

MODELING AND SIMPLIFIED NUMERICAL SIMULATION OF THE (N¹⁵) ISOTOPIC SEPARATION COLUMN USING THE OPERATOR MATRIX (M_{dp_x})

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Abstract: Continuing the papers (Axente et al, 1994; Colosi et al, 2002; Colosi et al, 2003; Bogdan, 2005), are presented significant aspects of modeling and numerical simulation of a nonlinear partial differential equation (npde), used for study of the (N¹⁵) isotopic separation column. The originality of the paper is the definition and use of operator matrix (M_{dp_x}), which, beside the disadvantage of a relatively high volume of calculus, cumulates as the main advantage the *quasi-general applicability* of the method for linear or nonlinear partial differential equations.

Key words: partial differential equations, state variables, Taylor series, modeling and numerical simulation

1. INTRODUCTION

To study the (N¹⁵) isotopic separation column, it is used the following nonlinear partial differential equation (npde):

$$(a_{00} + a_{01}y) \cdot \frac{\partial y}{\partial p} + a_{10} \cdot \frac{\partial y}{\partial t} + a_{02} \cdot \frac{\partial^2 y}{\partial p^2} = \varphi(t, p) \quad (1)$$

where (t), (p) and $y = y(t, p)$ represents the time, column high and the (N¹⁵) isotope concentration, respectively. In the hypothesis of null productivity it is noted: $a_{00} = (\alpha - 1) \cdot L$, $a_{01} = 2(\alpha - 1) \cdot L$; $a_{10} = h + H$ and $a_{02} = -L^2/K$, where $\alpha = 1.055$; $h = 2.8$ atom N/m³; $H = 430$ atom N / m³; $L = 1382.4$ atom N / day; $K = 4060.8$ atom / day·m. The integration domains are between the limits: $t_0 = 0$ days; $t_f = 14$ days; $p_0 = 0$ m; $p_f = 7$ m; the (N¹⁵) initial concentration is $y_{00} = 0.365$ mol/m³; and the final concentration $y_{ff} = 8.2$ mol/m³.

Introducing the notations: $y = x_{00}$; $\frac{\partial y}{\partial t} = x_{10}$;

$\frac{\partial y}{\partial p} = x_{01}$; $\frac{\partial^2 y}{\partial p^2} = x_{02}$, the equation (1) became:

$$(a_{00} + a_{01} \cdot x_{00}) \cdot x_{01} + a_{10} \cdot x_{10} + a_{02} \cdot x_{02} = \varphi(t, p) \quad (2)$$

which, in the hypothesis of numerical integration with respect to time (t), allow the state vector $\mathbf{x}(1 \times 1)$ and implicit the state variable $x_{00} = y$ by form

$$\mathbf{x} = x_{00} \quad (3)$$

The known initial conditions (IC) are $\mathbf{x}_{IC} = x_{00IC} = x_{00}(t_0, p)$ and the final conditions (FC) and the possible boundary conditions (BC) are expressed by: $\mathbf{x}_{FC} = x_{00FC} = x_{00}(t_f, p)$ and $\mathbf{x}_{BC} = x_{00BC} = x_{00}(t, p_f)$, respectively.

The goal is the numerical integration of the (npde) (2) with respect to time (t_k) for different column high

(p), with the convenient choose of the parameters which define the forced solution, until $x_{00}(t_k, p=\text{const}) = y(t_k, p=\text{const})$ is close enough to the experimental curves, interpreted by the technologist.

2. THE OPERATOR MATRIX (\mathbf{M}_{dpx})

The definition and the use of the operator matrix (\mathbf{M}_{dpx}) is presented in (Colosi et al, 2002). In the following are detailed the matrix for the example (2):

$$\mathbf{M}_{\text{dpx}} = \begin{matrix} \begin{matrix} \xrightarrow{1} \\ \xrightarrow{M} \end{matrix} \\ \begin{matrix} \updownarrow n \\ \updownarrow N \end{matrix} \end{matrix} \left[\begin{array}{c|c} \mathbf{x} & \mathbf{x}_P \\ \mathbf{x}_T & \mathbf{x}_{TP} \end{array} \right] = \begin{matrix} \begin{matrix} \xrightarrow{1} & \xrightarrow{M} \\ \updownarrow 1 \\ \updownarrow N \end{matrix} \\ \left[\begin{array}{c|c} x_{00} & x_{0P} \\ x_{10} & x_{1P} \\ x_{20} & x_{2P} \\ \vdots & \vdots \\ x_{1+N,0} & x_{1+N,P} \end{array} \right] \end{matrix} \quad (4)$$

The matrix is partitioned for $n=1$ state variables, as follows:

- $\mathbf{x}(1 \times 1)$, the state vector (variable)
- $\mathbf{x}_T(N \times 1)$, the (N) time derived state vector
- $\mathbf{x}_P(1 \times M)$ matrix, which contains the total number of (M) partial differential – with respect to the variable (p) – of the state vector $\mathbf{x}(1 \times 1)$. Because at the calculus start ($t=t_0$) $\mathbf{x}_{IC} = \mathbf{x}_{0IC} = \mathbf{x}_{00}(t_0, p)$ is known, it can be operated with respect to (p) the (M) partial differential.
- $\mathbf{x}_{TP}(N \times M)$ matrix is successively calculated from the first element of the vector (\mathbf{x}_T), which results from the explicit form of (x_{10}) from (2) at $t=t_0$:

$$x_{10} = \frac{1}{a_{10}} \cdot [\varphi(t_0, p) - (a_{00} + a_{01}x_{00})x_{01} - a_{02} \cdot x_{02}]_{t_0} \quad (5)$$

with the note that all the components (x_{\dots}) from the right member are known from (\mathbf{x}_{IC}).

To calculate the first line of the matrix (\mathbf{x}_{TP}), respectively (\mathbf{x}_{1P}), are operated (M) partial differentials with respect to (p), with the note that all the partial results will be take from the previous calculated row, disposed above the current line.

This algorithm is repeated for (N) rows, after which it is finally obtained the operating matrix, at the start sequence (k-1)

$$\mathbf{M}_{\text{dpx},k-1} = \begin{matrix} \begin{matrix} \xrightarrow{1} & \xrightarrow{M} \\ \updownarrow 1 \\ \updownarrow N \end{matrix} \\ \left[\begin{array}{c|c} \mathbf{x}_{k-1} & \mathbf{x}_{P,k-1} \\ \mathbf{x}_{T,k-1} & \mathbf{x}_{TP,k-1} \end{array} \right] \end{matrix} \quad (6)$$

respectively.

The elements of the matrix ($\mathbf{M}_{\text{dpx},k-1}$) from (6) allow the approximation by (truncated) Taylor series of the

vector (\mathbf{x}_k) and the matrix ($\mathbf{x}_{P,k}$) form the obvious equations:

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \sum_{T=1}^{\omega} \frac{\Delta t^T}{T!} \mathbf{x}_{T,k-1} \quad (7)$$

$$\mathbf{x}_{P,k} = \mathbf{x}_{P,k-1} + \sum_{T=1}^{\omega} \frac{\Delta t^T}{T!} \mathbf{x}_{TP,k-1} \quad (8)$$

where to the sequences (k-1) and (k) corresponds the time $t_k = t_{k-1} + \Delta t$, with the integration step (Δt) small enough and $\omega \geq 4$.

With the results (7) and (8) is completed the first line of the vector ($\mathbf{M}_{\text{dpx},k}$) for the new sequence (k)

$$\mathbf{M}_{\text{dpx},k} = \begin{matrix} \begin{matrix} \xrightarrow{1} & \xrightarrow{M} \\ \updownarrow 2 \\ \updownarrow N \end{matrix} \\ \left[\begin{array}{c|c} \mathbf{x}_k & \mathbf{x}_{PQR,k} \\ \mathbf{x}_{T,k} & \mathbf{x}_{TPQR,k} \end{array} \right] \end{matrix} \quad (9)$$

respectively.

The calculus details for ($\mathbf{x}_{T,k}$) and ($\mathbf{x}_{TP,k}$) are identical with the previous presented (k-1) sequence, in conformity with the relations (5), (6), resulting the matrix (9) at the new sequence (k) and time (t_k), which is formally identical with the matrix (6), considered at the previous sequence (k-1) and time (t_{k-1}).

3. EXAMPLE RUN ON COMPUTER

Knowing that the equation (1) or (2), for $\varphi(t, p) = 0$, represents the Cohen equation, the goal is the use of a forced solution by form (10), which approximate close enough the experimental step responses, which are interpreted by the technologist as realistic ones. It is considered that the experimental form

$$y = y_{00} + \left(J_{0T} + J_{1T} \cdot \varepsilon^{-t/T_1} + J_{2T} \cdot \varepsilon^{-t/T_2} \right) \cdot \left(J_{0P} + J_{1P} \cdot \varepsilon^{-p/P_1} + J_{2P} \cdot \varepsilon^{-p/P_2} \right) \cdot (y_{ff} - y_{00}) \quad (10)$$

is usual in numerous thermo-chemical processes, close to the isotopic separation columns specifics, where the concentrations $y_{00} = y(t_0, p_0) = 0.365$ and $y_{ff} = y(t_f, p_f) = 8.2$ corresponds to the initial time ($t_0=0$) at the base of the column ($p_0=0$) and to the final time ($t_f = 14$ days) at the top of the column, respectively.

Are considered: $J_{0T}=1$; $J_{1T} = -\frac{T_1}{T_1 - T_2}$;

$J_{2T} = -\frac{T_2}{T_2 - T_1}$; $J_{0P}=1$; $J_{1P} = -\frac{P_1}{P_1 - P_2}$;

$J_{2P} = -\frac{P_2}{P_2 - P_1}$, where (T_1) and (T_2) are time

constants in days, and (P_1) and (P_2) can be interpreted as “length constant” in (m).

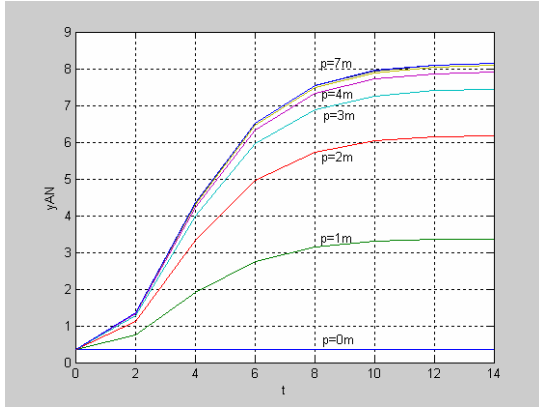


Figure 1. The analytical solutions

Replacing the forced solution (10) in (1) and (2), it is calculated $\varphi(t, p)$, which is used in (5) and in the following. After multiple testing of the solution (10) it is found out that for $T_1=1.3$ days, $T_2=1.7$ days, $P_1=0.7$ m and $P_2=0.9$ m, the analytical solutions family $y_{AN}(t, p)$, qualitatively presented in figure 1, is close to the experimental values and to the technologist appreciations to. As a result, for these parameters from (10), in conformity to the numerical simulation steps, based on the operator matrix (\mathbf{M}_{dpx}) , exposed above, the (npde) (1) and (2) was numerically integrated for $n=1$, $N=5$ and $M=9$.

In Table 1 is presented the analytical concentration values (y_{AN}) and the numerical approximated concentration values (x_{00}), with respect to time t (days), for different high p (m), with the integration step $\Delta t=0.01$. The same calculus was repeated for other integration steps, like is presented in Table 2.

The performance index of the numerical integration is defined by the cumulative relative error in percent:

$$\text{crepy} = 100 \cdot \frac{\sum_{k_0}^{k_f} |\Delta x_{00k}|}{\sum_{k_0}^{k_f} |y_{ANk}|} \quad (11)$$

where $\Delta x_{00k} = |y_{ANk} - x_{00k}|$ represents the absolute value of the sequential error between the analytical solution (y_{ANk}) and the numeric approximated solution (x_{00k}), between the limits $k_0=0$ and $k_f=t_f/\Delta t$. It can be remarked, from Table 2, that the decrease of (Δt) from (10^{-1}) to (10^{-4}) progressively decrease the maximal value of (crep) from 0.853% to $8 \cdot 10^{-4}\%$, for the same dimensions of the operator matrix $\mathbf{M}_{dpx}[(n+N) \times (1+M)] = \mathbf{M}_{dpx}[(1+5) \times (1+9)] = \mathbf{M}_{dpx}(6 \times 10)$, which certify the remarkable performances of this method, applied to nonlinear partial differential equation (npde) defined in (1) or (2). Of course, the decrease of dimensions (N) and especially (M) of the operator matrix (\mathbf{M}_{dpx}) contribute to (crep) with smaller values.

4. CONCLUSIONS

- 4.1. The paper is oriented strictly to the modeling and numerical simulation of a nonlinear partial differential equation by operator matrix (\mathbf{M}_{dpx}) , to approximate the concentration evolution $y(t, p)$ from the (N^{15}) isotopic separation column.
- 4.2. It is used the forced solution (10), with exponential evolutions, with respect to both the independent variables (t) and (p), assuring for $T_1=1.7$ days, $T_2=1.3$ days, $P_1=0.7$ m and $P_2=0.9$ m, a good approximation of the analytical solution $y_{AN}(t, p)$, with the experimental results and the technological specialist phenomenological interpretations.
- 4.3. The numerical approximation of the solution $x_{00}(t_k, p=\text{const})$, using the (\mathbf{M}_{dpx}) operator matrix method, leads to remarkable results, as results from Table 1 and Table 2, even at not too great dimensions of $\mathbf{M}_{dpx}(6 \times 10)$.
- 4.4. Not but that this method – considered original – needs a high volume of calculus, necessary to the program initialization, excel with quasi-general applicability for linear or nonlinear forms of partial differential equations.
- 4.5. The logical scheme based on this method is simple and flexible, without special programming methods.

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Table 1

t(days) p(m)		2	4	6	8	10	12	14	crep
7	y_{AN}	3.367	6.181	7.443	7.918	8.083	8.138	8.156	0.085
	x_{00}	3.385	6.190	7.447	7.920	8.084	8.138	8.156	
6	y_{AN}	3.347	6.142	7.396	7.868	8.032	8.086	8.104	0.085
	x_{00}	3.365	6.151	7.400	7.869	8.032	8.086	8.104	
5	y_{AN}	3.290	6.031	7.261	7.724	7.885	7.939	7.956	0.085
	x_{00}	3.307	6.041	7.265	7.726	7.886	7.939	7.956	
4	y_{AN}	3.133	5.729	6.893	7.331	7.484	7.534	7.550	0.085
	x_{00}	3.150	5.738	6.897	7.333	7.484	7.534	7.551	
3	y_{AN}	2.738	4.963	5.961	6.337	6.467	6.511	6.525	0.084
	x_{00}	2.753	4.971	5.964	6.338	6.468	6.511	6.525	
2	y_{AN}	1.898	3.335	3.979	4.222	4.306	4.334	4.343	0.081
	x_{00}	1.907	3.339	3.981	4.223	4.306	4.334	4.343	
1	y_{AN}	0.749	1.110	1.272	1.333	1.354	1.361	1.363	0.062
	x_{00}	0.752	1.111	1.272	1.333	1.354	1.361	1.363	
0	y_{AN}	0.365	0.365	0.365	0.365	0.365	0.365	0.365	0
	x_{00}	0.365	0.365	0.365	0.365	0.365	0.365	0.365	

Table 2

Δt	0.1	0.01	0.005	0.002	0.001	0.0001
crep max	0.853	$8.5 \cdot 10^{-2}$	$4.2 \cdot 10^{-2}$	$1.7 \cdot 10^{-2}$	$8 \cdot 10^{-3}$	$8 \cdot 10^{-4}$