I. THE USE OF SPLINE-FUNCTIONS TO CALCULATE THE STEADY-STATE CONCENTRATION PROFILE IN COUNTERCURRENT EXTRACTION COLUMNS

By

K. KOLLÁR-HUNEK, J. HUNEK* and J. SAWINSKY*

Department of Mathematics of the Faculty of Chemical Engineering

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In previous works [1—3] the one dimensional diffusion model has been used to describe the steady-state concentration profile along an extraction column. The equations of the model are as follows:

$$\frac{d^2x}{dz^2} + A_1 \frac{dx}{dz} + B_1 x + C_1 y = 0$$
$$\frac{d^2x}{dz^2} + A_2 \frac{dy}{dz} + B_2 y + C_2 x = 0 \tag{1}$$

The boundary conditions are:

$$\frac{dx}{dz} + A_1 x = D_1 \quad \text{and} \quad \frac{dy}{dz} = 0 \quad \text{if} \quad z = 0$$
$$\frac{dy}{dz} + A_2 y = D_2 \quad \text{and} \quad \frac{dx}{dz} = 0 \quad \text{if} \quad z = 1 \tag{2}$$

In the present work an approximate solution to the above differential equation system has been obtained by using Spline functions.

In our calculations the coefficients $A_1 \ldots D_1$, $A_2 \ldots D_2$ have been fixed constants. However, the calculations may be carried out for coefficients which are functions of column length, z. If the condition of linearity is given up, the calculations become more complicated [4].

The approximate solution of the differential equation system was obtained by cubic polynomial univariant Spline functions. The Spline function was defined in terms of its first derivative [5] [6]:

A distribution interval between [0; 1] may be

$$\Delta: 0 = z_1 < z_2 < \ldots < z_j < \ldots < z_n = 1$$

where

$$z_j = (j - 1) \cdot h \qquad \text{and} \qquad h = \frac{1}{n-1} \tag{3}$$

*Department of Chemical Engineering, Technical University, Budapest

In the case the form of Spline function is:

$$S_\Delta(z) = g_j + S_j(z - z_j) + \left(3\,\frac{g_{j+1} - g_j}{h^2} - \frac{S_{j+1} - 2S_j}{h}\right)(z - z_j)^2 + \left(\frac{S_{j+1} + S_j}{h^2} - 2\,\frac{g_{j+1} - g_j}{h^3}\right)(z - z_j)^3 \quad (4)$$

if $\quad z_j \leq z \leq z_{j+1} \quad (j = 1, 2, \ldots (n-1))$

A Spline function in this form (4) can be applied for $X(z)$ as well as for $Y(z)$ concentration functions. Thus, altogether $4n$ $(j = 1, 2, \ldots, n)$ parameters have to be determined with the symbols X_j and Y_j for the constants g_j, and SX_j and SY_j for S_j.

The determining equations are the following:

$$\frac{1}{h}\cdot SX_{j-1} + \frac{4}{h}\cdot SX_j + \frac{1}{h}\cdot SX_{j+1} + \frac{3}{h^2}\,X_{j-1} - \frac{3}{h^2}\cdot X_{j+1} = 0$$

$$\frac{1}{h}\cdot SY_{j-1} + \frac{4}{h}\cdot SY_j + \frac{1}{h}\cdot SY_{j+1} + \frac{3}{h^2}\,Y_{j-1} - \frac{3}{h^2}\cdot Y_{j+1} = 0$$

$$j = 2, 3, \ldots (n-1) \quad (5a)$$

$$\left(-\frac{4}{h} + A_1\right)\cdot SX_j - \frac{2}{h}\cdot SX_{j+1} + \left(-\frac{6}{h^2} + B_1\right)\cdot X_j + \frac{6}{h^2}\cdot X_{j+1} + C_1\cdot Y_j = 0$$

$$j = 1, 2, \ldots (n-1)$$

$$\left(\frac{4}{h} + A_1\right)\cdot SX_n + \frac{2}{h}\cdot SX_{n-1} + \left(-\frac{6}{h^2} + B_1\right)\cdot X_n + \frac{6}{h^2}\cdot X_{n-1} + C_1\cdot Y_n = 0 \quad (5b)$$

$$\left(-\frac{4}{h} + A_2\right)\cdot SY_j - \frac{2}{h}\cdot SY_{j+1} + \left(-\frac{6}{h^2} + B_2\right)\cdot Y_j + \frac{6}{h^2}\cdot Y_{j+1} + C_2\cdot X_j = 0$$

$$j = 1, 2, \ldots (n-1)$$

$$\left(\frac{4}{h} + A_2\right)\cdot SY_n + \frac{2}{h}\cdot SY_{n-1} + \left(-\frac{6}{h^2} + B_2\right)\cdot Y_n + \frac{6}{h^2}\cdot Y_{n-1} + C_2\cdot X_n = 0 \quad (5c)$$

and
$$SX_1 + A_1 \cdot X_1 = D_1$$
$$SX_n = 0$$
$$SY_1 = 0$$
$$SY_n + A_2 \cdot Y_n = D_2 \quad (5d)$$

Among these equations the continuity of the first and second derivatives of the Spline functions is described by (5a). The differential equation system (1) gives (5b) and (5c) and the boundary conditions (2) results in (5d).

Equation system (5) obviously consists of 4n equations having 4n unknown parameters. This linear equation system has been solved by the Gaussian method.

Table I

No. of dataset	N_{ez}	Pe_z	Pe_y	k	Note
1	2	2	2	2	In all
2	2	2	8	2	cases the
3	2	4	1	2	$f = 1$
4	2	4	4	2	$x_{in} = 1$
5	2	4	16	2	$y_{in} = 0$
6	8	4	1	2	
7	8	8	8	2	condition
8	4	2	8	4	is fulfilled
9	4	4	1	4	
10	4	4	4	4	

Table II

$h = 0.1$

Z	X Spline	X Literature	$\Delta X \cdot 10^4$	Y Spline	Y Literature	$\Delta Y \cdot 10^4$
0.00	0.7218	0.7218	0	0.2977	0.2970	7
0.05	0.6947	0.6947	0	0.2967	0.2960	7
0.15	0.6445	0.6445	0	0.2895	0.2888	7
0.50	0.5031	0.5032	—1	0.2372	0.2323	4
0.85	0.4167	0.4172	—5	0.1562	0.1559	3
0.95	0.4068	0.4073	—5	0.1328	0.1326	2
1.00	0.4055	0.4059	—4	0.1208	0.1206	2
	$\Sigma\|\Delta X\| = 0.0015$			$\Sigma\|\Delta Y\| = 0.0032$		

h = 0.04 x

Z	X Spline	X Literature	$\Delta X \cdot 10^4$	Y Spline	Y Literature	$\Delta Y \cdot 10^4$
0.00	0.7219	0.7218	1	0.2971	0.2970	1
0.05	0.6948	0.6947	1	0.2961	0.2960	1
0.15	0.6445	0.6445	0	0.2890	0.2888	2
0.50	0.5032	0.5032	0	0.2324	0.2323	1
0.85	0.4171	0.4172	—1	0.1560	0.1559	1
0.95	0.4073	0.4073	0	0.1326	0.1326	0
1.00	0.4059	0.4059	0	0.1207	0.1206	1
	$\Sigma\lvert\Delta X\rvert = 0.0003$			$\Sigma\lvert\Delta Y\rvert = 0.0007$		

The calculation of the concentration profile was done by the approximate method using the Spline functions for the model parameter values given in Table 1. The calculation results have been compared with those published by McMULLEN, MIYAUCHI and VERMEULEN [7].

This comparison is shown in Table 2 for the results of dataset No 1. with two different values of the distribution interval *h*.

Summary

The axial mixing has a considerable effect on the concentration profile and consequently on the effectivity of an extraction column. The present work presents the Spline-approximative solution of the differential equation system of the one dimensional diffusion model for calculating concentration profiles.

The accuracy of the method has been shown by comparing the results to the ones calculated by the exact solution [7]. The advantage of our present method is that it can be extended for models with non-constant coefficients, too.

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Klára KOLLÁR-HUNEK
dr. József HUNEK
dr. János SAWINSKY

H-1521 Budapest

Notation

f phase ratio
$g_j = S_\Delta(z_j)$ value of $S_\Delta(z)$ at z_j
h length of the distribution interval
k distribution coefficient
n number of dividing points of the length z
N_{0x} true Number of Transfer Units
Pe Peclet number
$S(z)$ Spline function for distribution
SX first derivative of $X(z)$ Spline function
SY first derivative of $Y(z)$ Spline function
x concentration in the raffinate phase
y concentration in the extract phase
z dimensionless length of the column
X dimensionless concentration in the raffinate phase
Y dimensionless concentration in the extract phase

Subscripts

in inlet
j serial number of dividing point of the length z
o overall
x raffinate phase
y extract phase