

Analytical Modeling of an ^{15}N Isotope Separation Column by Second-Order Quasi-Linear Equations with Two Independent Variables

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Abstract—The presented process is an isotope separation column for ^{15}N , which represents a space propagation process modeled by the proposed method. Cohen's equation was approached by a second-order differential equation in relation to time t and also second-order in relation to the spatial variable s . This second order partial derivative equation was developed at an initial stage for which the variables $F_{0T}(t)$ and $F_{0S}(s)$ have been limited to two time constants (T_1, T_2), or space (S_1, S_2), resulting a family of curves of the ^{15}N $y_{00}(t, s)$ concentration.

Index Terms—Isotopic separation process, Cohen's equation, transcendent equations, M_{pdx} method.

I. INTRODUCTION

An isotope separation column for ^{15}N is modeled through a second order partial differential equation which is in relation to two independent variables, time and space. Among the multiple approximate solutions associated with the isotopic separation phenomena expressed in relation to the time (t) and the propagation space (s), it is considered the following overdamped version represented in the following equation [1], [2]:

$$y_{00}(t, s) = \tilde{y}_{00} + F_{0T}(t) \cdot F_{0S}(s) \cdot (\tilde{y}_{ff} - \tilde{y}_{00}) \quad (1)$$

The two exponentially increasing evolutions represented in the following figure are limited to being approximated by two time constants T_1 respective T_2 and two space constants S_1 respective S_2 .

The ascending exponential functions represented by the following two relations for the final values $F_{0T}(t) \rightarrow 1$ respective $F_{0S}(s) \rightarrow 1$ [1]-[4].

$$F_{0T}(t) = 1 - \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t}{T_1}} - \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t}{T_2}} \quad (2)$$

$$F_{0S}(s) = 1 - \frac{S_1}{S_1 - S_2} \cdot \varepsilon^{-\frac{s}{S_1}} - \frac{S_2}{S_2 - S_1} \cdot \varepsilon^{-\frac{s}{S_2}} \quad (3)$$

Taking into consideration the relations (2) respectively (3),

the complete expression of the approximating solution represented in relation (1) is presented as follows [2], [4]:

$$y_{00}(t, s) = \tilde{y}_{00} + \left(1 - \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t}{T_1}} - \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t}{T_2}}\right) \cdot \left(1 - \frac{S_1}{S_1 - S_2} \cdot \varepsilon^{-\frac{s}{S_1}} - \frac{S_2}{S_2 - S_1} \cdot \varepsilon^{-\frac{s}{S_2}}\right) \cdot (\tilde{y}_{ff} - \tilde{y}_{00}) \quad (4)$$

Considering the elements of the Cartesian system, namely $p = 0$ and $q = 0$, it follows that $s = r$ corresponds to the height of the column, $s_0 = 0$ respective $s_f = 7$ represents the final height of the column.

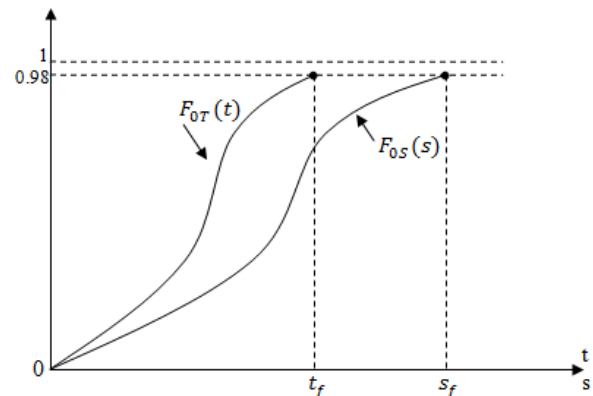


Fig. 1. Evolution of increasing functions.

With $t = t_0 = 0$ and $t = t_f = 14$ are noted the initial and final moments of the isotopic separation process.

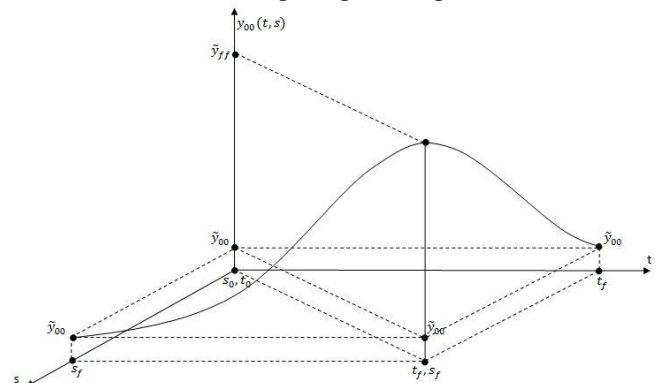


Fig. 2. Representation of the approximating solution

Where with \tilde{y}_{00} respective \tilde{y}_{ff} are noted the concentrations of the ^{15}N isotope in liquid phase, more precisely:

- $\tilde{y}_{00} = (t_0, s_0) = 0.365\%$

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- $\tilde{y}_{ff} = (t_f, s_f) = 8.2\%$

The relation represented in (4) is exemplified in Figure 2, this relation becoming:

- $y_{00}(t_0, s_0) = y_{00}(t_0, s_f) = y_{00}(t_f, s_0) = \tilde{y}_{00} = 0.365\%$
- $y_{00}(t_f, s_f) = \tilde{y}_{ff} = 8.2\%$

II. GENERAL OVERVIEW OF ANALYTICAL MODELING USING THE M_{PDX} METHOD

The simplified representation from Fig. 2 leads to an intuitive interpretation of the evolution $y_{00}(t, s)$ which represents the concentration of the isotope ^{15}N in the liquid form, in relation to the time (t) and the propagation height $s = r$ of the separation column. With the approximating solution $y_{00}(t, s)$ from (1), the partial derivatives expressed in relation (6) lead to much more unitary and systematized expressions than those resulting in M_{PDX} , presented in [3], directly associated with Cohen's equation.

$$y_{ij} = \frac{\partial^{i+j} y}{\partial t^i \partial s^j} \quad (6)$$

As a result, the following relations will be presented as follows [1], [2], [4]:

$$y_{ij} = F_{iT}(t) \cdot F_{jS}(s) \cdot (\tilde{y}_{ff} - \tilde{y}_{00}) \quad (7)$$

$$F_{iT}(t) = \frac{\partial^i F_{0T}(t)}{\partial t^i} = (-1)^i \left(\frac{1}{T_1^i} \cdot \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t}{T_1}} + \frac{1}{T_2^i} \cdot \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t}{T_2}} \right) \quad (8)$$

$$F_{jS}(s) = \frac{\partial^j F_{0S}(s)}{\partial s^j} = (-1)^j \left(\frac{1}{S_1^j} \cdot \frac{s_1}{s_1 - s_2} \cdot \varepsilon^{-\frac{s}{S_1}} + \frac{1}{S_2^j} \cdot \frac{s_2}{s_2 - s_1} \cdot \varepsilon^{-\frac{s}{S_2}} \right) \quad (9)$$

The results represented by the relations (7), (8) and (9) allow the partial derivation automatically with propagation indices, which further simplifies the calculations for the new expression of the M_{PDX} matrix. It can be shown that the approximate solution $y_{00}(t, s)$ verifies a second order partial derivatives equation in relation to (t) and (s) such as [5]-[9]:

$$a_{00} \cdot y_{00} + a_{10} \cdot y_{10} + a_{01} \cdot y_{01} + a_{02} \cdot y_{02} + a_{11} \cdot y_{11} + a_{20} \cdot y_{20} = K_y \cdot \varphi_{0.00} \cdot u_0 \quad (10)$$

where the K_y represents the proportionality constant, $\varphi_{0.00} = \varphi_{0.00}(t, s)$, u_0 is constant. The coefficients ($a_{...}$) are considered dependent both on time constants on space constants. Since the numerical integration will operate in relation to the time (t), according to which the equation (10) is second order, it results that the state vector consists two variables, respectively [5], [6]:

$$x(2 \times 1) = \begin{bmatrix} y_{00} \\ y_{10} \end{bmatrix} \quad (10)$$

As a result, the new general expression of the matrix of partial derivatives of state vector for the same $1 + M = n + N = 7$ become [1]-[4]:

$$M_{dpx} = \begin{bmatrix} x & x_s \\ x_T & x_{TS} \end{bmatrix} = \begin{bmatrix} y_{00} & y_{01} & y_{02} & y_{03} & y_{04} & y_{05} & y_{06} \\ y_{10} & y_{11} & y_{12} & y_{13} & y_{14} & y_{15} & y_{16} \\ y_{20} & y_{21} & y_{22} & y_{23} & y_{24} & y_{25} & y_{26} \\ y_{30} & y_{31} & y_{32} & y_{33} & y_{34} & y_{35} & y_{36} \\ y_{40} & y_{41} & y_{42} & y_{43} & y_{44} & y_{45} & y_{46} \\ y_{50} & y_{51} & y_{52} & y_{53} & y_{54} & y_{55} & y_{56} \\ y_{60} & y_{61} & y_{62} & y_{63} & y_{64} & y_{65} & y_{66} \end{bmatrix} \quad \begin{matrix} n = 2 \\ N = 5 \end{matrix} \quad \begin{matrix} 1 \\ M = 6 \end{matrix} \quad (11)$$

The two maximum order of partial derivation related to time (t), more precisely (N) and related to space (s), more precisely (M), are increased in order to provide lower approximation errors for the iterative calculation based on the Taylor Series. The calculation of the vector $x_T(5 \times 1)$ is obtained from the pivot element (y_{20}) which is derivate by $i = 1, 2, 3, N = 4$ in relation to time (t) resulting [7]-[9]:

$$y_{2+i,0} = \frac{1}{a_{20}} [K_y \cdot \varphi_{0.i0} \cdot u_i \cdot (a_{00} \cdot y_{i0} + a_{10} \cdot y_{1+i,0} + a_{01} \cdot y_{i1} + a_{02} \cdot y_{i2} + a_{11} \cdot y_{1+i,1})] \quad (12)$$

The calculation of the matrix $x_{ST}(5 \times 1)$ is obtained from the pivot element (y_{20}) which is successively derivate by $i = 1, 2, 3, N = 4$ in relation to time (t) and $j = 1, 2, 3, 4, 5, M = 6$ in relation to propagation space (s). As a result, these partial derivatives in relation to (t) and (s) are also obtained from the pivot element in the general form [1], [2]:

$$y_{2+i,j} = \frac{1}{a_{20}} [K_y \cdot \varphi_{0.ij} \cdot u_i \cdot (a_{00} \cdot y_{ij} + a_{10} \cdot y_{1+i,j} + a_{01} \cdot y_{i,j+1} + a_{02} \cdot y_{i,j+2} + a_{11} \cdot y_{1+i,j+1})] \quad (13)$$

III. VARIANTS OF APPROXIMATION OF STRUCTURE PARAMETERS BY TRANSCENDENT EQUATIONS

Qualitative evolutions for $F_{0T}(t)$ and $F_{0S}(s)$ are presented in the picture below, where $F_{0T}(t) \rightarrow 1$ and $F_{0S}(s) \rightarrow 1$ such as:

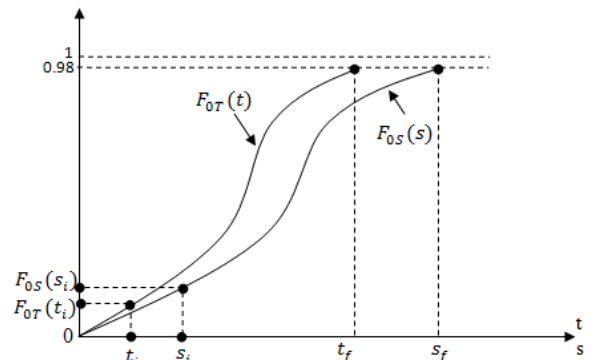


Fig. 3. Qualitative evolution of $F_{0T}(t)$ and $F_{0S}(s)$ functions.

The inflection abscises correspond to the following relations [1], [2], [5], [6]:

$$t_i = \frac{T_1 \cdot T_2}{T_2 - T_1} \ln \left(\frac{T_2}{T_1} \right) \quad (14)$$

$$s_i = \frac{S_1 \cdot S_2}{S_2 - S_1} \ln \left(\frac{S_2}{S_1} \right) \quad (15)$$

For the relations (2), (3), (14) and (15) the following notations are taken into consideration [1], [2], [5], [6]:

$$\lambda_T = \frac{T_2}{T_1} > 1 \quad (16)$$

$$\mu_T = \frac{t_f}{T_1 + T_2} > 1 \quad (17)$$

$$\lambda_S = \frac{S_2}{S_1} > 1 \quad (18)$$

$$\mu_S = \frac{s_f}{S_1 + S_2} > 1 \quad (19)$$

The approximation of these parameters is based on knowing the abscises (t_i), (t_f) and ordinate $F_{0T}(t) \rightarrow 1$ resulting the approximation of both T_1 and T_2 , but also knowing the abscises (s_i), (s_f) and ordinate $F_{0S}(t) \rightarrow 1$ resulting the approximation of both S_1 and S_2 . This is based on the numerical solution of the following transcendent equation [1], [2], [5], [6]:

$$F_{0T}(t_f) - \left(1 + \frac{1}{\lambda_T - 1} \cdot \varepsilon^{coef1} - \frac{\lambda_T}{\lambda_T - 1} \varepsilon^{coef2} \right) = DIF \quad (20)$$

where:

$$coef1 = -\frac{\lambda_T \ln \lambda_T}{\lambda_T - 1} \cdot \frac{t_f}{t_i} \quad (21)$$

$$coef2 = -\frac{\ln \lambda_T}{\lambda_T - 1} \cdot \frac{t_f}{t_i} \quad (22)$$

The start of calculations started with $\lambda_T = 1 + \Delta\lambda_T$ for $\Delta\lambda_T = 10^{-2} \sim 10^{-4}$ providing iterative increasing for (λ_T) until the difference (DIF) changes its mark, at which time the (DIF) is canceled, and (λ_T) corresponds to the solution of the transcendent equation. From (16), (17), (18) and (19) results the following relations which corresponds to the approximation of time constants (T_1) and (T_2) with an error, as low as the step ($\Delta\lambda_T$). [1], [2]:

$$\mu_T = \frac{\lambda_T \ln \lambda_T}{\lambda_T^2 - 1} \cdot \frac{t_f}{t_i} \quad (23)$$

$$T_1 = \frac{t_f}{\mu_T (1 + \lambda_T)} \quad (24)$$

$$T_2 = \lambda_T \cdot T_1 \quad (25)$$

The program developed for the numerical integration of transcendental equations is presented in the following [1], [2]:

L1: $t_f = 25$, $F_{0Tf} = 0.979$, $t_i = 3$, $F_{AS} = 230$, F_{0Ti} = informative

L2: $\Delta\lambda = 0.001$, $\lambda = 1 + \Delta\lambda$, $\lambda_{max} = 20$

$$L3: coef1 = -\frac{\lambda \ln \lambda}{\lambda - 1} \cdot \frac{t_f}{t_i} \quad coef2 = -\frac{\ln \lambda}{\lambda - 1} \cdot \frac{t_f}{t_i}$$

$$L4: DIF1 = [F_{0T}(t_f) - \left(1 + \frac{1}{\lambda_T - 1} \cdot \varepsilon^{coef1} - \frac{\lambda_T}{\lambda_T - 1} \varepsilon^{coef2} \right)] \cdot$$

F_{AS}

$$L5: \lambda = \lambda + \Delta\lambda$$

$$L6: coef1 = -\frac{\lambda \ln \lambda}{\lambda - 1} \cdot \frac{t_f}{t_i} \quad coef2 = -\frac{\ln \lambda}{\lambda - 1} \cdot \frac{t_f}{t_i}$$

$$L7: DIF2 = [F_{0T}(t_f) - \left(1 + \frac{1}{\lambda_T - 1} \cdot \varepsilon^{coef1} - \frac{\lambda_T}{\lambda_T - 1} \varepsilon^{coef2} \right)] \cdot$$

F_{AS}

$$L8: DIF = DIF1 \cdot DIF2$$

$$L9: \text{IF } DIF < 0 \text{ goto L12}$$

$$L10: \text{IF } \lambda \geq \lambda_{max} \text{ goto L16}$$

$$L11: \text{goto L3}$$

$$L12: \mu = \frac{\lambda \ln \lambda}{\lambda^2 - 1} \cdot \frac{t_f}{t_i}, T_1 = \frac{t_f}{\mu(1 + \lambda)}, T_2 = \lambda \cdot T_1$$

$$L13: F_{0Tf}(t) = 1 - \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t_f}{T_1}} - \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t_f}{T_2}}$$

$$L14: F_{0Ti}(t) = 1 - \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t_i}{T_1}} - \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t_i}{T_2}}$$

$$L15: \text{Print } \mu, T_1, T_2, F_{0Tf}, F_{0Ti}$$

$$L16: \text{STOP}$$

$$L17: t = 0, \Delta t = t_f/10$$

$$L18: F_{0T}(t) = 1 - \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t}{T_1}} - \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t}{T_2}}$$

$$L19: y_{00} = F_{0T} \cdot F_{AS}$$

$$L20: F_{1T}(t) = \frac{1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t}{T_1}} - \frac{1}{T_2 - T_1} \cdot \varepsilon^{-\frac{t}{T_2}}$$

$$L21: F_{2T}(t) = \frac{1}{T_1(T_1 - T_2)} \cdot \varepsilon^{-\frac{t}{T_1}} - \frac{1}{T_1(T_2 - T_1)} \cdot \varepsilon^{-\frac{t}{T_2}}$$

$$L22: \text{IF } t \geq t_f + \Delta t \text{ goto L25}$$

$$L23: \text{Print } t, F_{0T}, F_{1T}, F_{2T}, y_{00}$$

$$L24: t = t + \Delta t \text{ goto L18}$$

$$L25: \text{STOP}$$

$$L26: \text{END}$$

The transcendent equation calculates T_1 and T_2 from t_i , t_f , $F_{0T}(t_f)$ respectively F_{AS} , the value of the asymptote. The corresponding curves are shown in the figure below:

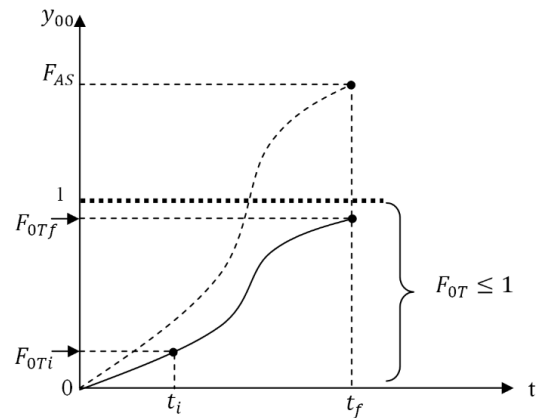


Fig. 4. Evolution of $F_{0Ti}(t)$ and $F_{0Tf}(t)$ function of the value of the asymptote.

Formally identical, space constants are also approximated resulting the following equations:

$$F_{0S}(s_f) - \left(1 + \frac{1}{\lambda_S - 1} \cdot \varepsilon^{coef1} - \frac{\lambda_S}{\lambda_S - 1} \varepsilon^{coef2} \right) = DIF \quad (26)$$

$$coef1 = -\frac{\lambda_S \ln \lambda_S}{\lambda_S - 1} \cdot \frac{s_f}{s_i} \quad (27)$$

$$\text{coef2} = -\frac{\ln \lambda_S \cdot \frac{s_f}{s_i}}{\lambda_S - 1} \quad (28)$$

$$\mu_S = \frac{\lambda_S \ln \lambda_S \cdot \frac{s_f}{s_i}}{\lambda_S^2 - 1} \quad (29)$$

$$S_1 = \frac{s_f}{\mu_S(1 + \lambda_S)} \quad (30)$$

$$S_2 = \lambda_S \cdot S_1 \quad (31)$$

IV. CORRECTION OF STRUCTURAL PARAMETERS IN RELATION TO PROPAGATION DEPTH

For the usual propagation case with stationary values $y_\alpha = y_{00}(t_{f\alpha}, s_0)$ and $y_\beta = y_{00}(t_{f\beta}, s_f)$, it is observed that $t_{f\beta} > t_{f\alpha}$. As a result, for this propagation inertia, which is increasing at the output s_f in comparison to the input s_0 , it follows that for the time constants the following relation is noted [1], [2], [5], [6]:

$$T_{1\beta} + T_{2\beta} > T_{1\alpha} + T_{2\alpha} \quad (32)$$

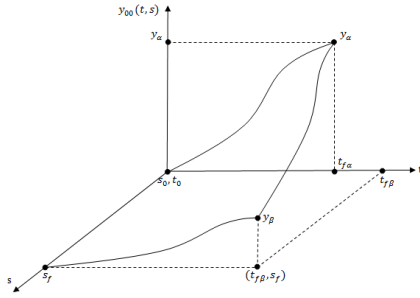


Fig. 5. Evolution of structural parameters.

The increasing trend for T_1 , which is also formally identical for T_2 , is approximated either as a dotted line, like the relation (33) or as a full exponential, like (34), as follows:

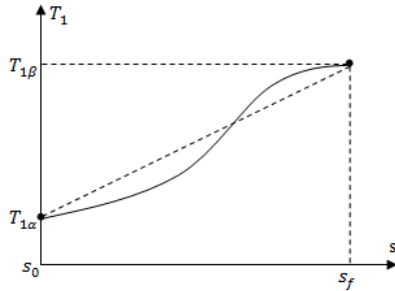


Fig. 6. Increasing evolution of T_1

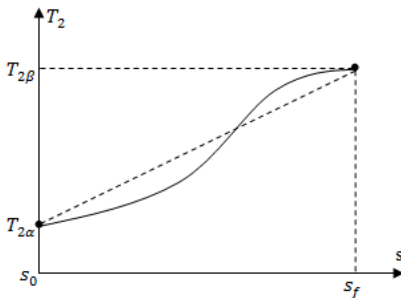


Fig. 7. Increasing evolution of T_2

$$T_1 = J_0 + J_1 \cdot s \quad (33)$$

$$T_1 = J_0 + J_1 \cdot \varepsilon^{-\frac{s}{s_1}} + J_2 \cdot \varepsilon^{-\frac{s}{s_2}} \quad (34)$$

From the conditions that the relations (33) and (34) verify the values $T_1(s_0) = T_{1\alpha}$ and $T_1(s_f) = T_{1\beta}$, but also the values $T_2(s_0) = T_{2\alpha}$ and $T_2(s_f) = T_{2\beta}$ results the following approximations represented in the relations, where (35) and (36) are linear approximations and (37) and (38) are exponentially approximations[1], [2], [5], [6]:

$$T_1 = T_{1\alpha} + \frac{T_{1\beta} - T_{1\alpha}}{s_f - s_0} \cdot s \quad (35)$$

$$T_2 = T_{2\alpha} + \frac{T_{2\beta} - T_{2\alpha}}{s_f - s_0} \cdot s \quad (36)$$

$$T_1 = T_{1\alpha} + \frac{T_{1\beta} - T_{1\alpha}}{\varepsilon^{-\frac{s_f}{s_1}} - \varepsilon^{-\frac{s_0}{s_1}}} \cdot \varepsilon^{-\frac{s}{s_1}} \quad (37)$$

$$T_2 = T_{2\alpha} + \frac{T_{2\beta} - T_{2\alpha}}{\varepsilon^{-\frac{s_f}{s_2}} - \varepsilon^{-\frac{s_0}{s_2}}} \cdot \varepsilon^{-\frac{s}{s_2}} \quad (38)$$

However, for both approximations, linear or exponential, the same approximate solution remains valid [1], [2], [5], [6]:

$$y_{00}(t, s) = K_y \cdot \left(1 - \frac{T_1}{T_1 - T_2} \cdot \varepsilon^{-\frac{t}{T_1}} - \frac{T_2}{T_2 - T_1} \cdot \varepsilon^{-\frac{t}{T_2}} \right) [y_\beta + (y_\alpha - y_\beta) \cdot \left(\frac{s_1}{s_1 - s_2} \cdot \varepsilon^{-\frac{s}{s_1}} - \frac{s_2}{s_2 - s_1} \cdot \varepsilon^{-\frac{s}{s_2}} \right)] \quad (39)$$

If $t_{f\beta} = t_{f\alpha}$ then $T_{1\beta} = T_{1\alpha}$ and $T_{2\beta} = T_{2\alpha}$ which emphasise the same propagation inertia in relation with time t , both on input $s = s_0$ and on output $s = s_f$.

Through a specialized detail for $F_{0T}(t)$ and $F_{0S}(s)$ with more than two time and space constants, the achieved performances for the concentration $y_{00}(t, s)$ are very close to the results experimentally found in the literature.

V. CONCLUSION

In this article, the presented process is an isotope separation column for ^{15}N , which represents a space propagation process modeled by the proposed method, more precisely a new approach of Cohen's equation, by a second-order differential equation in relation to time t and also second-order in relation to the spatial variable s .

At the initial stage of development, for the partial derivative equation of second order in relation to time t and space constant s , the variables $F_{0T}(t)$ and $F_{0S}(s)$ are limited at two, where time constants are (T_1, T_2) and space constants are (S_1, S_2) , in this way resulting a family of curves of the ^{15}N $y_{00}(t, s)$ concentration.

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