Revista Mexicana de Ingeniería Química

NEW ADD-IN FOR ENGINEERING SIMULATIONS IN SPREADSHEETS USING HOMOTOPY CONTINUATION METHODS

NUEVO COMPLEMENTO PARA SIMULACIONES DE INGENIERÍA EN HOJAS DE CÁLCULO USANDO MÉTODOS DE CONTINUIDAD HOMOTÓPICA

L. Díaz-Montes[1], R. Barrera-Zapata[1]*, H. Jiménez-Islas[2]

[1]*Grupo CERES, Departamento de ingeniería química, Facultad de ingeniería, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia*

[2]*Departamento de Ingeniería Bioquímica. Tecnológico Nacional de México, Instituto Tecnológico de Celaya, Ave. Tecnológico y A. García Cubas s/n. Celaya, Gto. CP 38010. México*

Abstract

Solving models represented by non-linear equations is a common situation in engineering and can be a challenging task. Homotopy Continuation Methods have shown globally convergent behavior, capable of finding all the possible roots of algebraic systems. Based on these methods, a new Microsoft Office Excel add-in was developed, *SphereSolver*, aiming to enhance the ability to use this easily obtainable software as a simulation computing platform for engineering problems. *SphereSolver* was applied over different types of engineering models and the non-linear equations were solved successfully each time. Selected problems were solved with *SphereSolver* and compared with other solution tecniques, e.g., classical Newton's method, Fixed Point homotopy or Affine Homotopy. It was observed that using *SphereSolver* the solution for selected problems was improved, i.e., the interval of convergence is extended massively and/or additional roots can be found. It can be concluded that *SphereSolver* is a new and efficient tool that can be used within Microsoft Excel for solving engineering problems where other software or traditional tools could fail or present limitations.

Keywords: engineering non-linear models, homotopy continuation methods, excel add-in, hyperspherical path tracking.

Resumen

Resolver modelos matemáticos representados por ecuaciones no lineales es común en la ingeniería y puede ser una tarea difícil. Los métodos de Continuidad Homotópica han mostrado ser globalmente convergentes y capaces de encontrar todas las posibles raíces de sistemas algebraicos. Con base en este tipo de métodos, se presenta un nuevo complemento para Microsoft Office Excel, *SphereSolver*, desarrollado con el objetivo de mejorar la capacidad de este software común, como una plataforma de computación de simulación para problemas de ingeniería. *SphereSolver* se aplicó sobre diferentes tipos de modelos de ingeniería y en todos los casos, las ecuaciones no lineales se resolvieron con éxito. La solución con *SphereSolver* a los problemas seleccionados se comparó con otras técnicas de solución, por ejemplo, el método clásico de Newton, Homotopía de punto fijo y Homotopía Afín. Se observó que usando *SphereSolver* el intervalo de convergencia se extiende masivamente y / o se pueden encontrar raíces adicionales, es decir, se mejoró la solución. Se concluye que *SphereSolver* es una herramienta eficiente que se puede utilizar en Microsoft Excel para resolver problemas de ingeniería donde otros programas o herramientas tradicionales pueden fallar o presentar limitaciones.

Palabras clave: modelos de ingeniería no lineales, métodos de continuidad homotópica, complemento de excel, seguimiento hiperesférico.

1 Introduction

The solution of systems of non-linear equations is a common practice in engineering, and transcendental functions are usually part of these models (Jiménez-Islas *et al*., 2014; Rodríguez and Niño, 2016). Newton-

like methods are a classical approach used in these cases, though they are locally convergent, i.e., they require an initial approximation *close enough* to the solution to find the value of the vector that satisfies a given convergence criterion (Davis, 1984). Homotopy Continuation Methods (HCMs) have emerged as an alternative strategy, which uses the local convergence

* *Corresponding author. E-mail*: rolando.barrera@udea.edu.co
Tel. +57 +4 2198564

properties of such methods in a gradual deformation scheme (Allgower and Georg, 1990). They have been shown to be accurate, robust, and able to converge from almost any arbitrary starting point. These techniques have been successfully applied to solve polynomial systems of equations, constrained and unconstrained optimization problems, and non-linear partial differential equations. Therefore, the applications of HCMs to solve engineering models have been numerous, including phase separation and transport phenomena problems, among others (Jalali *et al,.* 2008; Menglong and Zhenxin, 2008; Laiadi and Merzougui, 2012; Yang *et al.*, 2012; Jimenez-Islas *et al.*, 2013; Torres-Muñoz *et al.*, 2015).

The solution of systems of non-linear equations is a common practice in engineering, and transcendental functions are usually part of these models (Jiménez-Islas *et al.*, 2014; Rodríguez and Niño, 2016). Newton-like methods are a classical approach used in these cases, though they are locally convergent, i.e., they require an initial approximation *close enough* to the solution to find the value of the vector that satisfies a given convergence criterion (Davis, 1984). Homotopy Continuation Methods (HCMs) have emerged as an alternative strategy, which uses the local convergence properties of such methods in a gradual deformation scheme (Allgower and Georg, 1990). They have been shown to be accurate, robust, and able to converge from almost any arbitrary starting point. These techniques have been successfully applied to solve polynomial systems of equations, constrained and unconstrained optimization problems, and non-linear partial differential equations. Therefore, the applications of HCMs to solve engineering models have been numerous, including phase separation and transport phenomena problems, among others (Jalali *et al,.* 2008; Menglong and Zhenxin, 2008; Laiadi and Merzougui, 2012; Yang *et al.*, 2012; Jimenez-Islas *et al.*, 2013; Torres-Muñoz *et al.*, 2015).

HCMs are recognized by their potential as a reliable and efficient seeker of all the set of possible roots of a multivariable function from one starting point (Rahimian *et al.* 2011). The general problem that faces HCMs is to find the solution x_F of the system of equations $F(x_F) = 0$, where the mapping $F : \Re^n \rightarrow \Re^n$ represents a set of equations, which in the general case includes transcendental functions. The basic idea of HCMs is fully described in the literature and deals with the gradual deformation from an auxiliary function, $E(x)$, to the function to be solved, $F(x)$, where x_E, such as $E(x_E) = 0$, is known. This deformation is developed using an artificial

parameter t that establishes specific conditions to be satisfied by the homotopic function, $H(t, x)$, i.e., Eq. (1) (Cveticanin *et al.*, 2012; Ward and King, 2012).

$$H(t,x) = \begin{cases} E(x) & \text{if } t = 0 \\ F(x) & \text{if } t = 1 \end{cases} \tag{1}$$

Thus the standard convex homotopic function, Eq. (2), is stated (Verschelde and Cools, 1994; Thompson, 2006).

$$H(t,x) = (1-t)E(x) + tF(x) \tag{2}$$

Starting from $t = t_0 = 0$, if a small increment Δt is applied over t_0, such as $t_1 = t_0 + \Delta t \rightarrow t_1 \approx t_0 \rightarrow H(t_1, x) \approx H(0, x)$, it is expected that $x_(H, 1) \approx x_E$, where $H(t_1, x_{H,1}) = 0$. Once the value of x_{H1} is obtained, t is slightly changed again, such as $t_2 = t_1 + \Delta t \rightarrow t_2 \approx t_1 \rightarrow H(t_2, x) \approx H(t_1, x)$, and therefore $x_(H, 2) \approx x_(H, 1)$, where $H(t_2, x_{H,2}) = 0$. Following this pattern, an increase in t is made such as $t_{k+1} = t_k + \Delta t \rightarrow t_{k+1} \approx t_k \rightarrow H(t_{k+1}, x) \approx H(t_k, x)$, using $x_{H,k}$ as the initial trial in a locally convergent numerical method to find the vector $x_{H,k+1}$. Following this strategy, every time $t = 1$ is reached, a solution of the problem $F(x) = 0$ is found.

Different types of HCMs can be obtained according to the specific form of the auxiliary function $E(x)$, the numerical method used to solve $H(t_k, x_{H,k}) = 0$ for each discretized value t_k, and the selected homotopic path tracking method (Menglong and Zhenxin, 2008; Jimenez-Islas *et al.*, 2013). Some typical auxiliary functions found in the literature include Fixed Point Homotopy (Eq. (3)), Affine Homotopy (Eq. (4)) and Newton or global Homotopy (Eq. (5)).

$$E(x) = x - x_0 \tag{3}$$
$$E(x) = A \cdot (x - x_0) \tag{4}$$
$$E(x) = F(x) - F(x_0) \tag{5}$$

Where x_0 is a known value (initial estimate) and A is a scaling matrix, e.g., Jacobian matrix.

Regarding to the numerical method used to solve $H(t_k, x_{H,k}) = 0$ for each discretized value t_k, the basic Predictor-Corrector approach is recommended (Wayburn and Seader, 1987). Taking the total derivative with respect to t of the homotopic function given by Eq. (2), the Initial Value Problem, IVP (Eq. (6)), is obtained (Georg, 1981).

$$\frac{dx_H}{dt} = [t \cdot J_F(x_H) + (1-t) \cdot J_E(x_H)]^{-1} \cdot [E(x_H) - F(x_H)],$$

$$x_H(t = 0) = x_E \tag{6}$$

Where $J_F(x_H)$ and $J_E(x_H)$ represent the derivative or Jacobian matrix of the original function and the auxiliary function, respectively.

In a basic Predictor-Corrector scheme, instead of directly using the solution obtained at point k as the initial guess for the problem for the next point $k + 1$, a simple strategy such as Euler's method is applied over the IVP given by Eq. (6) using the new initial condition $x_H(t_k) = x_{H,k}$, and this numerical result is used as the initial guess for the problem at the next point $k + 1$.

By other side, among different homotopic path tracking methods discussed in the literature, the circle tracking method, generalized as hyperspheres, exhibited the best behavior (Yamamura, 1993; Jiménez-Islas, 1996). The hypersphere that is represented by Eq. (7) must be solved for each discretized point k following the algorithm described in Table 1.

$$\|x - x_{H,k}\|^2 + (t - t_k)^2 = R^2 \tag{7}$$

Fig. 1 shows how, for a two-dimensional x_H, the tangent line from the center of the sphere given by Euler's predictor intersects the surface of the sphere, and this point feeds a locally convergent method that finds the intersection of the path with the sphere. A detailed analysis of this tracking method is presented by Oliveros-Muñoz and Jiménez-Islas, (2013).

One known problem of HCMs appears when the homotopic path presents *turning points* as described by Watson (2001), where an inappropriate step increase could skip roots of the homotopic path.

Such situation can be avoided by using the arc length p as alternative tracking parameter (Klopfenstein, 1961), wherein x and t are taken as functions of this new parameter. Hence, the total derivative of each component of the homotopic function $H(t, x) = 0$ regarding to "p" will be described by Eq. (8).

$$\begin{bmatrix} \frac{dH_1}{dp} \\ \vdots \\ \frac{dH_n}{dp} \end{bmatrix} = \begin{bmatrix} \frac{\partial H_1}{\partial x_1}\frac{dx_1}{dp} + \cdots + \frac{\partial H_1}{\partial x_n}\frac{dx_n}{dp} + \frac{\partial H_1}{\partial t}\frac{dt}{dp} + \frac{\partial H_1}{\partial p} \\ \vdots \\ \frac{\partial H_n}{\partial x_1}\frac{dx_1}{dp} + \cdots + \frac{\partial H_n}{\partial x_n}\frac{dx_n}{dp} + \frac{\partial H_n}{\partial t}\frac{dt}{dp} + \frac{\partial H_n}{\partial p} \end{bmatrix} = 0 \tag{8}$$

where $x = [x_1 \cdots x_n]^T$ and $H(t, x) = [H_1 \cdots H_n]^T$.

Considering that $\partial H_1/\partial p = \cdots = \partial H_n/\partial p = 0$, and using the compact notation of Eq. (9), Eq. (10) can be obtained.

$$J_{Hx}\frac{dx}{dp} = -\frac{dt}{dp}\frac{\partial H}{\partial t} \tag{9}$$

$$\frac{dx}{dp} = -\frac{dt}{dp}[J_{Hx}]^{-1}\frac{\partial H}{\partial t} \tag{10}$$
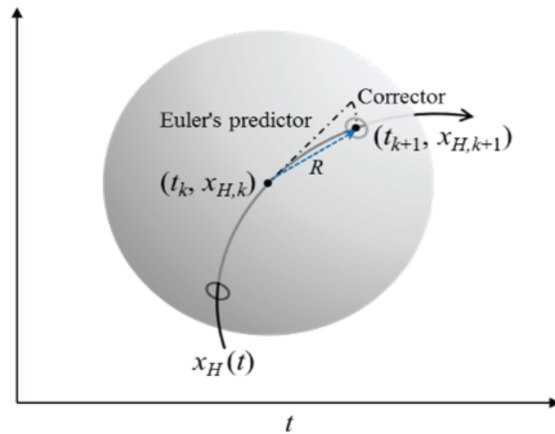

Fig. 1. Euler's predictor for hyperspheres as homotopic path tracking method.

Table 1. Algorithm steps for hyperspheres as homotopic path tracking method.

Step	Description
1. Hypersphere setting	Taking the point $(t_k, x_{H,k})$ as the center of the sphere, with an established radius R, Eq. (7) is set.
2. Euler's predictor step	Applying Euler's method over Eq. (6) a tangent line is formed, and the intersection point of this line and the hypersphere surface is obtained.
3. Corrector step	The point obtained from step 2 is used as an initial trial to find the simultaneous solution of $H(t, x) = 0$ and Eq. (7), using a locally convergent Newton-like method as a corrector strategy. The solution will be the next point $(t_{k+1}, x_{H,k+1})$ of the homotopic path.
4. Loop	The point $(t_{k+1}, x_{H,k+1})$ is set as the center of a new hypersphere, and the tracking strategy continues with step 1.

On the other hand, the approximate calculation of dt/dp can be performed using the determinant of the homotopic Jacobian matrix (Oliveros-Muñoz and Jiménez-Islas, 2013), Eq. (11).

$$\frac{dt}{dp} = (-1)^{n+1} \cdot det(J_{Hx}) \qquad (11)$$

In a Predictor-Corrector scheme, Euler's method is applied over the problem at the center of the sphere. Thus, for a given change in the new path tracking parameter, Δp, the initial estimate that feeds the locally convergent method, t^0, and the vector, x^0, are found using eqs. (12) and (13), respectively. This approach permit to follow any n-dimensional homotopic path only in terms of $t(p)$.

$$t^0 = t + \frac{dt}{dp}\Delta p \qquad (12)$$

$$x^0 = x + \frac{dx}{dp}\Delta p \qquad (13)$$

When this approach is combined with the hypersphere radius R (Eq. (7)), the change in the arc length can be described by Eq. (14), where the sign for the square root is set according to the positive or negative advance of p (Oliveros-Muñoz and Jiménez-Islas, 2013).

$$\Delta p = \pm \sqrt{\frac{R^2}{1 + \|\frac{dx}{dp}\|^2 + \left(\frac{dt}{dp}\right)^2}} \qquad (14)$$

According to the literature survey, it was found that different computational tools have been developed based on HCMs, most of them implemented in scientific computation packages as Matlab (Thompson, 2006; Lee *et al.*, 2008); while the use of HCMs as an add-in for the widely known software Microsoft Excel Office is scarce and limited to Fixed Point and Affine Homotopies (Henao and Velásquez, 2004), without including hyperspheres as homotopic path tracking method, neither arc length p as alternative tracking parameter.

In this contribution, a new code for HCMs developed in Visual Basic for Applications 7.1©, to be used as Microsoft Office Excel add-in (named *SphereSolver*) is presented. *SphereSolver* uses Newton Homotopy (Eq. (5)) as auxiliary equation, hyperspheres as the tracking device of the homotopic path; arc length p as alternative tracking parameter; and second-order finite central differences to approximate the required derivatives. The simplicity associated to the use of widely known software as Microsoft Office Excel improves the range of applications for the HCMs methods in solving engineering problems. In the next section, the software is presented and then a problem is proposed as case study. For comparison proposes, the case study is analyzed by using different approaches, i.e., classical Newton´s method; Fixed Point Homotopy, Affine Homotopy, and the *SphereSolver*. Finally, it is illustrated the use of *SphereSolver* for solving different kinds of typical engineering problems.

2 Software presentation

Microsoft Excel© by Microsoft© can be considered a low-cost program with uses in several engineering applications (Huddleston *et al.*, 2004; Wong and Zhou, 2004; Bhattacharjya, 2010; Le Roux *et al.*, 2010). Excel is widely available and easily adaptable to individual needs for solving engineering problems. Although several add-ins and templates have been developed in Excel, as far as we know, there have been no tools capable of finding several roots of system of non-linear equations using a globally convergent method. The newly developed add-in *SphereSolver* was designed with a friendly user interface, and with default settings suitable for users who are not familiar with the numerical method. The size of the add-in is 143 kB.

The code was developed in Visual Basic for Applications 7.1©. A description of the main algorithm is included as supporting material. The developed add-in uses Newton Homotopy; hyperspheres as the tracking device of the homotopic path; and second-order finite central differences to approximate the required derivatives.

To use the developed add-in, Microsoft Office Excel spreadsheets are used to set up the model that contains the system of equations to be solved. Specific information shown in Figs. 2 and 3 is related with the case study described in the next section. As shown in Fig. 2, at least two set of cells are required to capture the information of the model from the spreadsheet. The first set contains n cells, where the different values that the unknown variables adopt during the execution of the algorithm are downloaded (cell D7, Fig. 2). The initial values for the HCM are recommended to be entered there. The second set contains other n cells, where the formulas of the system of equations are introduced. They must depend directly or indirectly on the first set of cells (cell F7, Fig. 2). In general, *SphereSolver* changes the values of the cells that

represent the unknown variables as the homotopic path is followed, and the solution will be the values that satisfies the equations with in a convergence criterion.

	A	B	C	D	E	F	G
	Given parameters			*Intermediate calculations*			
	P_c (atm)	37.5		a	286.1048		
	T_c (K)	425.2		b	0.080605		
	R	0.08205					
	P (atm)	50		*Variables*		*Functions*	
	T (K)	298.15		v		F(v)= 0	
				1		=\$B\$4*\$B\$6/(D7-\$E\$3)-	
						\$E\$2/(\$B\$6^0.5*D7*(D7	
						\$E\$3))-\$B\$5	

Fig. 2. Example of a set up in a spreadsheet used to capture the information of a model (case study presented in the next section).
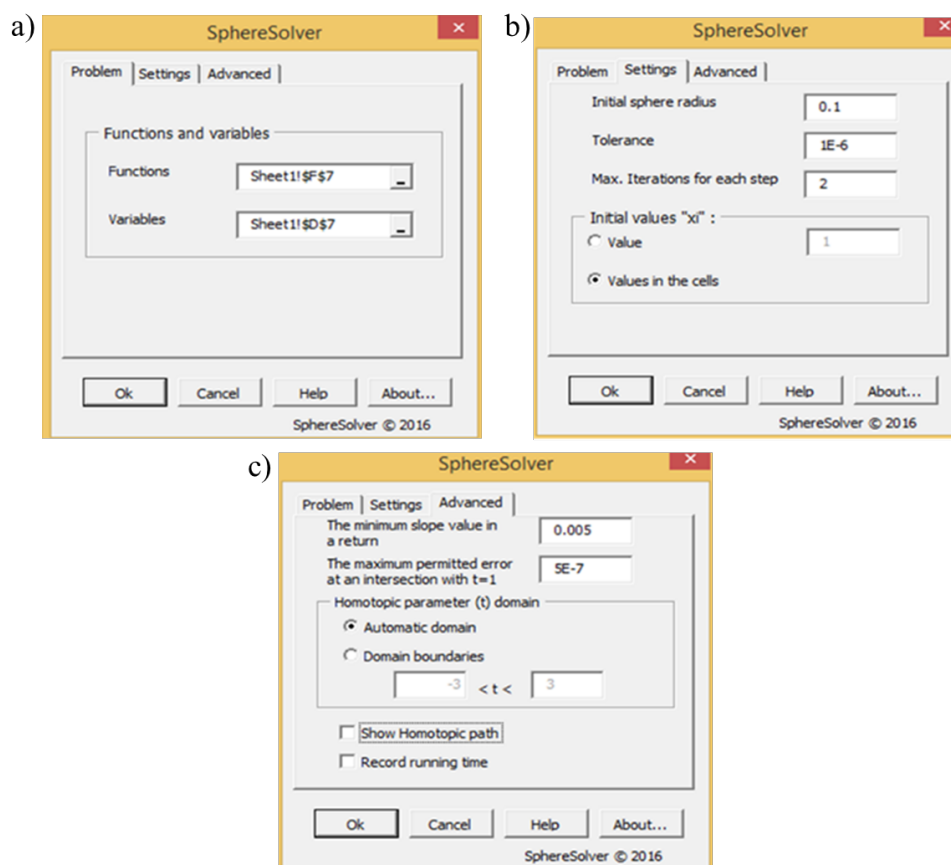
Fig. 3. *SphereSolver*'s interface. a) Page to capture the information of the system of equations from an Excel Office spreadsheet. b) Page to acquire basic numerical parameter values. c) Page to set advanced parameters for the HCM.

After installation, the add-in can be executed from the Excel Office ribbon with the name *SphereSolver*. The interface consists of three pages: *Problem* (Fig. 3a), *Settings* (Fig. 3b) and *Advanced* (Fig. 3c). In *Problem* (Fig. 3a), using two different reference selection controls, the cells containing the functions and the variables are captured. In *Settings* (Fig. 3b), some basic settings for the HCM are entered, i.e., tolerance of convergence (ε), the initial value of the radius (R_{init}) and the maximum number or iterations in the correction step (I_{max}). In this page the user has the option of taking one particular initial value for all the variables, or taking the values initially entered in the spreadsheet. Finally in *Advanced* (Fig. 3c), advanced numerical parameters can be entered, i.e., the minimum slope value of both sides of a return and the maximum error at an intersection with the hyperplane $t = 1$. The option to set the domain for the homotopic parameter t is also available for users which are familiar with the HCMs and the homotopic function behavior. In this study, the machine used has an Intel(R) Core(TM) i7-4510U CPU @ 2.00GHz 60 GHz processor and 8.00 GB RAM installed. Because the developed add-in is intended for a wide variety of users, the characteristics of the machine are intentionally easy to obtain.

3   Case of study

Redlich-Kwong (Eq. (15)) represents one of the most classical and widely used equations of state in the calculation of thermodynamic properties required in several chemical engineering applications (Murdock, 1993).

$$P = \frac{RT}{v - b} - \frac{a}{T^{1/2}v(v + b)} \qquad (15)$$

where parameters a and b are functions of the critical properties of the gas, and can be described by eqs. (16) and (17), respectively (Murdock, 1993).

$$a = \frac{0.42748023354R^2T_c^{2.5}}{P_c} \qquad (16)$$

$$b = \frac{0.086640349965RT_c}{P_c} \qquad (17)$$

The case study consists in applying the Redlich-Kwong model (Eq. (15)) to estimate the molar volume v of n-butane with the conditions and parameters given in Table 2 (Smith *et al.* 2005).

3.1   Use of the classical Newton's method in the case study

Eq. (15) is written as a function of molar volume, Eq. (18)

$$F(v) = \frac{RT}{v - b} - \frac{a}{\sqrt{T}v(v + b)} - P = 0 \qquad (18)$$

A plot $F(v)$ (Eq. 18) using condition from Table 1 reveals several asymptotes (Fig. 4).

To apply classical Newton's method (Ramírez *et al.* 2006; Bürgisser and Cucker, 2013) and find the root of the function given by Eq. (18), the derivative with respect to the unknown variable v is required, i.e., Eq. (19).

$$F'(v) = -\frac{RT}{(v - b)^2} + \frac{a(2v + b)}{\sqrt{T}[v(v + b)]^2} \qquad (19)$$

Iterations with the classical Newton's method are given by $v_{k+1} = v_k - F(v_k)/F'(v_k)$, in this case represented by Eq. (20).

$$v_{k+1} = v_k - \frac{\left[\frac{RT}{v_k-b} - \frac{a}{\sqrt{T}v_k(v_k+b)} - P\right]}{\left[\frac{-RT}{(v_k-b)^2} + \frac{a(2v_k+b)}{\sqrt{T}[v_k(v_k+b)]^2}\right]} \qquad (20)$$

Table 2. Values for Redlich-Kwong cubic equation.

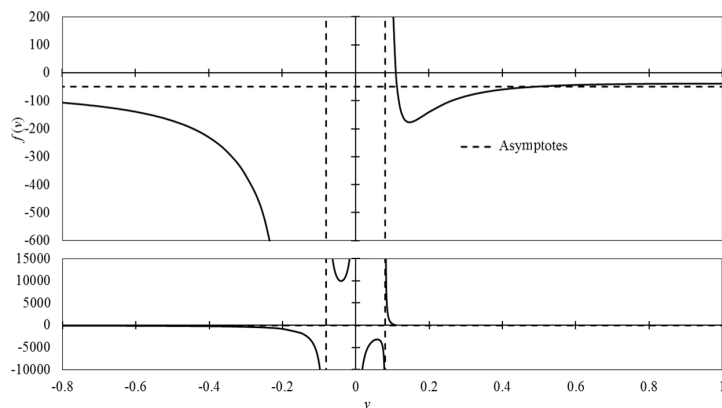| Parameter	Name	Units	Value
P	Pressure	atm	50
T	Temperature	K	298.15
P_c	Critical pressure	atm	37.5*
T_c	Critical temperature	K	425.2*
R	Universal gas constant	L·atm/mol K	0.08205

* Taken from (Smith *et al.*, 2005)

Fig. 4. Graph of the function $F(v) = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)} - P$ using conditions from Table 1.
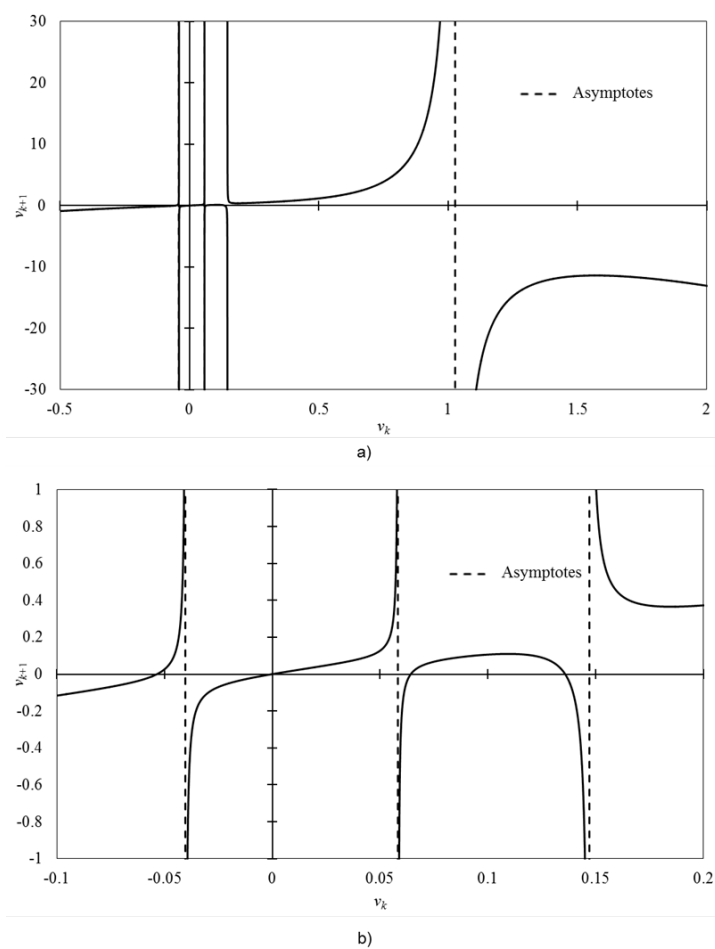

a)

b)

Fig. 5. Estimative of v_{k+1} as a function of the estimate v_k of Newton's method (Eq. (18) with conditions from Table 1); a) Higher scale; b) Smaller scale.

Typical drawbacks of Newton's method are related with the adequate choice of the initial guess. Fig. 5 shows the behavior of the first estimate as a function of the initial value for Newton's method in two different scales. The sequence reveals only one continuous interval containing the root where convergence can be achieved, i.e., from 0.0806047752495982 to 0.127396259816616. In other words, the initial estimate must go from -26.41% to 16.31% of the solution. Thus, the interval of convergence of Newton's method for this case of study is tight. Importantly, the common initial value for the molar volume in a real model is the one obtained from the ideal gas equation, and in this case it is v=RT/P=0.48926415 L/mol, which falls outside the interval of convergence.

3.2 Use of the Fixed Point Homotopy in the case study

Using the same case study, when the molar volume obtained from the ideal gas equation is used as the initial estimate (i.e., $x_0 = v_0 = RT/P$ =0.48926415, $t = 0$), and Fixed Point Homotopy (eqs. (2) and (3)) is applied; the homotopic path shown in Fig. 6 is obtained.

In Fig. 6, the portion of the homotopic path that is above the horizontal asymptote comes from the point ($x_H = x_E = v_0$ =0.48926415,$t = 0$). Due to the horizontal asymptote, there is no continuous path that connects the initial point to the desired root at $t = 1$. Setting the Homotopy function equal to 0, and combining eqs. (2) and (3), Eq. (21) can be obtained.

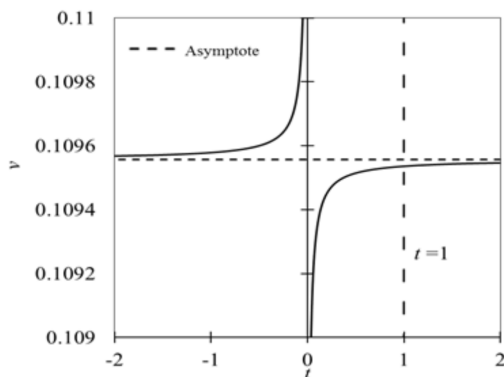$$t = \frac{(x - x_0)}{(x - x_0) - F(x)} \tag{21}$$

Fig. 6. Homotopic path for the study case of the Redlich-Kwong cubic equation under the conditions given in Table 1 using Fixed Point Homotopy.

Thus, when $x - x_0 = F(x)$, t becomes $\pm\infty$. Hence, the horizontal asymptote in Fig. 6 is due to the type of Homotopy itself, and not due to the nature of the original function.

For the given set of parameters (Table 1), the horizontal asymptote occurs at v =0.109557347 L/mol, which is 0.0195% away from the root. In other words, for Fixed Point Homotopy, following the path in the real domain from the initial estimate will not lead to the answer at $t = 1$.

3.3 Use of the Affine Homotopy in the case study

The homotopic path for the implicit equation $H(x_H, t) = 0$ using Affine Homotopy (Eqs. (2) and (4)) over the case of study is shown in Fig. 7. It is observed that the homotopic path presents similar behavior to the Fixed Point Homotopy (Fig. 6). In a similar fashioned way, the horizontal asymptote occurs when the denominator of the Eq. (22) equals 0, i.e., when $F'(x)(x - x_0) = F(x)$.

$$t = \frac{F'(x_0)(x - x_0)}{F'(x_0)(x - x_0) - F(x)} \tag{22}$$

For the case study this scenario is at v= 0.111378181943983 L/mol, 1.68% away from the root. Although not shown in Fig. 7, if the path from the initial estimate is followed upwards, it leads to a vertical asymptote at $t = 1$, and the other path has a horizontal asymptote at the mentioned point. This same behavior was observed for the Fixed Point Homotopy.
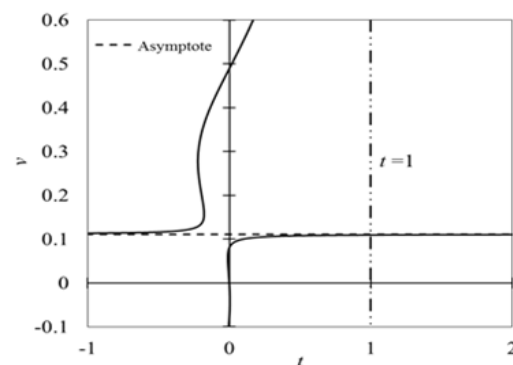

Fig. 7. Homotopic path for the study case of the Redlich-Kwong cubic equation under the conditions given in Table 1 using Affine Homotopy.
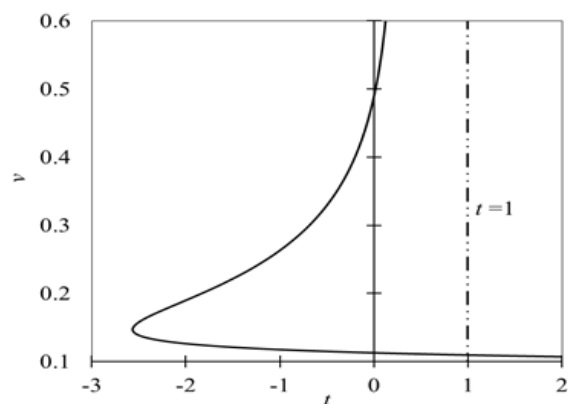
Fig. 8. Homotopic path for the study case of the Redlich-Kwong cubic equation under the conditions given in Table 1 using Newton Homotopy.

According to the previous analysis, for the Fixed Point Homotopy or Affine Homotopy, there is no continuous path from the initial value $v_0 = 0.48926415$ to the solution of the problem at $v = 0.109535967857868$. Again, as observed for Fixed Point Homotopy, the horizontal asymptotes analyzed do not rise from the nature of the function but from the type of homotopy.

3.4 Use of the Newton Homotopy in the case study

Using the Newton Homotopy over the case study, i.e., combination of eqs. (2) and (5), a path from the initial estimate, $v_0 = 0.48926415$, to the solution of the problem exists, as shown in Figure 8.

This case study has shown the advantage of using the Newton Homotopy over the Fixed Point and Affine Homotopy. According to the results, the convergence interval will be the same continuous domain of the function $F(v)$, given by Eq. (18), where the root is contained. For other initial values, a similar homotopic path could be found, but due to the discontinuities created by the nature of the original function, it will not be possible to obtain the

root in a continuous path. Thus, the new practical continuous interval of convergence that contains the root is from $b = 0.0806047752495982$ to ∞. Further results are shown in the use of *SphereSolver*, which include Newton Homotopy with in the code.

3.5 Use of the SphereSolver in the case study

The *SphereSolver* presented in Section 2 was also used with the case study, using several initial values for the HCM. Three of them are shown in Table 3, with their corresponding performance within the application. The initial value of the first case in Table 3 was obtained using the ideal gas equation of state, which is common for this type of problem and, as previously shown, is not useful in this case when Fixed Point Homotopy or Affine Homotopy are used. Even when more initial values were used (with *SphereSolver*), they presented similar behavior.

As analyzed in Section 3.1, the highest continuous interval where the classic Newton's method converges is from 0.0806047752495982 to 0.127396259816616, i.e., the initial estimate must go from -26.41% to 16.31% of the solution. Using *SphereSolver* (which applies Newton Homotopy), any value higher than 0.0806047752495982 can be used where a horizontal asymptote exists due to the nature of the original function and not the type of HCM, will go from the initial value to the root of the equation at $t = 1$, i.e., the interval of convergence is extended massively.

4 Additional engineering problems solved with *SphereSolver*

Three additional engineering models that include non-linear system of equations were selected to be solved by using *SphereSolver*.

Table 3. Performance of *SphereSolver* over the case study with three different initial values. Initial sphere radius: 0.1. Tolerance: 1×10^{-6}. Max. Iterations for each step: 2. Max. error for t = 1: 5×10^{-7}.

Case	Initial value	Time [s]	Number of Spheres	Norm
1	0.48926	39.93	393	3.42×10^{-7}
2	10	33.45	337	1.87×10^{-10}
3	20	35.46	360	4.91×10^{-7}

Table 4. Value of parameters for the adiabatic equilibrium temperature model, taken from Fogler (2016).

Parameter	Name	Units	Value
H_A^0	Heat of formation for A at 298 K	cal/mol	-40,000
H_B^0	Heat of formation for B at 298 K	cal/mol	-60,000
C_{PA}	Heat capacity of A at 298 K	cal/mol K	50
C_{PB}	Heat capacity of B at 298 K	cal/mol K	50
R	Universal gas constant	cal/mol K	1.987
K_e	Equilibrium constant at 298 K	—	100,000

Table 5. Tests of *SphereSolver* solving Eq. (23) by using different initial guess. Minimum slope in a return: 0.005. Max. error for $t = 1 : 5 \times 10^{-7}$.

Case	Initial value	Initial sphere radius	Tolerance	Max. Iterations	Time (s) for each step	Spheres	Norm
1	100	10	1×10^{-3}	2	140.84	517	7×10^{-8}
2	10000	1000	1×10^{-6}	5	29.55	113	4×10^{-7}
3	100000	10000	1×10^{-3}	5	26.18	125	8×10^{-4}
4	30	100	1×10^{-3}	5	22.09	93	4×10^{-7}
5	30	10	1×10^{-3}	5	22.6	94	1×10^{-7}

Selected models include the adiabatic equilibrium temperature in a chemical reactor, the Benzene production in a plant performance evaluation, and an electronic circuit with two-tunnel exponential diodes. Depending on the nature of the functions, different aspects are highlighted for each simulation, i.e., severe non-linearity, restricted convergence with traditional methods, several sets of possible solutions, and so on.

4.1 Chemical reactor: Adiabatic equilibrium temperature

The highest conversion that can be achieved in reversible reactions is obtained at the equilibrium temperature. Fogler (2016) presents an example for an elementary solid-catalyzed liquid-phase reaction $A \leftrightarrow B$, where the adiabatic equilibrium temperature T is determined when pure A is fed to the reactor at a temperature of 3000 K. The resulting Eq. (23), which deduction is presented by Fogler (2016), should be solved to find the adiabatic equilibrium temperature. Supplied information is given in Table 4.

$$F(T) = \frac{K_e \exp\left[\frac{(H_B^0 - H_A^0)}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]}{1 + K_e \exp\left[\frac{(H_B^0 - H_A^0)}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]} - \frac{C_{PA}(T - T_0)}{-(H_B^0 - H_A^0)} = 0 \tag{23}$$

A typical approach for solving the problem is by using Newton's method, in such case, the derivative of Eq. (23), (Eq. (24)), should be considered.

$$\frac{dF}{dt} = \frac{K_e \exp\left[\frac{(H_B^0 - H_A^0)}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]}{\left(1 + K_e \exp\left[\frac{(H_B^0 - H_A^0)}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]\right)^2} \frac{(H_B^0 - H_A^0)}{RT^2} - \frac{C_{PA}}{-(H_B^0 - H_A^0)} \tag{24}$$

Fig. 9 shows the behavior of the function convergence. For the Newton's method, it is achieved if the initial trial is within the interval $400.569432 < T < 522.389085$, which is -13% to +13.46% away from the root at $T = 460.399642820735$. In Fig. 9, the dotted vertical lines are part of the convergence interval for Newton's method

Alternatively, *SphereSolver* add-in was used to solve the non-linear equation under different initial guess. The convergence criteria were satisfied in each occasion, and the performance of the method for five different cases is reported in Table 5.

4.2 Plant performance evaluation: Benzene production

The hydrodealkylation of toluene to benzene is an important petrochemical process; an industrial process for this transformation is shown in Fig. 10 (Henao, 2010).
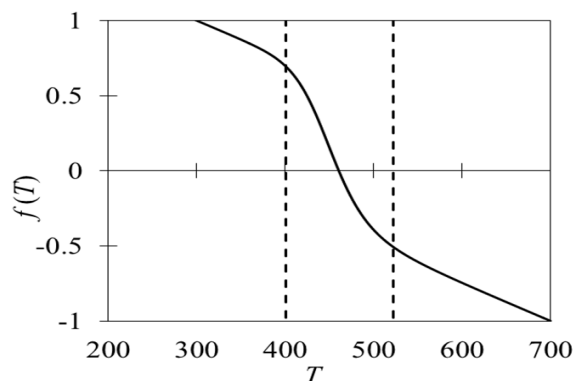
Fig. 9. Graph of the function given by Eq. (23). Values wherein the dotted vertical lines are part of the convergence interval for Newton's method.
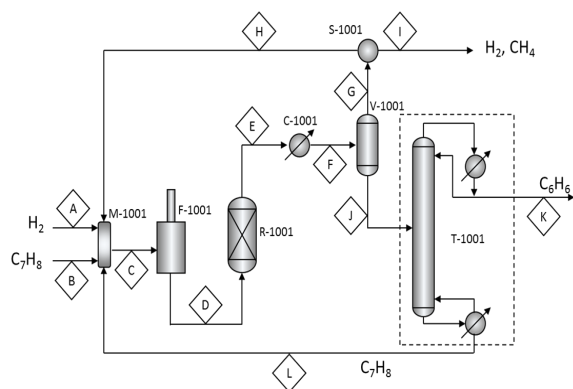

Fig. 10. Hydrodealkylation toluene plant for producing benzene.

The global reaction uses toluene and hydrogen as reactants to obtain bencene and methane as products by the chemical reaction: $C_6 H_5 CH_3 + H_2 \rightarrow C_6 H_6 + CH_4$. The system of equations that represents the process at T=620°C and P=3400 KPa is depicted in Table 6. Table 7 presents the meanings of the variables used in the model.

Resulting non-linear system includes 44 equations and 58 unknowns. To fix the degrees of freedom, the information in Table 8 is used. Upon setting these values, the system of equations becomes a performance evaluation. Henao (2010) reported one solution of this problem. Using *SphereSolver* add-in, three solutions were found (Table 9). The answer that satisfies the equilibrium conditions will be the one that represents the phenomena most accurately, but this question is beyond the scope of the current research.

Taking into account that this system of equations is multivariable, the representation of the homotopic

path in terms of the homotopic parameter *t* and the unknown variables is not practical. As shown in the Introduction section, the arc length *p* of the Homotopy function could be used as a new parameter to represent the path. In this manner, a graph of *p* vs. *t* describes the hotomopic path accurately, and each intersection with the horizontal line *t* = 1 represents a root of the original function. A wide set of initial values were tested, and at least one of the roots listed in Table 8 was always found. In Fig. 11, different homotopic paths are shown, where the same initial value, X_o, were used for all unknown variables. Most of them, except for $X_o = 6$, led to the three possible roots. For $X_o = 6$, only one root was found showing that the initial value of the homotopic path is still a relevant subject and must be explored in future researches.

4.3 Electronic circuits: Circuit with two-tunnel exponential diodes

Torres-Munoz *et al.* (2014), presents a circuit with two tunnel diodes, one voltage source and a resistor in series. Using the Kirchoff's current law, with E=1, R=20Ω, $I_p = 100 \times 10^{-3}$, $V_p = 50 \times 10^{-3}$, $I_0 = 1 \times 10^{-9}$ and $q/RT = 40$, eqs. (25) - (27) are obtained.

$$f_1 = \frac{1}{20} - \frac{v_1}{20} + I_{v_1} = 0 \tag{25}$$

$$f_2 = -\frac{1}{20} + \frac{v_1}{20} + 2(v_1 - v_2)e^{1-20v_1+20v_2}$$
$$+ 1 \times 10^{-9} e^{40v_1 - 40v_2} = 0 \tag{26}$$

$$f_3 = 2(v_1 - v_2)e^{1-20v_1+20v_2} + 1 \times 10^{-9} e^{40v_1 - 40v_2}$$
$$- 2v_2 e^{1-20v_2} - 1 \times 10^{-9} e^{40v_2} = 0 \tag{27}$$

Torres-Muñoz *et al.*, (2014) reported 5 solutions to this system of equations. Using *SphereSolver* with 0.5 as the initial value for all three variables, 9 solutions were found (Table 10). Therefore, it is demonstrated again that *SphereSolver* is a powerful tool for solving different kind of engineering problems.

Conclusions

SphereSolver, an add-in for use in Microsoft Office Excel© to solve systems of non-linear equations, was developed and applied to several engineering models. The Newton Homotopy Method was chosen over Affine and Fixed Point Homotopy as the main algorithm.

Table 6. Equations for benzene production model. Index 1, 2, 3, 4 refers to toluene; hydrogen; benzene; and methane, respectively.

| Unit	Type of equation	Equations
Mixer M-1001	Material balances	$C_1 = A_1 + B_1 + H_1 + L_1$ $C_2 = A_2 + B_2 + H_2 + L_2$ $C_3 = A_3 + B_3 + H_3 + L_3$ $C_4 = A_4 + B_4 + H_4 + L_4$
Furnace F-1001	Material balances	$D_1 = C_1$ $D_2 = C_2$ $D_3 = C_3$ $D_4 = C_4$
Reactor R-100 (Continuous stirred-tank reactor model)	Material balances	$E_1 = D_1 - r \cdot V$ $E_2 = D_2 - r \cdot V$ $E_3 = D_3 + r \cdot V$ $E_4 = D_4 + r \cdot V$
	Reaction kinetics equations	$r = kc_{1,E}c_{2,E}^{1/2}$ $k = k_0 \exp(-E_a/RT_E)$ $c_{1,E} = \frac{P_E}{RT_E}\left(\frac{E_1}{E_1+E_2+E_3+E_4}\right)$ $c_{2,E} = \frac{P_E}{RT_E}\left(\frac{E_2}{E_1+E_2+E_3+E_4}\right)$
Cooler C-1001	Material balances	$F_1 = E_1$ $F_2 = E_2$ $F_3 = E_3$ $F_4 = E_4$
Vessel V-1001	Material balances	$G_1 + J_1 = F_1$ $G_2 + J_2 = F_2$ $G_3 + J_3 = F_3$ $G_4 + J_4 = F_4$
	Operation equations	$G_1 = 0.0001 \cdot F_1$ $G_2 = 0.99 \cdot F_2$ $G_3 = 0.001 \cdot F_3$ $G_4 = 0.95 \cdot F_4$
Splitter S-1001	Material balances	$H_1 + I_1 = G_1$ $H_2 + I_2 = G_2$ $H_3 + I_3 = G_3$ $H_4 + I_4 = G_4$
	Operation equations	$H_1 = \alpha \cdot G_1$ $H_2 = \alpha \cdot G_2$ $H_3 = \alpha \cdot G_3$ $H_4 = \alpha \cdot G_4$
Distillation Tower T-1001	Material balances	$K_1 + L_1 = J_1$ $K_2 + L_2 = J_2$ $K_3 + L_3 = J_3$ $K_4 + L_4 = J_4$
	Operation equations	$K_1 = 0.0001J_1$ $K_2 = 0.9999 \cdot J_2$ $K_2 = 0.999 \cdot J_3$ $K_2 = 0.9999 \cdot J_4$
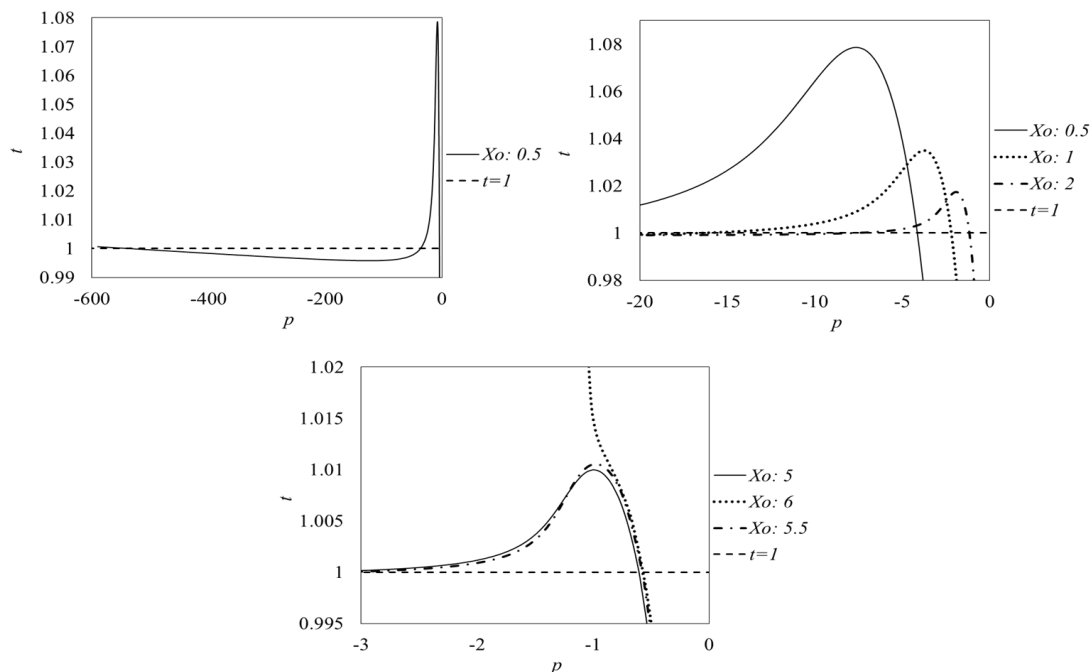
Fig. 11. Discretized homotopic path t vs. p for differential initial conditions, X_o, and different scales.

Table 7. Notation for the benzene production model.

Name	Definition
X_i	Molar flow of substance i in stream X, for $i = 1,..4$
V	Reactor volume
$c_{i,X}$	Molar concentration of substance i in stream X
T_E	Stream E temperature
P_E	Stream E pressure
r	Reaction rate
k	Reaction rate coefficient
α	Molar flow ratio of stream H to stream G
R	Universal gas constant: 8.314 kJ/kmol K

Table 8. Parameter values for the benzene production model.

Parameter	Units	Value
k_0	kmol$^{1/2}$/m$^{3/2}$ h	2.268×10^{14}
E_a	kJ/K kmol	2.18×10^5
V	m^3	100
α	-	0.7
T_E	K	893.15
P_E	kPa	3 400
A_1, A_3, A_4	kmol/h	0
A_2	kmol/h	130
B_2, B_3, B_4	kmol/h	0
B_1	kmol/h	100

Table 9. List of solutions for the benzene production model.

Variable	Units	Solution 1	Solution 2	Solution 3
C_1	kmol/h	225.4	15 524.9	532 750.5
C_2	kmol/h	197.76	202.25	354.04
C_3	kmol/h	0.17016	0.16678	0.05234
C_4	kmol/h	198.48	194.53	61.05
D_1	kmol/h	225.4	15 524.9	532 750.5
D_2	kmol/h	197.76	202.25	354.04
D_3	kmol/h	0.17016	0.16678	0.05234
D_4	kmol/h	198.48	194.53	61.05
E_1	kmol/h	125.4	15 427.0	532 719.8
E_2	kmol/h	97.77	104.25	323.29
E_3	kmol/h	100.15	98.16	30.80
E_4	kmol/h	298.46	292.53	91.80
F_1	kmol/h	125.4	15 427.0	532 719.8
F_2	kmol/h	97.77	104.25	323.29
F_3	kmol/h	100.15	98.16	30.80
F_4	kmol/h	298.46	292.53	91.80
G_1	kmol/h	0.013	1.543	53.272
G_2	kmol/h	96.80	103.21	320.05
G_3	kmol/h	0.1002	0.0982	0.0308
G_4	kmol/h	283.54	277.90	87.21
H_1	kmol/h	0.0088	1.0799	37.2904
H_2	kmol/h	67.76	72.25	224.04
H_3	kmol/h	0.0701	0.0687	0.0216
H_4	kmol/h	198.478	194.530	61.045
I_1	kmol/h	0.0038	0.4628	15.9816
I_2	kmol/h	29.039	30.963	96.016
I_3	kmol/h	0.0300	0.0294	0.0092
I_4	kmol/h	85.062	83.370	26.162
J_1	kmol/h	125.4	15 425.4	532 666.5
J_2	kmol/h	0.978	1.043	3.233
J_3	kmol/h	100.05	98.06	30.77
J_4	kmol/h	14.923	14.626	4.590
K_1	kmol/h	0.013	1.543	53.267
K_2	kmol/h	0.978	1.042	3.233
K_3	kmol/h	99.954	97.965	30.743
K_4	kmol/h	14.922	14.625	4.589
L_1	kmol/h	125.4	15 423.9	532 613.2
L_2	kmol/h	0.000098	0.000104	0.000323
L_3	kmol/h	0.100054	0.098063	0.030773
L_4	kmol/h	0.001492	0.001463	0.000459
$c_{1,E}$	kmol/m^3	0.092370	0.443639	0.457490
$c_{2,E}$	kmol/m^3	0.071992	0.002998	0.000278
r	kmol/m^{3}h	0.999837	0.979947	0.307518
k	kmol$^{1/2}$/m$^{3/2}$h	40.342	40.342	40.342

The proposed algorithm uses hyperspheres as a tracking method for the homotopic path, which has been proven to be a reliable method, following the path without losing it. The other two main elements of the algorithm are Euler's tangent plane as a predictor and Newton's method as the locally convergent method for the corrector step at each discretized point of the homotopic path.

Table 10. List of solutions for the circuit with two-tunnel exponential diodes.

Solution #	I_{v1}	v_1	v_2	Norm
1	-0.0282803	0.43439597	0.4285488	4.70×10^{-7}
2	-0.0421756	0.15648531	0.14713161	2.99×10^{-7}
3	-0.0488741	0.02252113	0.01126054	1.98×10^{-7}
4	-0.0421755	0.15648584	0.00935372	1.99×10^{-7}
5	-0.0336138	0.32772635	0.16386296	2.18×10^{-7}
6	-0.0189197	0.62160289	0.41818366	8.27×10^{-7}
7	-0.0099145	0.80171369	0.40085755	5.44×10^{-7}
8	-0.0189198	0.62159913	0.20341635	6.88×10^{-7}
9	-0.0282804	0.4343955	0.00584709	4.31×10^{-7}

Based on the obtained results, *SphereSolver* is shown to be a powerful tool for developing simulations in Microsoft Excel office, finding the solutions of the system of non-linear equations that represents the corresponding model. By comparison on the use of *SphereSolver* for solving the case study (section 3) and additional engineering problems (section 4) it is concluded that *SphereSolver* improves the numerical solution by increasing the interval range of the possible initial values that lead to the solution of the problems and/or increasing the amount of found roots.

SphereSolver uses Microsoft Excel Office ©, thus it offers a user-friendly spreadsheet environment, where models represented by algebraic equations (including transcendental functions) are introduced easily, presenting the information and results in an organized and personalized set up.

Acknowledgements

References

Allgower, E. L. and Georg, K. (1990). *Numerical Continuation Methods: An Introduction*, Springer, Berlin.

Bhattacharjya, R. K. (2010). Solving groundwater flow inverse problem using spreadsheet solver. *Journal of Hydraulic Engineering 16*, 472-477.

Bürgisser, P. and Cucker, F. (2013). Homotopy Continuation and Newton's Method. En: *Condition: The Geometry of Numerical Algorithms*, (P. Bürgisser, and F. Cucker, eds.), Pp. 283-294. Springer Science & Business Media.

Cveticanin, L., Kalami-Yazdi, M. and Askari, H. (2012). Analytical approximations to the solutions for a generalized oscillator with strong nonlinear terms. *Journal of Engineering Mathematics 77*, 211-223.

Davis, M. E. (1984). *Numerical Methods and Modeling for Chemical Engineers*, John Wiley & Sons, New York.

Fogler, H. S. (2016). *Elements of Chemical Reaction Engineering*, fifth ed., Pearson Education, New Jersey.

Georg, K. (1981). On tracing an implicitly defined curve by quasi-Newton steps and calculating bifurcation by local perturbations. *SIAM Journal on Scientific & Statistical Computing 2*, 35-50.

Henao, C. A. and Velásquez, J. A. (2004). Simulación de Procesos Químicos Empleando MS Excel® (I) -Aplicación de Métodos Homotópicos. *Ingeniería Química 26*, 16-22.

Henao, C. A. (2010). *Simulación and Evaluación de Procesos Químicos: Herramientas Básicas para la Síntesis de Procesos*, 1a ed., Universidad Pontificia Bolivariana, Medellín.

Huddleston, D., Alarcon, V. and Chen, W. (2004). Water distribution network analysis using Excel. *Journal of Hydraulic Engineering 130*, 1033-1035.

Jalali, F., Seader, J. D. and Khaleghi, S. (2008). Global solution approaches in equilibrium and stability analysis using homotopy continuation in the complex domain. *Computers & Chemical Engineering 32*, 2333-2345.

Jiménez-Islas, H. (1996). SEHPE: Programa para la solución de sistemas de ecuaciones no lineales mediante método homotópico con seguimiento hiperesférico. *Avances en Ingeniería Química 6*, 174-179.

Jimenez-Islas, H., Martinez-Gonzalez, G. M., Navarrete-Bolanos, J. L., Botello-Alvarez, J. E., and Oliveros-Muñoz, J. M. (2013). Nonlinear homotopic continuation methods: a chemical engineering perspective review. *Industrial & Engineering Chemistry Research 52*, 14729-14742.

Jiménez-Islas, H., Calderon-Ramírez, M., Molina-Herrera, F., Martínez-Gonzalez, G., Navarrete-Bolanos, J. and Castrejon-González, E. (2014). Algoritmo de bajo consumo de RAM para resolver problemas de convección natural 3-d, usando colocación ortogonal. *Revista Mexicana de Ingeniería Química 13*, 259-277.

Klopfenstein, R. (1961). Zeros of nonlinear functions. *Journal of the ACM 8*, 366-373.

Laiadi, D. and Merzougui, A. (2012). Homotopy method to predict liquid-liquid equilibria for ternary mixtures of (water + carboxylic acid + organic solvent). *Fluid Phase Equilibria 313*, 114-120.

Le Roux, J. P., Demirbilek, Z. and Flemming, B. W. (2010). WAVECALC: an Excel-VBA spreadsheet to model the characteristics of fully developed waves and their influence on bottom sediments in different water depths. *Geo-Marine Letters 30*, 549-560.

Lee, T. L., Li, T. Y. and Tsai, C. H. (2008). HOM4PS-2.0: a software package for solving polynomial systems by the polyhedral homotopy continuation method. *Computing 83*, 109-133.

Menglong, S. and Zhenxin, L. (2008). Modified homotopy methods to solve fixed points of self-mapping in a broader class of nonconvex sets. *Applied Numerical Mathematics 58*, 236-248.

Murdock, J. W. (1993). *Fundamental Fluid Mechanics for the Practicing Engineer*, first ed., CRC Press, New York.

Oliveros-Muñoz, J. and Jiménez-Islas, H. (2013). Hyperspherical path tracking methodology as

correction step in homotopic continuation methods. *Chemical Engineering Science 97*, 413-429.

Rahimian, S. K., Jalali, F., Seader, J. D. and White, R. E. (2011). A robust homotopy continuation method for seeking all real roots of unconstrained systems of nonlinear algebraic and transcendental equations. *Industrial & Engineering Chemistry Research 50*, 8892-8900.

Ramírez, A. D., Rodriguez, D. and González, N. D. (2006). Estudio experimental and numérico de la morfología de mezclas PS/PEAD preparadas por extrusión. *Revista Mexicana de Ingeniería Química 5*, 67-78.

Rodríguez, R. and Niño, Z. (2016). Evaluación de herramientas computacionales gratuitas para la simulación de procesos de combustión en motores de encendido por chispa. *Revista Mexicana de Ingeniería Química 15*, 977-984.

Smith, J. M., van Ness, H. G., and Abbott, M. M. (2005). *Introduction to Chemical Engineering Thermodynamics*, 7th Ed., McGraw-Hill Book Co., New York.

Thompson, S. L. (2006). A friendly Fortran DDE solver. *Applied Numerical Mathematics 56*, 503-516.

Torres-Munoz, D., Vazquez-Leal, H., Hernandez-Martinez, L. and Sarmiento-Reyes, A. (2014). Improved spherical continuation algorithm with application to the double-bounded homotopy (dbh). *Computational and Applied Mathematics 33*, 147-161.

Torres-Muñoz, D., Hernandez-Martinez, L. and Vázquez-Leal, H. (2015). Spherical Continuation Algorithm with Spheres of Variable Radius to Trace Homotopy Curves. *International Journal of Computational and Applied Mathematics 2*, 1-13.

Verschelde, J. and Cools, R. (1994). Symmetric homotopy construction. *Journal of Computational and Applied Mathematics 50*, 575-592.

Ward J. P. and King, J. R. (2012). Thin-film modelling of biofilm growth and quorum sensing. *Journal of Engineering Mathematics 73*, 71-92.

Watson, L. (2001). Globally convergent homotopy methods. En: *Encyclopedia of Optimization*, (C. A. Floudas, P. M. Pardalos, eds.), Pp. 893-898, Springer, US.

Wayburn, T. L. and Seader, J. D. (1987). Homotopy continuation methods for computer-aided process design. *Computers & Chemical Engineering 11*, 7-25.

Wong, T. S. and Zhou, M. (2004). Determination of critical and normal depths using excel. En: *Critical Transitions in Water and Environmental*

Resources Management, (G. Sehlke, D. F. Hayes and D. K. Stevens, eds.), Pp. 1-8. American Society of Civil Engineers, Salt Lake City, UT, USA.

Yamamura, K. (1993). Simple algorithms for tracing solution curves. *IEEE Transactions on Circuits and Systems I 40*, 537-541.

Yang, F., Chen, K. and Yu, B. (2012). Homotopy method for a mean curvature-based denoising model. *Applied Numerical Mathematics 62*, 185-200.