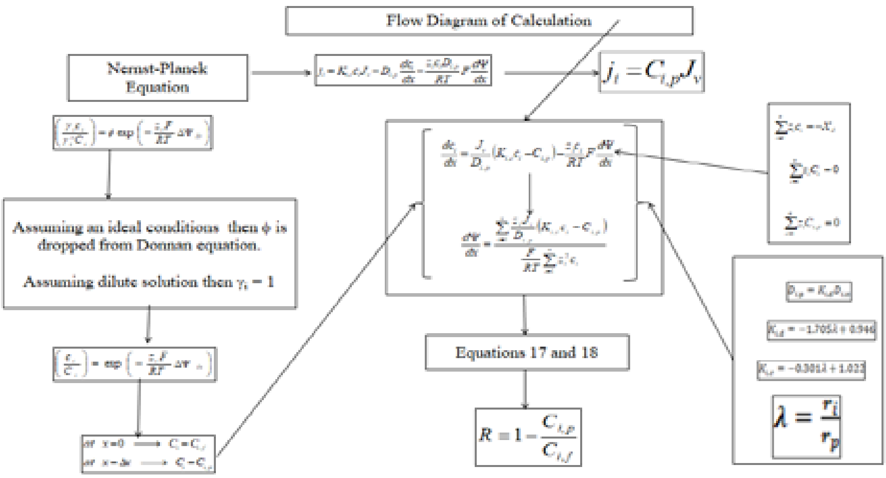

Figure 2. Flow diagram of calculation.

$$R = 1 - \frac{C_{i,p}}{C_{i,f}} \qquad (10)$$

The hindered diffusivity ($D_{i,p}$) and the hindrance factor for convection ($K_{i,c}$) can be obtained from the following equations (Morão et al., 2008; Janz and Bansal, 1982; Gao et al., 2007). The hindered diffusivity is

$$D_{i,p} = K_{i,d} \cdot D_{i,\infty} \qquad (11)$$

Where $K_{i,d}$ is the hindrance factor for diffusion and $D_{i,\infty}$ is the bulk diffusivity (m^2/s).

If the solute velocity inside the membrane pores is taken into consideration then the hindrance factor for convection ($K_{i,c}$) (Henley et al., 2011; Afonso and Pinho, 2000; Lefebvre et al., 2003; Wadley et al., 1995) is given as follows

$$K_{i,c} = (2 - \phi_i) G(\lambda_i, 0) \qquad (12)$$

Where ϕ is steric partitioning term and G is the hydrodynamic drag coefficient. The steric partitioning term (Bowen et al., 1997) was calculated as follows

$$\phi = (1 - \lambda)^2 \qquad (13)$$

The ratio of the stokes radius of component (i) to the pore radius ratio (λ) is given as follows (Fievet et al., 2002)

$$\lambda_i = \frac{r_i}{r_p} \qquad (14)$$

where r_p is the effective pore radius and r_i is the stokes radius of component (i). The hindrance factor for diffusion (Geraldes and Alves, 2008; Bowen and Mukhtar, 1996; Lefebvre et al., 2003) is given follows

$$K_{i,d} = K^{-1}(\lambda_i, 0) \qquad (15)$$

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

The Donnan equilibrium was assumed to apply at the feed/membrane interface and at the membrane/permeate interface. The Donnan equilibrium is given as (Morão et al., 2008; Gao et al., 2007)

$$\left(\frac{\gamma_i c_i}{\gamma_i^o C_i} \right) = \phi \exp\left(-\frac{z_i F}{RT} \Delta\Psi_D \right) \qquad (8)$$

where γ_i is the activity coefficient of ion (i) in the membrane, γ_i° is the activity of ion (i) in the bulk solution and ϕ is the steric partitioning term. Equation (8) defines the boundary conditions at both sides of the membrane. Assuming an ideal conditions then the steric partitioning was dropped from Donnan equation. Assuming that the solution is a dilute solution, and then the activity coefficient, to be accounted for inside the membrane by the effective membrane charge density, would be equal to unity. Hence, the Donnan equilibrium becomes as (Schäfer et al., 2005; Tsuru et al., 1991; Lefebvre et al., 2003)

$$\left(\frac{c_i}{C_i} \right) = \exp\left(-\frac{z_i F}{RT} \Delta\Psi_D \right) \qquad (9)$$

where C_i is the ion concentration in the solution (mol/m^3) and $\Delta\Psi_D$ is the Donnan potential (V). Then Equations (3) and (7) can be solved over the following conditions

$$at \quad x = 0 \longrightarrow C_i = C_{i,f}$$
$$at \quad x = \Delta x \longrightarrow C_i = C_{i,p}$$

where $C_{i,f}$ is the concentration of ion (i) in the feed (mol/m^3) and $C_{i,p}$ is the concentration of ion (i) in the permeate (mol/m^3). The rejection (R) of ion (i) is given as

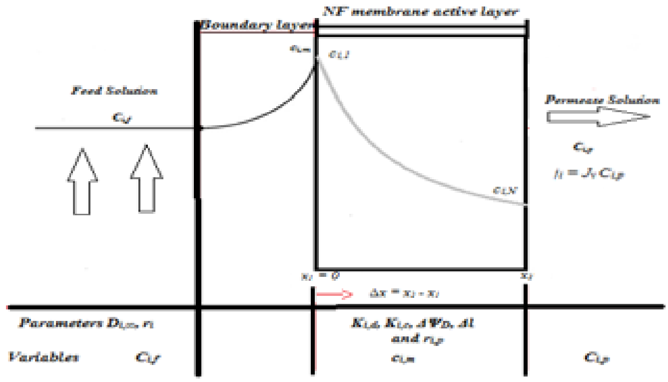

Figure 1. Ion transport through membrane active layer.

To obtain the potential gradient, several conditions were implied (Fievet et al., 2002; Bórquez and Ferrer, 2016; Lefebvre et al., 2003), (Figure 2). The electro-neutrality conditions are fulfilled in the following order: the feed, the membrane and permeate, as depicted in equations (4) and (5). The membrane effective charge (X_d) is assumed to be constant

$$\sum_{i=1}^{n} z_i c_i = -X_d \qquad (4)$$

where X_d is the effective membrane charge density (mol/m^3). The electro-neutrality condition in the bulk solution is given as

$$\sum_{i=1}^{n} z_i C_i = 0 \qquad (5)$$

The electro-neutrality condition in the permeate solution is given as

$$\sum_{i=1}^{n} z_i C_{i,p} = 0 \qquad (6)$$

By applying the conditions in Equations (4), (5) and (6) for Equation (3) and rearranging it, gives the electrical potential gradient as follows

- The Donnan equilibrium takes place at the membrane/feed interface, and the membrane/permeate interface.

The extended Nernst-Planck equation is given as (Schäfer et al., 2005; Morão et al., 2008; Hilal et al., 2004; Fievet et al., 2002)

$$j_i = K_{i,c} c_i J_v - D_{i,p} \frac{dc_i}{dx} - \frac{z_i c_i D_{i,p}}{RT} F \frac{d\Psi}{dx} \qquad (1)$$

where j_i is the flux of ion (i) based on the membrane area (mol/m^2.s), $K_{i,c}$ is the hindrance factor for convection inside the membrane, c_i is the concentration inside the membrane active layer (mol/m^3), J_v is the solution volume flux based on the membrane area (m^3/m^2.s), $D_{i,p}$ is the hindered diffusivity (m^2/s), x is the membrane active layer thickness, z_i is the valence of ion (i), R is the gas constant (J/mol.K), T is the absolute temperature (K), F is Faraday constant (C/mol) and Ψ is the electrical potential (V). Transport of ions through the membrane is obtained by implying a set of boundary conditions-as follows. The ions rejection is calculated by writing the Nernst-Planck equation in the form of concentration and potential gradients (Figure 1). To obtain the concentration gradient, the ion flux is related to its concentration as

$$j_i = C_{i,p} J_v \qquad (2)$$

where $C_{i,p}$ is the concentration of ion (i) in the permeate (mol/m^3). Substituting equation (2) into equation (1) and rearranging it gives the concentration gradient as follows

$$\frac{dc_i}{dx} = \frac{J_v}{D_{i,p}} \left(K_{i,c} c_i - C_{i,p} \right) - \frac{z_i c_i}{RT} F \frac{d\Psi}{dx} \qquad (3)$$

al., 2004; Bowen and Mohammad, 1998; Tsuru et al., 1991). The mathematical model was developed for a negatively charged membrane and one type of electrolyte system, i.e. charged solutes. The charged electrolyte system is in the form of a salt solution containing anions and cations species. The existence of a cation and an anion will give rise to the Donnan effect and consequently affect the separation performance together with the steric effect, (Hajarat, 2010). The model was used to run sodium chloride (NaCl), sodium sulphate (Na_2SO_4), magnesium chloride ($MgCl_2$), and magnesium sulphate ($MgSO_4$) for two different feed concentration values over a different volume flux based on the membrane area ($m^3/m^2.s$) values.

Theory

Extended Nernst-Planck Equation

The extended Nernst-Planck equation covers all of the three important aspects in transport mechanisms through nanofiltration membrane: diffusion, electro-migration and convection. The model development is based on two approaches: the irreversible thermodynamic approach and the hydrodynamic approach, which are governed by both the steric and the charge effects, which in turn govern the ion transport through nanofiltration membrane (Schäfer et al., 2005; Morão et al., 2008; Lefebvreet et al., 2003). The steric effect is caused by the difference between the membrane pore radius and the solute ion radius, while the Donnan effect is actually the result of the charge polarities between the membrane and the solute (Bandini, 2005). These combined effects influence the selectivity of the membrane. The concentration gradient and the electrical potential gradient cause ion diffusion across nanofiltration membranes, whilst the pressure difference causes convection of ions across nanofiltration membrane. Four assumptions were made

- The solution is assumed ideal.
- The membrane charge capacity is uniform.
- All the ions that exist in the membrane are transportable.

Introduction

Nanofiltration membranes have the potential to be used in many different applications such as water softening, removal of hardness, removal of heavy metals, and production of clean water. Nanofiltration has properties lying between those of ultrafiltration and reverse osmosis membrane.

The permeation of ions through nanofiltration membrane can be described by using the extended Nernst-Planck equation. The extended Nernst-Planck equation describes the solute concentration change inside the membrane and the change between the feed and the permeate concentrations, (Schäfer et al., 2005; Morão et al., 2008; Fievet et al., 2002). The transport of ions through nanofiltration membrane is described in terms of concentration gradient, electrical potential gradient and pressure difference across the membrane. The concentration and the electrical potential gradients give rise to ionic diffusion across the nanofiltration membrane, while pressure difference causes convection of ions across the membrane, (Schäfer et al., 2005; Morão et al., 2008).

A model is essential in predicting the membrane performance, understanding the separation mechanism for various substances, selecting the appropriate membrane for a specific application and process design and optimization. In this work, a mathematical modelling of the extended Nernst-Planck equation was used due to its description of the ionic transport mechanisms through nanofiltration membranes and to try to understand nanofiltration membrane separation behaviour, (Schäfer et al., 2005; Hilal et

نمذجة الأيونات النقل من خلال غشاء الترشيح النانومتر السيراميك

رشــا عامر حجرات

ملخص

تم استخدام معادلة Nernst-Planck الموسعة لوصف فصل الأيونات باستخدام غشاء الترشيح النانوي، حيث أن الفصل هو نتيجة التركيز والتدرجات الكهربائية وتدرجات الضغط عبر الغشاء. تم استخدام الترشيح الدقيق للسيراميك لدراسة تأثير الكاتيون والأنيون على سلوك الفصل. لفهم سلوك فصل الأيونات من محلول الملح الواحد ومحاليل الأملاح المختلطة. تم بناء نموذج لمحاكاة سلوك الفصل لمزيج من اثنين، وثلاثة، وأربعة أيونات. كانت الأيونات المستخدمة في النموذج هي Mg^{2+} و Na^{1+} و Cl^{1-} و SO_4^{2-}.

الكلمة الرئيسية: الأيونات، الغشاء، النمذجة، الترشيح الدقيق جدا.

Modelling Ions Transport through Ceramic Nanofiltration Membrane

Rasha Amer Hajarat*

Abstract

Extended Nernst-Planck equation was used to describe the separation of ions by using Nanofiltration membrane, where the separation is a result of concentration, electrical and pressure gradients across the membrane. Ceramic Nanofiltration was used to study the effect of a cation and an anion on the separation behaviour. To understand the separation behaviour of ions from single salt solution and mixed salts solutions, a model was built to simulate the separation behaviour of a mixture of two, three, and four ions. The used ions in the model were Mg^{2+}, Na^{1+}, Cl^{1-} and SO_4^{2-}.

Keyword: ions, membrane, modelling, nanofiltration.

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