# II. THE USE OF SPLINE-FUNCTIONS TO CALCULATE THE PARAMETERS OF THE ONE DIMENSIONAL DIFFUSION MODEL FROM THE CONCENTRATION PROFILE IN COUNTERCURRENT EXTRACTION

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In general, two mathematical models have been used to describe the steady-state concentration profiles in countercurrent extraction columns [1, 2]. In this work a method is given for the calculation of the parameters of the one dimensional diffusion model established by SCHLEICHER [3], MIYAUCHI and VERMEULEN [4] from concentration profile data. The method is based on our previously published approximate solution using Spline functions [6].

The differential equation system of the one dimensional diffusion model is based on the steady-state material balance of the distributed component:

$$\frac{dx}{dz} - \frac{1}{Pe_x} \cdot \frac{d^2x}{dz^2} + N_{0x}\left(x - \frac{y}{k}\right) = 0 \tag{1a}$$

$$f \cdot \left(-\frac{dy}{dz} - \frac{1}{Pe_y} \cdot \frac{d^2y}{dz^2}\right) - N_{0x}\left(x - \frac{y}{k}\right) = 0 \tag{1b}$$

The boundary conditions are

$$\left.\begin{aligned} x - \frac{1}{Pe_x} \cdot \frac{dx}{dz} &= x_{\text{in}} \\ \frac{dy}{dz} &= 0 \end{aligned}\right\} \quad \text{at} \quad z = 0$$

$$\left.\begin{aligned} \frac{dx}{dz} &= 0 \\ y + \frac{1}{Pe_y} \cdot \frac{dy}{dz} &= y_{\text{in}} \end{aligned}\right\} \quad \text{at} \quad z = 1$$

The problem for which the solution is described here is the calculation of the Number of Transfer Units, $N_{0x}$, and one of the Peclet numbers ($Pe_x$ or $Pe_y$) when the other Peclet number, the phase ratio, $f$, the distribution coeffi-

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cient, $k$, and the concentration profile data at $z_j$ points of the column, $x_j$ and $y_j$ ($j = 1, 2, \ldots n$), are given.

*Calculation of* $N_{0x}$ *and* $Pe_y$ ($\mathrm{Pe}_x$ is given)

A univariant cubic interpolating Spline function was determined to the given $\{z_j; x_j\}_{j=1}^n$ points with the boundary conditions

$$\left(\frac{dx}{dz}\right)_{z=0} = Pe_x(x_1 - x_{in}); \qquad \left(\frac{dx}{dz}\right)_{z=1} = 0 \tag{2a}$$

This Spline function can be differentiated twice and in this way gives a good approximation to the first and second derivatives of the $x(z)$ function. Using the Spline function in this way the values of $\frac{dx}{dz}$ and $\frac{d^2x}{dz^2}$ are calculated at points $z_j$ ($j = 1, 2, \ldots n$).

Furtheron the value of $N_{0x}$ was calculated accepting the average of the NTU values calculated from each point.

For the determination of $\mathrm{Pe}_y$ — the Spline function calculated to the $\{z_j; y_j\}_{j=1}^n$ points was required. From the function derivatives $\frac{d^2y}{dz^2}$ and $\frac{dy}{dz}$ can be calculated at points $z_j$ and in this way $\mathrm{Pe}_y$ can be determined from equation (1b).

The boundary condition of the Spline function $y(z)$ contains the unknown Peclet number. These conditions are the following

for the starting point

$$\left(\frac{dy}{dz}\right)_{z=0} = 0$$

and for the endpoint (2b)

$$\left(\frac{dy}{dz}\right)_{z=1} = Pe_y(y_{in} - y_n)$$

Combining equations (1b) and (2b) the following function is given

$$\mathrm{Pe}_y = \Phi(\mathrm{Pe}_y) \tag{3}$$

For the approximative solution of equation (3), a fixed point trial and error method seems to be applicable, but in this case it was found to be divergent. For this reason the method of regula falsi was applied for finding the root of equation (3a):

$$\Phi(\mathrm{Pe}_y) - \mathrm{Pe}_y = 0 \tag{3a}$$

*Calculation of $N_{0x}$ and $Pe_x$* ($Pe_y$ is given)

The method of calculation is similar to the previous case, but the equations (1a) and (1b), as well as (2a) and (2b) change their roles respectively and consequently in the equations (3) and (3a) the unknown parameter is $Pe_x$.

*The results of the calculations*

The values of the Number of Transfer Units and those of $Pe_y$ were determined from ten different concentration profile datasets at given $Pe_x$ values. $N_{0x}$ and $Pe_y$ values calculated accordingly were compared with the ones given in the literature [7]. This comparison is shown in Table 1. In all cases the values of $f = 1$; $x_{in} = 1$; $y_{in} = 0$ were used.

**Table I**

| Dataset | Input data | | $N_{0x}$ | | $Pe_y$ | |
|---|---|---|---|---|---|---|
| | $k$ | $Pe_x$ | Calculated | Lit. [7] | Calculated | Lit. [7] |
| 1 | 2 | 2 | 2.02 | 2 | 2.03 | 2 |
| 2 | 2 | 2 | 1.99 | 2 | 7.50 | 8 |
| 3 | 2 | 4 | 1.99 | 2 | 1.01 | 1 |
| 4 | 2 | 4 | 2.00 | 2 | 4.06 | 4 |
| 5 | 2 | 4 | 1.98 | 2 | 15.00 | 16 |
| 6 | 2 | 4 | 7.98 | 8 | 0.98 | 1 |
| 7 | 2 | 8 | 8.00 | 8 | 8.01 | 8 |
| 8 | 4 | 2 | 3.93 | 4 | 7.62 | 8 |
| 9 | 4 | 4 | 3.96 | 4 | 0.98 | 1 |
| 10 | 4 | 4 | 4.03 | 4 | 4.10 | 4 |

The calculations were performed using an ALGOL programm on an ODRA 1204 computer. The job time for the calculation of one dataset was 25—30 seconds and the maximum number of iteration steps was ten in the interval $0 \leq Pe_y \leq 100$.

Summarizing the results a calculation method was developed for the determination of the parameters ($Pe_x$ or $Pe_y$ and $N_{0x}$) of the one dimensional diffusion model from steady state concentration profile data in extraction columns. The method is based on the solution of the differential equation system and boundary conditions of the model by the use of Spline functions.

## Summary

For a given concentration profile in an extractor the parameters of the one dimensional diffusion model have been determined by using Spline functions. The accuracy of this method has been tested and is shown here by comparing the calculated parameters with ones used for the exact concentration profile calculations [7].

The advantage of our present method is that it can be extended for models with non-constant parameters as well.

## References

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## Notation

| | |
|---|---|
| $x$ | concentration in the raffinate phase |
| $y$ | concentration in the extract phase |
| $z$ | dimensionless length of the column |
| Pe | Peclet number |
| $N_{ox}$ | true number of transfer units |
| $k$ | distribution coefficient |
| $f$ | phase ratio |

Subscripts

| | |
|---|---|
| $o$ | overall |
| $x$ | raffinate phase |
| $y$ | extract phase |
| $in$ | inlet |