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MATHEMATICAL MODELLING OF ABSORPTION COLUMNS II. PARAMETER SENSITIVITY AND METHODS FOR ITS CALCULATION

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The idea "parameter sensitivity" is defined for various operational units and the models enabling their calculation have been described. The Piston Flow Model (P.F. Model), suitable for the description of two-phase countercurrent operational units has two dimensionless parameters, whereas the Axial Dispersed Plug Flow Model (A.D.P.F. Model) has four. In the case of both models, the number of physical quantities and figures characteristic of the working state included in these dimensionless parameters is very large.

This paper deals with the analytical solution used for the calculation of the sensitivities.

The theoretical connections are supplemented by a number of numerical examples, calculated by both analog and digital computers, presenting an illustration of the practical application of parameter sensitivity.

In the first paper [1] of this series, the mathematical modelling of a packed absorption column was described. An experimental method was presented for the determination of the absorbed component in both of the phases, along the packed column. The experimental results were processed on the basis of the P.F. Model and the A.D.P.F. Model. The mathematical models describe the modelled reality only with a limited accuracy. The inaccuracy of the models is brought about by two causes. Firstly, they can give only a phenomenological description of reality. The complicated connections and phenomena of a real system are attributed by the model to the collective influence of only two or three factors. For example, in a packed absorption column, the individual elements of the streaming liquid phase may move in any direction of space with a different and variable velocity. In the P.F. Model, this complicated flow pattern is ignored and the process is characterized by mean values. The A.D.P.F. Model characterizes the flow occurring in the real system by two parameters: the mean flow rate and the mixing coefficient. Accordingly, in both cases a schematic pattern is forced upon the reality.

The second reason for the inaccuracy of the parameters is the method of determination. The parameters of the models, such as rate, mixing coefficient, and transfer coefficient, etc., cannot be calculated, but the results of experiments carried out with a real apparatus are processed on the basis of the chosen model. The source of errors is, on the one hand, experimental errors, and, on the other, the errors of the calculation method.

It is our aim in the mathematical description of the operational units to present a description which is,for a given purpose, of adequate accuracy, and as simple as possible. Generally much experimental and calculation work is necessary to produce models which approximate the reality. It is not justified to carry this out if a simpler description also offers satisfactory accuracy. In the solution of such tasks, the knowledge of the parameter sensitivity of the model comes very useful.

The mathematical description of two-phase operational units is often possible by models of the same type, the only difference being the values of the parameters. This paper deals with the generally used P.F. and A.D.P.F. Models.

Studies on the sensitivity of operational units against changes in the parameters proved to be very useful in reactor technique. However, in the field of diffusion operations in chemical engineering there are practically no papers that deal with this problem.

Both for the researcher and the practical worker in the field, the knowledge of how far a change in some property of the apparatus or in the technological parameters may change, the operation of the apparatus is of real practical importance. Such and similar questions may be answered if the parameter sensitivity is known.

The problem of parameter sensitivity is also encountered in the solution of models describing the operational units. This knowledge may also be helpful in choosing the means and methods of calculation.

In the case of all models used in connection with the calculation of operational units, the dependent variables are in all phases the concentration and temperature of the component, and the independent variable is, when a stationary state is examined, the place co-ordinate. In addition to these, a number of parameters, such as e.g. the rate of the phases, transfer coefficients, retention, mixing coefficients, and the concentration of the components along the edges, etc., are applied in the models. This connection is expressed for the variable x_j by the function $x_j\,(z, p_1, p_2, p_i \dots p_n)$. In the case of a given set of parameter values $(p_1, p_2 \dots p_n)$ the sensitivity with respect to the parameter p_i can be defined by the following equation:

$$e_{j,i}\,(z, p_1, p_2 \dots p_n) = \frac{\partial x_j(z, p_1, p_2 \dots p_n)}{\partial p_i} \qquad (1)$$

where x_j is one of the dependent variables and p_i is the parameter with respect to which the sensitivity is examined. Often it is preferable to express this sensitivity in a dimensionless form:

$$E_{j,i} = \frac{p_i}{x_j(z,p_1,p_2,\dots p_n)}\, e_{j,i} \qquad (2)$$

This paper describes the calculation methods serving the determination of parameter sensitivity on the basis of the most frequently used models.

1. The Sensitivity of the P.F. Model

Two-phase operational units are very frequently described by the following model (cf. Equations (4) and (5) in [1], if A = 1):

$$\frac{dx}{dz} + \frac{\beta\omega Z}{v_L}(y - x) = 0 \tag{3}$$

$$\frac{dy}{dz} + \frac{\beta\omega ZH}{v_G}(y - x) = 0 \tag{4}$$

where

$$x = \frac{c_L}{Hc_{G,in}} ; \qquad y = \frac{c_G}{c_{G,in}}$$

The boundary conditions pertaining to the model are the following:

$$y(0) = 1 \tag{5}$$

$$x(1) = x_{in} \tag{6}$$

The model has two dimensionless parameters:

$$St_L = \frac{\beta\omega Z}{v_L} \qquad \text{and} \qquad St_G = \frac{\beta\omega ZH}{v_G}$$

The sensitivity of the model with respect to these two parameters will now be examined.

The following designations for the sensitivity are introduced:

$$e_{11} = \frac{\partial x}{\partial St_L}; \quad e_{21} = \frac{\partial y}{\partial St_L}; \quad e_{12} = \frac{\partial x}{\partial St_G}; \quad e_{22} = \frac{\partial y}{\partial St_G}$$

The functions $x(z)$ and $y(z)$ are obtained at given parameter values, by the solution of Equations (3) and (4) as well as condition Equations (5) and (6).

Let Equations (3), (4), (5) and (6) be differentiated with respect to St_L. In this case, the set of equations expressing the sensitivity with respect to St_L is obtained:

$$\frac{\partial^2 x}{\partial St_L \partial z} + St_L\left(\frac{\partial y}{\partial St_L} - \frac{\partial x}{\partial St_L}\right) + (y - x) = 0 \tag{7}$$

$$\frac{\partial^2 y}{\partial St_L \partial z} + St_G\left(\frac{\partial y}{\partial St_L} - \frac{\partial x}{\partial St_L}\right) + \frac{\partial St_G}{\partial St_L}(y - x) = 0 \tag{8}$$

The boundary conditions for this set of differential equations can be derived from Equations (5) and (6). The values y(0) and x(1), i.e. the concentration at which the phases enter the apparatus, are independent of the Stanton figures, and consequently the boundary condition can also be written in the following form:

$$\left.\frac{\partial y}{\partial St_L}\right|_{z=0} = 0 \tag{9}$$

$$\left.\frac{\partial x}{\partial St_L}\right|_{z=1} = 0 \tag{10}$$

With application of the signs introduced for the designation of the sensitivity, we may write:

$$\frac{\partial e_{11}}{\partial z} + St_L(e_{21} - e_{11}) + (y - x) = 0 \tag{11}$$

$$\frac{\partial e_{21}}{\partial z} + St_G(e_{21} - e_{11}) + \frac{\partial St_G}{\partial St_L}(y - x) = 0 \tag{12}$$

$$e_{21}(0) = 0 \tag{13}$$

$$e_{11}(1) = 0 \tag{14}$$

In a similar manner, the following set of differential equations is obtained for the sensitivity with respect to St_G:

$$\frac{\partial e_{12}}{\partial z} + St_L(e_{22} - e_{12}) + \frac{\partial St_L}{\partial St_G}(y - x) = 0 \tag{15}$$

$$\frac{\partial e_{22}}{\partial z} + St_G(e_{22} - e_{12}) + (y - x) = 0 \tag{16}$$

$$e_{22}(0) = 0 \tag{17}$$

$$e_{12}(1) = 0 \tag{18}$$

The values of the functions $x(z)$, $y(z)$, $e_{11}(z)$, $e_{12}(z)$, $e_{21}(z)$ and $e_{22}(z)$ are obtained from the solution of the set of Differential Equations (3) ... (18), at a given set of parameter values.

Functions $x(z)$ and $y(z)$ can be produced without solving the sensitivity equations. The sensitivities can be obtained without any difficulty if the functions $x(z)$ and $y(z)$ are known in an analytical way by solving the sets of differential equations or by derivating $x(z)$ and $y(z)$. For example, the following equation was obtained for the sensitivity of the concentration y with respect to St_L:

$$e_{21} = [1 - x(1)]\{[1 - \frac{\partial St_G}{\partial St_L} + \frac{1}{St_L} - \frac{1}{St_G}\frac{\partial St_G}{\partial St_L}]\exp(St_L - St_G) \times$$

$$\times[\exp[(St_L - St_G)z] - 1] + \frac{(1 - \frac{\partial St_G}{\partial St_L})\ z\ \exp[(St_L - St_G)z]}{\frac{St_G}{St_L} - \exp(St_L - St_G)}\}\frac{St_G}{St_L} \tag{19}$$

It is apparent from the above equation that the sensitivity is a function of the place co-ordinate z and different sensitivity values are obtained at different sets of parameter values.

It has been supposed in the foregoing [cf. Equations (3) and (4)] that the component equilibrium among the phases can be described by a straight line starting from the origo. Equilibrium conditions different from this pattern are often encountered in practice, and consequently the analytical solution of the above sets of differential equations is difficult. Furthermore, the claim for rapid calculations makes it preferable to carry out such a mass of calculations by a computer. In the following, an analog computer programme is shown for the calculation of the sensitivity. The analog computer enables the calculations to be carried out even in the case of nonlinear sets of equations. The linear case will be discussed here.

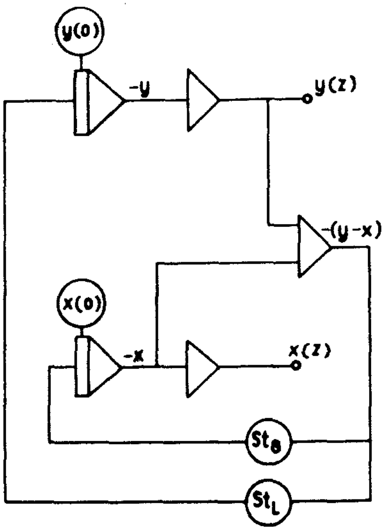

Fig.1. Programme for the solution of Differential Equations (3) and (4)

The analog computer program for the solution of differential Equations (3) and (4) is shown in Fig. 1. The conditional equations are such that only the initial value $y(0) = 1$ is known, but $x(0)$ is unknown, an iterative solution has to be chosen. In the course of this, the initial value fed to the integrator calculating the function is varied until the condition $x(1) = 0$ prescribed for the place $z=1$ is fulfilled. This procedure can, with some practice, be carried out rapidly. It should be noted here that there exists a method for the automation of the iteration.

Having determined the functions x and y, the sensitivity values can - after a similar iteration procedure - be determined with the help of the programme shown in Fig. 2.

Figs. 3 and 4 show the results of the calculations. The values of the functions x, y, e_{11}, e_{21}, e_{12}, and e_{22} are shown in both Figures. As it is apparent from Equations (11), (12), (15) and (16), the differential quotient of the St numbers with respect to each other also appears.

When calculating this differential quotient, different results will be obtained, depending on whether the change in the St number is due to the transfer coefficient ($\beta\omega$) or to the rate of the phase (v_L or v_G).

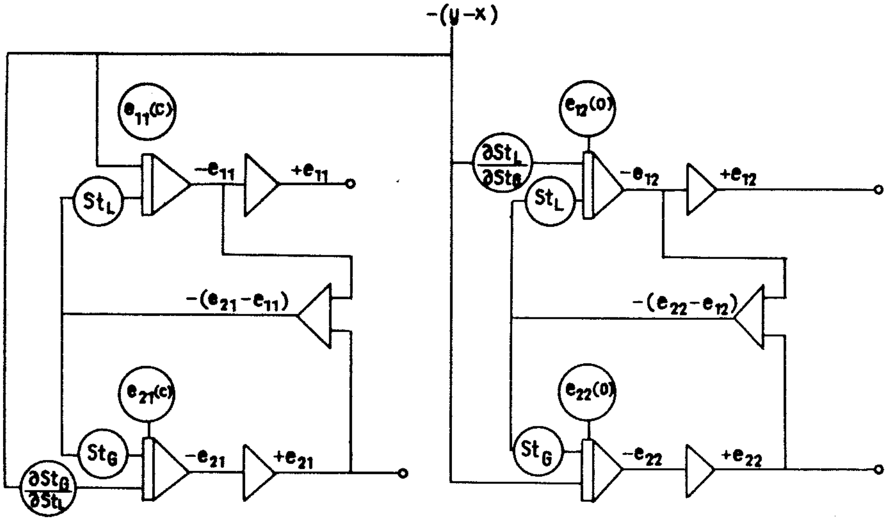

Fig. 2. Programme for the solution of Equations (11), (12), (15) and (16)

Since

$$\frac{\partial St_L}{\partial St_G} = \frac{\partial\left(\frac{\beta\omega Z}{v_L}\right)}{\partial\left(\frac{\beta\omega ZH}{v_G}\right)} \tag{20}$$

if $\beta\omega$ changes, but v_L and v_G are constant:

$$\frac{\partial St_L}{\partial St_G} = \frac{v_G}{v_L H} \tag{21}$$

if $\beta\omega$ is constant, we have

$$\frac{\partial St_L}{\partial St_G} = 0 \tag{22}$$

The sensitivity curves for a given system (St_L = 3.48; St_G = = 2.32) and for a case when the parameters St_L and St_G change on

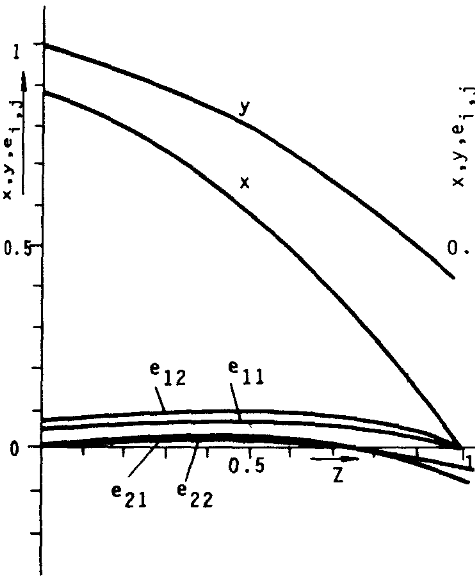

Fig.3. Sensitivity of the variables x and y with respect to St_L and St_G, if the value of $\beta\omega$ is varied (St_L = 3.48, St_G = 2.32)

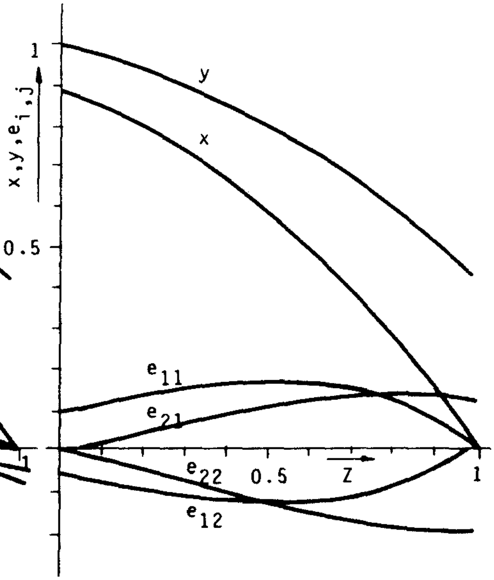

Fig.4. Sensitivity of the variables x and y with respect to St_L and St_G, if v_L or v_G is varied (St_L = 3.48, St_G = 2.32)

account of a change in the transfer coefficient, are shown in Fig. 3. Fig. 4 shows curves that are the result of changes in v_L and v_G. It is apparent from the Figures that the sensitivity curves possess an extreme value. The position of the latter depends on the ratio St_L/St_G. If the ratio $St_L/St_G > 1$, the extreme value at a high z value, whereas it is found at a low z value if $St_L/St_G <$ < 1.

2. Sensitivity of the A.D.P.F. Model

This model is frequently applied for the description of co--current or counter-current two-phase operational units. The analytical method of the determination of the parameter sensitivity will be presented here. The model will be described in general for a system in which the equilibrium function is a linear one, but the straight line does not necessarily start from the origo.

The diffusion model may be described in the general form with dimensionless quantities by the following Equation [1]:

$$a_1 \frac{d^2x}{dz^2} + \frac{dx}{dz} + a_2(a_5y + a_6 - x) = 0 \tag{23}$$

$$a_3 \frac{d^2y}{dz^2} - \frac{dy}{dz} - a_4(a_5y + a_6 - x) = 0 \tag{24}$$

Boundary conditions:

$$z = 0, \quad a_3 \frac{dy}{dz} - y + 1 = 0 \tag{25}$$

$$\frac{dx}{dz} = 0 \tag{26}$$

$$z = 1, \quad a_1 \frac{dx}{dz} + x - a_7 = 0 \tag{27}$$

$$\frac{dy}{dz} = 0 \tag{28}$$

Parameters $a_1 \ldots a_7$ are present in the differential equation and the boundary conditions. Parameters a_8 and a_9 mean the initial values of the functions x and y and are interesting from the point of view of the calculation.

The set of differential equations pertaining to the sensitivity and the conditional equations may be obtained by the derivation of Equations (24) ... (29). Accordingly, the expression of the sensitivity with respect to parameter a_i (i = 1, 2 ... 9) is the following:

$$a_1 \frac{d^2e_{1,i}}{dz^2} - \frac{de_{1,i}}{dz} + a_2(a_5e_{2,i} - e_{1,i}) + b_1 \frac{d^2x}{dz^2} + b_7y - b_2x + b_8 = 0 \tag{29}$$

$$a_3 \frac{d^2e_{2,i}}{dz^2} - \frac{de_{2,i}}{dz} - a_4(a_5e_{2,i} - e_{1,i}) + b_3 \frac{d^2y}{dz^2} - b_9y + b_4x - b_{10} = 0 \tag{30}$$

The boundary condition of the set of differential equations is the following:

Condition A (i = 1, 2 ... 7):

if $z = 0$, we have $a_3 \frac{de_{2,i}}{dz} - e_{2,i} + b_3 \frac{dy}{dz} = 0$

and $\frac{de_{1,i}}{dz} = 0$ (31)

if $z = 1$, we have $a_1 \frac{de_{1,i}}{dz} + e_{1,i} + b_1 \frac{dx}{dz} - f_o = 0$

and $\frac{de_{2,i}}{dz} = 0$ (32)

Condition B (i = 8, 9):

if $z = 0$, we have

$$e_{1,i} = f_1$$

$$e_{2,i} = f_2$$

$$\frac{de_{1,i}}{dz} = 0 \qquad (33)$$

and

$$\frac{de_{2,i}}{dz} = f_4$$

where: $e_{1,i} = \frac{\partial x}{\partial a_i}$; $e_{2,i} = \frac{\partial y}{\partial a_i}$

The meaning of the quantities a_i, b_i and f_i is apparent from Table 1.

Equations (23) ... (33) together represent the A.D.P.F. Model of the parameter sensitivity with the initial and boundary conditions. The part pertaining to x and y can be separated within the model and the solution can be written in the following form:

$$x = \sum_{i=1}^{4} c_i \exp(\lambda_i z) \qquad (34)$$

$$y = \frac{1}{a_5} \sum_{i=1}^{4} (1 - \frac{\lambda_i}{a_2} - \frac{a_1}{a_2} \lambda_i^2) c_i \exp(\lambda_i z) - \frac{a_6}{a_5}$$

where λ_i represents the four solutions of the equation

Table 1. Parameter Sensitivity of the A.D.P.F. Model (Symbols)

$a_1 = 1/Pe_L$; $a_2 = St_L$; $a_3 = 1/Pe_G$; $a_4 = St_G$; $a_5 = A$; $St_L = \frac{\beta\omega Z}{v_L}$

$a_6 = x_o^*$; $a_7 = x_{in}$; $St_G = \frac{\beta\omega Z}{v_G}\frac{H}{A}$; $a_8 = x(o)$; $a_9 = y(o)$

Parameters / b_i and f_i	$E_L H_L$	$E_G H_G$	$(\beta\omega)$	v_L	v_G	Z	x_{in}	x(o)	y(o)
	a_1	a_3	a_2	a_2	a_4	a_2	a_7	a_8	a_9
$b_1 = \frac{\partial a_1}{\partial a_i}$	1	0	0	$\frac{a_1}{a_2}$	0	$-\frac{a_1}{a_2}$	0	0	0
$b_2 = \frac{\partial a_2}{\partial a_i}$	0	0	1	1	0	1	0	0	0
$b_3 = \frac{\partial a_3}{\partial a_i}$	0	1	0	0	$\frac{a_3}{a_4}$	$-\frac{a_3}{a_2}$	0	0	0
$b_4 = \frac{\partial a_4}{\partial a_i}$	0	0	$\frac{a_4}{a_2}$	0	1	$\frac{a_4}{a_2}$	0	0	0
$b_7 = \frac{\partial a_2 a_5}{\partial a_i}$	0	0	a_5	a_5	0	a_5	0	0	0
$b_8 = \frac{\partial a_2 a_6}{\partial a_i}$	0	0	a_6	a_6	0	a_6	0	0	0

$b_9 = \frac{\partial a_4 a_5}{\partial a_i}$	0	0	$\frac{a_4 a_5}{a_2}$	0	a_5	$\frac{a_4 a_5}{a_2}$	0	0	0
$b_{10} = \frac{\partial a_4 a_6}{\partial a_i}$	0	0	$\frac{a_4 a_6}{a_2}$	0	a_6	$\frac{a_4 a_6}{a_2}$	0	0	0
$f_o = \frac{\partial a_7}{\partial a_i}$	0	0	0	0	0	0	0	0	0
$f_1 = \frac{\partial a_8}{\partial a_i}$	-	-	-	-	-	-	-	1	0
$f_2 = \frac{\partial a_9}{\partial a_i}$	-	-	-	-	-	-	-	1	0
$f_4 = \frac{1}{a_3} (f_2 - b_3 \frac{da_9}{dz})$	-	-	-	-	-	-	-	0	$\frac{1}{a_3}$

$$a_1a_3\lambda^4 + (a_3 - a_1)\lambda^3 - (a_1a_4a_5 + a_2a_3 + 1)\lambda^2 + (a_2 - a_4a_5)\lambda = 0 \tag{35}$$

of the fourth degree, and c_i represents the solutions of the linear set of equations with four unknowns

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix} \begin{vmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{vmatrix} = \begin{vmatrix} b_1' \\ b_2' \\ b_3' \\ b_4' \end{vmatrix} \tag{36}$$

The elements of the matrices are the following:

$$\begin{aligned} a_{1i} &= (1 + a_1\lambda_i) \exp \lambda_i \\ a_{2i} &= (1 - a_3\lambda_i)(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2) \\ a_{3i} &= \lambda_i \\ a_{4i} &= \lambda_i(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2)\exp \lambda_i \end{aligned} \tag{37}$$

and

$$b_1' = a_7, \quad b_2' = 1, \quad b_3' = 0, \quad b_4' = 0.$$

When $x(z)$ and $y(z)$ are known, the sensitivity model is an inhomogenous differential equation of the fourth degree with constant coefficients. The coefficients of the argumentum of the exponential terms causing the inhomogenous part are identical to the roots of the characteristic equation of the homogenous equation, and consequently the functions $e_{1,i}(z)$ and $e_{2,i}(z)$ take the following form:

$$e_{1,i}(z) = \sum_{i=1}^{4} (K_i + Q_i z) \exp(\lambda_i z) \tag{38}$$

$$e_{2,i}(z) = \frac{1}{a_5} \sum_{i=1}^{4} (1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2)(K_i - L_i + Q_i z)\exp(\lambda_i z) - \frac{b_8 - b_7 \frac{a_6}{a_5}}{a_2 a_5} \tag{39}$$

Expressions K_i, L_i and Q_i of the equations can be obtained in the following way:

$$L_i = \frac{[b_1\lambda_i^2 + \frac{b_7}{a_5}(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2) - b_2]c_i + (1 + 2\,a_1\lambda_i)Q_i}{a_2 - \lambda_i - a_1\lambda_i^2}$$

$$i = 1,\ 2,\ 3,\ 4$$

$$Q_i = c_i\,[\frac{(a_4a_5 - a_3\lambda_i^2 + \lambda_i)[b_1\lambda_i^2 + \frac{b_7}{a_5}(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2) - b_2]}{3\,a_1a_3\lambda_i^3 + 2(a_3 - a_1)\lambda_i^2 - (a_2a_3 + a_1a_4a_5 + 1)\lambda_i} +$$

$$+ \frac{a_2a_5[(\frac{b_3}{a_5}\lambda_i^2 - \frac{b_9}{a_5})(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2) + b_4]}{3\,a_1a_3\lambda_i^3 + 2(a_3 - a_1)\lambda_i^2 - (a_2a_3 + a_1a_4a_5 + 1)\lambda_i}],\quad i = 1,\ 2,\ 3$$

$$Q_4 = \frac{[a_4(b_7 - b_2a_5) + a_2(b_4a_5 - b_9)]c_4 + a_4(a_5b_8 - a_6b_7) + a_2(a_6b_9 + a_5b_{10})}{a_2 - a_4a_5}$$

The values of K_i are given by a set of equations similar to Equation (36), in which the elements of the matrices are the following:

Condition A:

a_{ji} is the same as in Equation (37)

$$b_1' = f_o - \sum_{i=1}^{4}\{[1 + a_1(1 + \lambda_i)]Q_i + b_1\lambda_i c_i\}\exp\lambda_i$$

$$b_2' = \frac{a_5b_8 - a_6b_7}{a_2a_5} + \sum_{i=1}^{4}\{(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2)[L_i(1 - a_3\lambda_i) + b_3\lambda_i c_i + a_3Q_i]\}$$

$$b_3' = -\sum_{i=1}^{n} Q_i$$

$$b_4' = \sum_{i=1}^{4}(1 - \frac{1}{a_2}\lambda_i - \frac{a_1}{a_2}\lambda_i^2)[\lambda_i L_i - (\lambda_i + 1)Q_i]\exp\lambda_i$$

Condition B:

$$a_{1i} = 1$$

$$a_{2i} = (1 - \frac{1}{a_2} \lambda_i - \frac{a_1}{a_2} \lambda_i^2$$

$$a_{3i} = \lambda_i$$

$$a_{4i} = (1 - \frac{1}{a_2} \lambda_i - \frac{a_1}{a_2} \lambda_i^2) \lambda_i$$

$$b_1' = f_1$$

$$b_2' = a_5 f_2 + \frac{a_5 b_8 - a_6 b_7}{a_2 a_5} + \sum_{i=1}^{4} L_i (1 - \frac{1}{a_2} \lambda_i - \frac{a_1}{a_2} \lambda_i^2)$$

$$b_3' = - \sum_{i=1}^{4} Q_i$$

$$b_4' = a_5 f_4 + \sum_{i=1}^{4} [(1 - \frac{1}{a_2} \lambda_i - \frac{a_1}{a_2} \lambda_i^2) \lambda_i L_i - a_5 Q_i]$$

The solutions of the shape of (34), (38) and (39) can be used only if $a_2 \neq a_4 a_5$ and $a_1 \neq 0$ and $a_3 \neq 0$.

Table 1 contains the values of b_i and f_i for a few given parameters. The meaning of the parameters a_i is given in the Table. The first row contains only such physical quantities with respect to which the sensitivity was studied. The second row shows the a_i parameters which contain these physical quantities. The values of the quantities b_i and f_i vary with respect to which parameter the sensitivity is examined. These values are found in the Table.

In many cases the operational units are such that the coefficients of the differential equations are not constant. For example, the rate of one of the phases varies or the equilibrium connection is a non-linear one. Accordingly, digital computer programmes were prepared in which the set of differential equations was solved with the Runge-Kutta method.

The sort of differential equations pertaining to the sensitivities was solved, for the parameters given in Table 2, with the

Table 2. Parameter sensitivity of the ADPF Model

$Pe_L = 10$; $Pe_G = 10$; $St_L = 4.0$; $St_G = 2.0$; $x_{in} = 0.0$; $A = 1$; $x^*_o = 0$

z	x	y	E_{1,D_L}	E_{2,D_L}	E_{1,D_G}	E_{2,D_G}	$E_{1,\beta\omega}$	$E_{2,\beta\omega}$	E_{1,v_L}	E_{2,v_L}	E_{1,v_G}	E_{2,v_G}	$E_{1,x(o)}$	$E_{2,x(o)}$
0.0	0.84	0.97	-0.044	-0.005	-0.038	-0.028	0.183	0.004	-0.297	-0.040	0.196	0.069	1.0	0
0.1	0.83	0.95	-0.035	-0.008	-0.039	-0.032	0.191	0.010	-0.333	-0.083	0.216	0.113	1.1	-0
0.2	0.79	0.92	-0.025	-0.010	-0.042	-0.037	0.211	0.014	-0.399	-0.128	0.255	0.161	1.6	-1
0.3	0.74	0.89	-0.018	-0.011	-0.044	-0.042	0.236	0.016	-0.474	-0.175	0.301	0.212	2.5	-4
0.4	0.69	0.85	-0.010	-0.011	-0.046	-0.047	0.264	0.014	-0.557	-0.225	0.349	0.267	4.9	-15
0.5	0.62	0.81	0.000	-0.008	-0.046	-0.051	0.294	0.009	-0.647	-0.277	0.399	0.328	12.0	-52
0.6	0.55	0.77	0.019	-0.004	-0.045	-0.055	0.328	-0.003	-0.749	-0.331	0.447	0.392	34.0	-177
0.7	0.47	0.72	0.050	0.003	-0.039	-0.054	0.364	-0.024	-0.867	-0.386	0.493	0.461	109.0	-590
0.8	0.38	0.66	0.110	0.014	-0.030	-0.044	0.404	-0.058	-1.016	-0.439	0.532	0.527	355	-1959
0.9	0.27	0.61	0.243	0.028	-0.015	-0.014	0.448	-0.106	-1.235	-0.485	0.559	0.576	1169	-6490
1.0	0.14	0.58	0.702	0.038	-0.004	0.019	0.487	-0.139	-1.754	-0.507	0.569	0.589	3860	-21149

above-mentioned method. The Table contains the sensitivity data with respect to a few more important parameters as a function of z.

3. The Application of Parameter Sensitivity

The knowledge of parameter sensitivity enables a deeper insight to be gained into the properties of the model and the operational unit described by it. From the point of view of unit operations, it provides assistance in the choice among the models describing the operational unit and in judging the merit of a given model. In practical work, it helps to estimate the accuracy of the calculations.

A few numerical examples, illustrating the application of the concept of sensitivity, are presented in the following.

In **design work**, the values of the parameters are taken from the literature. The sensitivity offers a possibility for the estimation of the degree of accuracy that can be claimed of the data taken from the literature.

In the vicinity of a p_s set of values of the parameters we may write

$$x(z,p) = x(z,p_s) + E_{1,i}(z,p_s)\,\frac{x(z,p_s)}{p_i}\,\Delta p_i$$

and after rearrangement we obtain

$$\frac{x(z,p) - x(z,p_s)}{x(z,p_s)} = E(p_s,z)_{1,i}\,\frac{\Delta p_i}{p_i}$$

This equation enables the calculation of the error of the variable x if the relative error of the parameter $(\Delta p_i/p_i)$ is known. A similar procedure may also be applied in the case of the variable y.

Let us estimate the error made with the application of the data given in Table 2, if the expression, taken from the literature, for the calculation of $(\beta\omega)$ is of an accuracy of ± 10 %. The calculation should be carried out for the place z = 1. In this place, the sensitivity is (cf. Table 2) $E_{1,\beta\omega} = 0.487$ and $E_{2,\beta\omega} = -0.139$. Accordingly

$$\frac{x(z,p) - x(z,p_s)}{x(z,p_s)} = 0.1 \cdot 0.487 \approx 0.049$$

$$\frac{y(z,p) - y(z,p_s)}{y(z,p_s)} = -0.1 \cdot 0.139 \approx -0.014$$

that is, an error of 10 % in the value of $(\beta\omega)$ results in an error of 4.9 % and 1.4 %, resp. in the calculation of the x and y values in the case of the given system. Similar calculations can also be carried out for the other parameters.

From the point of view of the operator it is interesting to know the effect, for example, of fluctuations in the rate of the phases (v_L and v_G) on the composition of the phases leaving the operational unit. Let us consider a deviation of + 10 % from the predetermined value. In the case of the set of parameters presented in Table 2, this causes the following deviations in the x(o) and y(1) values:

$$\frac{x(o,p) - x(o,p_s)}{x(o,p_s)} = -0.1 \cdot 0.297 \approx -0.030$$

$$\frac{y(1,p) - y(1,p_s)}{y(1,p_s)} = -0.1 \cdot 0.507 \approx -0.050$$

As can be seen, this results in a deviation of 3 % and 5 %, respectively. A change of 10 % in the v_G value results, after a similar calculation, in deviations of 2 % and 6 %, respectively.

In research work the aim is frequently to determine the values of the parameters from the experimental data. If for example we want to determine the D_L mixing coefficient from measured values of $x(t)$, and the latter can be determined only with an accuracy of 10 %, the error made in the calculation of the parameter is the following:

$$\frac{\Delta D_L}{D_L} = \frac{\frac{\Delta x}{x}}{E_{1,D_L}(1)} = \frac{0.1}{0.7} \approx 0.14$$

Accordingly, it can be calculated with an error of 14 % from the data referring to the place $z = 1$. The same parameter, when calculated from the measured values of y, could be determined only with an error of 25 %. The sensitivity with respect to E_G is such that its value could be determined with an error even greater than the previous one.

In modelling operational units, a boundary value problem is usually encountered. If we want to use a digital or analog computer in the calculations, the values of the functions taken at the initial points ($z = o$) have to be given and the solution which satisfies the boundary conditions has to be found by the iteration method. Table 2 also contains the sensitivities with respect to $x(o)$.The absolute value of these is so high that a small deviation from the actual value in the determination of $x(o)$ and $y(o)$ causes a large error in the values of $x(z)$ and $y(z)$. This is the explanation of the fact that two-phase countercurrent operational units cannot be modelled with an analog computer. With the latter, the setting of the $x(o)$ and $y(o)$ values is possible only to a limited accuracy (1-2 %) and even such a small deviation from the actual value causes $x(z)$ and $y(z)$ values to be obtained that are technically unreal. This difficulty is considerably decreased by the use of digital computers, due to the high degree of accuracy that can be realized.

The above examples clearly illustrate the importance and wide range of applicability of the knowledge of the sensitivity.

SYMBOLS USED

a_i parameters (cf. Table 1)

D axial mixing coefficient (m^2/sec)

$e_{j,i}$ sensitivity of the j^{th} dependent variable to alter the value of the i^{th} parameter

$E_{j,i}$ dimensionless sensitivity of the j^{th} dependent variable according to the i^{th} parameter

H Henry-constant (dimensionless)

Pe Peclet-number (dimensionless)

St Stanton-number (dimensionless)

v linear flow rate of the phase (m/sec)

Z length of the column (m)

z space co-ordinate along the length of the column (dimensionless)

x concentration of the absorbed component in the liquid phase (dimensionless)

y concentration of the absorbed component in the gaseous phase (dimensionless)

x_o axis section of equilibrium line (dimensionless)

$\beta\omega$ component transfer coefficient, as referred to unit volume (sec^{-1})

Indices

j refers to the dependent variable (the concentration in the liquid phase is j = 1, that in the gaseous phase is j = 2) i refers to the parameter

L liquid phase

G gaseous phase

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РЕЗЮМЕ

Авторами определяется понятие чувствительности параметра для диффузионных элементов процесса, и рассматриваются модели для его вычисления. Модель идеального вытеснения для двухфазных противоточных элементов процесса содержит два, а диффузионная модель, имеющая в виду и осевое смешивание, четыре безразмерных параметра. В обоих моделях используется много физических величин а также величин, характеризующих заводские условия в выражениях безразмерных параметров.

В работе описывается и аналитическое решение для вычисления чувствительностей.

Теоретические выражения дополняются числовыми примерами, решаемыми на аналоговых и цифровых вычислительных машинах, и таким образом, показывается и практическое применение чувствительности параметра.