

Dynamic models of absorbers

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In this paper three mathematical models of absorbers describing the flow of individual phases as a cascade of ideally stirred regions with countercurrent are presented and verified. The algorithms and programs enabling us to find out the values of parameters on the basis of jump response data (response to jump in gaseous phase) have been elaborated for a computer. The results ensuing from experimental data have shown that the models and methods of calculation proposed in this contribution are more convenient for significant axial stirring than the models of absorbers with axial dispersion flow.

В работе предложены и проверены три математические модели адсорбентов, описывающие потоки отдельных фаз, как каскады идеально смешанных областей с обратным потоком. Были разработаны алгоритмы и программы для вычислительной машины, позволяющие находить значения параметров на основе данных скачковых отзвов (отзывы на скачок в подвижной фазе). Результаты обработки экспериментальных данных показали, что для случая значительного аксиального перемешивания являются модели и способ расчета, предложенные в данной работе, более удовлетворительными, чем модели адсорбентов с аксиальным дисперсионным потоком.

We frequently use mathematical models which describe the behaviour of real absorber with certain precision for design, intensification, and optimization of absorbers.

For physicochemical description of absorber we have to know the character of substance transfer as well as the flow of individual phases. The rate of substance transfer is to be expressed by different relationships [1] the derivation of which is

frequently based on the film theory. In the simplest models, it may be assumed that the flow in the gaseous as well as liquid phase is piston flow [1, 2]. If the stirring is, however, in one or both phases significant, we must use some more intricate hydrodynamic model. If the axial stirring is respected, it is convenient to use an axial dispersion model [1, 3, 4]. The use of axial dispersion model has the advantage in that the axial stirring is characterized by one parameter, *i.e.* the Peclet number. On the other hand, the use of this model for simulating the dynamic behaviour of absorber requires solution of a system of differential equations, which is rather tedious. In order to avoid this problem, we decided to simulate the flow of individual phases as a cascade of perfectly stirred regions with countercurrent. Below are described three linear models which are suited to identification of the parameters of flow model, mean retention times, and product of the coefficient of substance transfer and interfacial area. We give a comparison with axial dispersion model which enables us to appreciate the suitability for use. The presented models of absorbers were used for processing the measurements carried out with a laboratory countercurrent absorber.

1. General characteristics of the derived models and conditions of their use

The presented models were derived for description of the dynamics of countercurrent packed absorber. Their common feature is the use of a cascade of perfectly stirred regions with countercurrent and the assumption of validity of the film theory [1, 2]. The models belong among the class of two-phase models.

The models were derived for the following conditions:

- a) Isothermal regime.
- b) Axially symmetric system.
- c) Zero radial component of concentration gradient of the investigated substance in individual phases.
- d) Influence on the change in phase volume and thus in volume flow of absorption or desorption is negligible.
- e) Uniform distribution of retention of the gaseous and liquid phase along the column.
- f) The rate of substance transfer may be described by the expression

$$\dot{f} = (K a) \Delta L (m c_G - c_L) \quad (1)$$

where \dot{f} — quantity of the substance transferred through the interface in the section ΔL [kmol s⁻¹] of absorption column;

$K a$ — product of the overall coefficient of substance transfer and interfacial surface referred to unit length of absorption column [m²s⁻¹]. It is assumed that its value does not vary along the column;

- ΔL — section of the absorption column [m];
 m — equilibrium coefficient in the relation $c_L^x = m c_G$;
 c_L^x — equilibrium concentration in the liquid phase [kmol m⁻³];
 c_L — concentration of the investigated component in the liquid phase [kmol m⁻³];
 c_G — concentration of the investigated component in the gaseous phase [kmol m⁻³].

g) The flow of individual phases may be described with a model of a cascade of perfectly stirred regions with countercurrent.

Under these assumptions, the substance balance of individual cascade members may be expressed by a system of linear differential equations

$$\frac{d\mathbf{X}}{dt} = \mathbf{A} \mathbf{X} + \mathbf{B} \mathbf{U} \quad (2)$$

$$\mathbf{Y} = \mathbf{C} \mathbf{X}$$

The individual symbols mean:

- \mathbf{X} — vector of variables of dimension r which will be discussed in more detail for individual models;
 \mathbf{A} — matrix of the system of dimensions $r \cdot r$;
 \mathbf{B} — matrix which determines the input in the system, dimension $r \cdot 2$;
 \mathbf{U} — input vector (gaseous and liquid phase);
 \mathbf{Y} — output vector (gaseous and liquid phase);
 \mathbf{C} — matrix determining output from the system $2 \cdot r$.

The system of differential equations (2) may be solved analytically but owing to incoherence of matrices and their ample dimensions (up to 90) which were needed for simulating a real absorber, a numerical solution was more convenient. First of all, we applied the Runge—Kutta method of the fourth order with the Merson modification [5] and automatic step regulation. However, this method appeared to be unsuitable because the stable solution necessitated a very small step owing to which the time necessary for calculation increased very much. The application of the semiimplicit Euler method was more profitable. The calculation was always stable for obtaining the solution with equal precision as by the Runge—Kutta method while the time necessary for calculation was 10—20 times shorter than the time required by the Runge—Kutta method.

The basis of the semiimplicit method is the following relationship

$$(\mathbf{E} - w h \mathbf{A}) \mathbf{X}^{i+1} = [\mathbf{E} + (1 - w) h \mathbf{A}] \mathbf{X}^i + h \mathbf{B} \mathbf{U} \quad (3)$$

where \mathbf{E} , w , \mathbf{X}^{i+1} , \mathbf{X}^i are unit matrix, weight for the implicit Euler method $w \in \langle 0, 1 \rangle$, vector of the solution sought for in the $(i + 1)$ -th step, and vector of the solution in the i -th step, respectively.

By multiplying eqn (3) with the expression $(\mathbf{E} - w h \mathbf{A})^{-1}$ we obtained an explicit specification for \mathbf{X}^{i+1} . However, this arrangement is not convenient because the matrices \mathbf{A} , $(\mathbf{E} - w h \mathbf{A})$, and $[\mathbf{E} + (1 - w h \mathbf{A})]$ are band matrices or can be resolved into band submatrices. It was better to solve the system of linear algebraic equations for each step while the resolution of matrices into lower and upper triangle matrices was used

$$(\mathbf{E} - w h \mathbf{A}) = \mathbf{A}^x = \mathbf{A}_D \mathbf{A}_H \quad (4)$$

After this resolution the solution of the system of linear algebraic equations may be found according to the following relations

$$\mathbf{A}_D \mathbf{Z} = [\mathbf{E} + (1 - w) h \mathbf{A}] \mathbf{X}^i + h \mathbf{B} \mathbf{U} \quad (5)$$

$$\mathbf{A}_H \mathbf{X}^{i+1} = \mathbf{Z}$$

where \mathbf{Z} is an auxiliary vector.

It is typical of resolution (4) that, provided \mathbf{A}^x is a band matrix with $2k + 1$ diagonals of nonzero elements, we can so perform the resolution that \mathbf{A}_D has k subdiagonals and units on main diagonal and \mathbf{A}_H has a main diagonal and k overdiagonals.

As for matrix \mathbf{A} with variable elements, the relations called factorization [5] proved to be very good.

1.1. Equal number of cascade members in both phases

This model is represented in Fig. 1. The substance quantity which is absorbed in one fictitious member in a time unit is given by the expression

$$\dot{f}_k = \beta (m c_{G,k} - c_{L,k}) \quad (6)$$

$$\beta = (K a) L / n$$

where L , n , $c_{G,k}$, $c_{L,k}$ are the length of absorption column, number of cascade members, concentration in the gaseous phase in the k -th member of cascade, and concentration in the liquid phase in the k -th member of cascade, respectively.

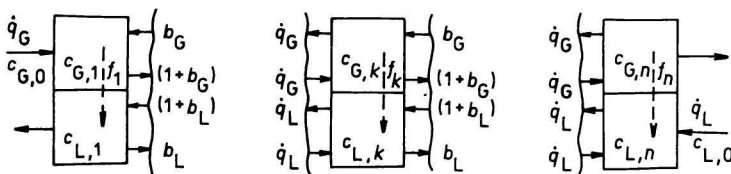


Fig. 1. Model of absorber with equal number of cascade members.

The substance balances for individual members are

$$\begin{aligned}
 V_G \frac{dc_{G,1}}{dt} &= -(1 + b_G) \dot{q}_G c_{G,1} + b_G c_{G,2} - \beta(m c_{G,1} - c_{L,1}) + \dot{q}_G c_{G,0} \\
 V_L \frac{dc_{L,1}}{dt} &= -(1 + b_L) \dot{q}_L c_{L,1} + (1 + b_L) \dot{q}_L c_{L,2} + \beta(m c_{G,1} - c_{L,1}) \\
 V_G \frac{dc_{G,k}}{dt} &= (1 + b_G) \dot{q}_G c_{G,k-1} - (1 + 2b_G) \dot{q}_G c_{G,k} + b_G \dot{q}_G c_{G,k+1} + \\
 &\quad + \beta(m c_{G,k} - c_{L,k}) \quad k = 2, 3, \dots, n-1 \\
 V_L \frac{dc_{L,k}}{dt} &= b_L \dot{q}_L c_{L,k-1} - (1 + 2b_L) \dot{q}_L c_{L,k} + (1 + b_L) \dot{q}_L c_{L,k+1} + \\
 &\quad + \beta(m c_{G,k} - c_{L,k}) \quad k = 2, 3, \dots, n-1 \\
 V_G \frac{dc_{G,n}}{dt} &= (1 + b_G) \dot{q}_G c_{G,n-1} - (1 + b_G) \dot{q}_G c_{G,n} - (1 + b_G) \dot{q}_G c_{G,n+1} + \\
 &\quad + \beta(m c_{G,n} - c_{L,n}) \\
 V_L \frac{dc_{L,n}}{dt} &= b_L \dot{q}_L c_{L,n-1} - (1 + b_L) \dot{q}_L c_{L,n} + \beta(m c_{G,n} - c_{L,n}) + \dot{q}_L c_{L,0} \quad (7)
 \end{aligned}$$

Let us assume that it holds in the time moment $t_0 = 0$ $c_{G,k} = c_{L,k} = 0$, $k = 1, 2, \dots, n$ and a jump change of $c_{G,0}$ from 0 to $c_{G,max}$ takes place in this time moment. In this case, the solution of eqns (7) enables us to obtain the jump responses in the gaseous and liquid phase as responses to a jump at the input of the gaseous phase. For calculation, it is convenient to rearrange eqns (7). We divide the equations for individual members of the gaseous phase by $c_{G,max}$ and the equations for individual members of the liquid phase by $c_{L,max} = m c_{G,max}$. This rearrangement ensures that the values of solution vary in the interval 0—1.

The matrices for the system of linear differential equations are

$$\mathbf{A} = \begin{matrix}
 \begin{matrix} \gamma_2 & \gamma_1 & \gamma_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 \lambda_1 & \lambda_2 & 0 & \lambda_3 & 0 & 0 & 0 & 0 & 0 & 0 \\
 \gamma_3 & 0 & \gamma_5 & \gamma_1 & \gamma_4 & 0 & 0 & 0 & 0 & 0 \\
 0 & \gamma_4 & \lambda_1 & \lambda_5 & 0 & \lambda_3 & 0 & 0 & 0 & 0 \\
 \dots & & & & & & & & & \\
 0 & 0 & \gamma_3 & 0 & \gamma_5 & \gamma_1 & \gamma_4 & 0 & \dots & 0 \\
 0 & 0 & 0 & \lambda_4 & \lambda_1 & \lambda_5 & 0 & \lambda_3 & 0 & 0 \\
 \dots & & & & & & & & & \\
 0 & & & & & & 0 & \gamma_3 & 0 & \gamma_2 & \gamma_1 \\
 0 & \dots & & & & & 0 & 0 & \lambda_4 & \lambda_1 & \lambda_2 \end{matrix} \\
 \end{matrix} \quad (8)$$

$$\mathbf{B}^T = \begin{bmatrix} \gamma_6 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & \lambda_6 \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{U}^T = (c_{L,0} c_{G,0}) \quad \mathbf{Y}^T = (c_{G,n} c_{L,1})$$

$$\mathbf{X}^T = (c_{G,1} c_{L,1} c_{G,2} c_{L,2} \dots c_{G,k} c_{L,k} \dots c_{G,n} c_{L,n})$$

where

$$\begin{aligned} \lambda_1 &= \frac{\beta}{V_L}, & \lambda_2 &= -\frac{(1+b_L)\dot{q}_L + \beta}{V_L}, & \lambda_3 &= -\frac{(1+b_L)\dot{q}_L}{V_L} \\ \lambda_4 &= \frac{b_L\dot{q}_L}{V_L}, & \lambda_5 &= -\frac{(1+2b_L)\dot{q}_L + \beta}{V_L}, & \lambda_6 &= \frac{\dot{q}_L}{V_L} \\ \gamma_1 &= \frac{\beta m}{V_G}, & \gamma_2 &= -\frac{(1+b_G)\dot{q}_G + \beta m}{V_G}, & \gamma_3 &= \frac{(1+b_G)\dot{q}_G}{V_G} \\ \gamma_4 &= \frac{b_G\dot{q}_G}{V_G}, & \gamma_5 &= -\frac{(1+2b_G)\dot{q}_G + \beta m}{V_G}, & \gamma_6 &= \frac{\dot{q}_G}{V_G} \end{aligned} \quad (9)$$

1.2. Different number of cascade members

The model with equal number of cascade members is convenient if the stirring in both phases is not too different. In case of very different stirring, the model represented in Fig. 2 is more adequate.

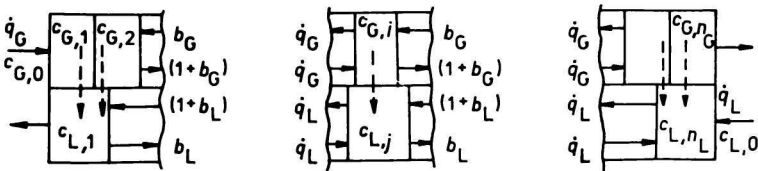


Fig. 2. Model of absorber with different number of cascade members.

Owing to nonequal number of cascade members the substance balances are more difficult to express than for the preceding model. In order to make their expression clearer, we shall introduce the following variables

$$\beta = (K a) L / n_G, \quad P = n_G / n_L \quad (10)$$

$n_{G,k}$ — the last member of the liquid phase which adjoins the k -th member of the gaseous phase;

$n_{L,k}$ — the last member of the gaseous phase which adjoins the k -th member of the liquid phase;

$g_{k,i}$ — the portion of interfacial surface by which the i -th member of the liquid phase adjoins the k -th member of the gaseous phase;

$l_{k,i}$ — the portion of interfacial surface by which the i -th member of the gaseous phase adjoins the k -th member of the liquid phase.

Then it holds for substance balances

$$V_G \frac{dc_{G,1}}{dt} = -(1 + b_G) \dot{q}_G c_{G,1} + b_G \dot{q}_G c_{G,2} - \beta(m c_{G,1} - \sum_{i=1}^{n_{G,k}} g_{k,i} c_{L,i}) + \dot{q}_G c_{G,0}$$

$$V_G \frac{dc_{G,k}}{dt} = (1 + b_G) \dot{q}_G c_{G,k-1} - (1 + 2b_G) \dot{q}_G c_{G,k} + b_G \dot{q}_G c_{G,k+1} + \beta \left(m c_{G,k} - \sum_{i=n_{G,k-1}}^{n_{G,k}} g_{k,i} c_{L,i} \right) \quad k=2, 3, \dots, n_{G-1}$$

$$V_G \frac{dc_{G,n_G}}{dt} = (1 + b_G) \dot{q}_G c_{G,n_{G-1}} - (1 + b_G) \dot{q}_G c_{G,n_G} + \beta \left(m c_{G,n_G} - \sum_{i=n_{G,n_{G-1}}}^{n_{G,n_G}} g_{n_G,i} c_{L,i} \right)$$

$$V_L \frac{dc_{L,1}}{dt} = -(1 + b_L) \dot{q}_L c_{L,1} + (1 + b_L) \dot{q}_L c_{L,2} + \beta p \left(m \sum_{i=1}^{n_{L,1}} l_{1,i} c_{G,i} - c_{L,1} \right)$$

$$V_L \frac{dc_{L,k}}{dt} = b_L \dot{q}_L c_{L,k-1} - (1 + 2b_L) \dot{q}_L c_{L,k} + (1 + b_L) \dot{q}_L c_{L,k+1} + \beta p \left(m \sum_{i=n_{L,k-1}}^{n_{L,k}} l_{k,i} c_{G,i} - c_{L,k} \right) \quad k=2, 3, \dots, n_{L-1}$$

$$V_L \frac{dc_{L,n_L}}{dt} = b_L \dot{q}_L c_{L,n_{L-1}} - (1 + b_L) \dot{q}_L c_{L,n_L} + \beta p \left(m \sum_{i=n_{L,n_{L-1}}}^{n_{L,n_L}} l_{n_L,i} c_{G,i} - c_{L,n_L} \right) + \dot{q}_L c_{L,0} \quad (11)$$

An arrangement with the following vector of variables appeared to be suitable for the system of differential equations

$$\mathbf{X}^T = (c_{G,1} c_{G,2} \dots c_{G,n_G} c_{L,1} c_{L,2} \dots c_{L,n_L}) \quad (12)$$

where n_G , n_L are the numbers of cascade members in the gaseous and liquid phase, respectively.

The matrix \mathbf{A} for eqn (2) may be regarded as a block matrix

$$\mathbf{A} = \left[\begin{array}{c|c} \mathbf{A}_1 & \mathbf{A}_2 \\ \hline \mathbf{A}_3 & \mathbf{A}_4 \end{array} \right] \quad (13)$$

where \mathbf{A}_1 and \mathbf{A}_4 are tridiagonal matrices which express the cascade models of perfectly stirred regions with countercurrent for the gaseous or liquid phase. Matrices \mathbf{A}_2 and \mathbf{A}_3 are related with the concentration change due to interfacial transport. For n_G and n_L matrix \mathbf{A}_2 contains in one line maximally two nonzero elements. For numerical solution, it is convenient to put the nonzero elements of matrix \mathbf{A}_2 into vector \mathbf{P} in the order from the left at the top to the right at the bottom. The work also requires the auxiliary vector

$$\mathbf{Q} = (k_1 k_2 \dots k_i \dots k_{n-1} k_n) \quad (14)$$

which contains the information how many elements of vector \mathbf{P} belong to a given column of matrix \mathbf{A}_2 . Matrix \mathbf{A}_3 is transposed to matrix \mathbf{A}_2 by dimensions and position of nonzero elements.

For numerical calculation of jump responses the following procedure proved to be excellent:

1. In particular step of solution the equations for the gaseous phase were solved first while the values of concentration in the liquid phase were regarded as constant and equal to the values in preceding step of solution. The error due to this assumption is very small for poorly soluble gases and can be theoretically diminished down to the zero value by decreasing the integration step.

2. The values of concentration in the gaseous phase obtained, the values of concentration in the liquid phase were calculated while the values of concentration in the i -th member of cascade of the gaseous phase were calculated according to the equation

$$c_{G,k} = w c_{G,k}^{i+1} + (1-w) c_{G,k}^i \quad (15)$$

where exponents $i+1$ and i denote the solution in the $(i+1)$ -th and i -th step of solution, respectively.

This resolution made possible to regard the interfacial transport as inputs with variable values so that only matrix \mathbf{A}_1 or \mathbf{A}_4 could be taken for matrix \mathbf{A} in eqn (2). The testing of the precision of calculation was carried out both by decreasing the integration step h and by overall substance balance in steady state.

The substance balances as well as the entire algorithm of response solution for the model with different number of cascade members are also valid for the model with equal number of cascade members. However, if the model with equal number of cascade members satisfies, the use of the model with different number of cascade members is less effective because the time necessary for calculation is longer by 30% approximately. The accuracy in a certain step was practically equal (deviations less than 0.01%).

1.3. Piston flow and a cascade of perfectly stirred regions with countercurrent

If the axial stirring of the phase is low, the number of cascade members and thus the dimension of linear differential equations and laboriousness of solution considerably increases. Let us assume that the poorly stirred phase is the gaseous phase and this poor stirring may be neglected. We shall consider a piston flow. For simplicity, we shall confine ourselves to the case when the influence of absorption or desorption on concentration in the gaseous phase is negligible. The model of absorber obtained by introducing these assumptions is represented in Fig. 3.

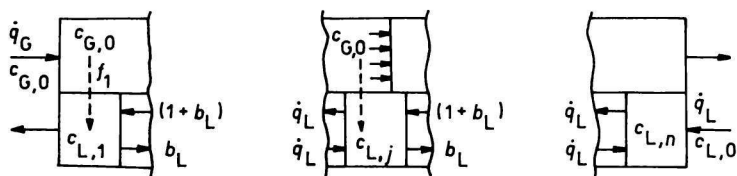


Fig. 3. Model of absorber with cascade and countercurrent for the liquid phase and piston flow for the gaseous phase.

The substance balances of the investigated component have the following form

$$V_L \frac{dc_{L,1}}{dt} = -(1+b_L) \dot{q}_L c_{L,1} = (1+b_L) \dot{q}_L c_{L,2} + \beta s_1 (m c_{G,0} - c_{L,1})$$

$$V_L \frac{dc_{L,k}}{dt} = b_L \dot{q}_L c_{L,k-1} - (1+2b_L) \dot{q}_L c_{L,k} + (1+b_L) \dot{q}_L c_{L,k+1} + \beta s_k (m c_{G,0} - c_{L,k}) \quad k=2, 3, \dots, n$$

$$V_L \frac{dc_{L,n}}{dt} = b_L \dot{q}_L c_{L,n-1} - (1+b_L) \dot{q}_L c_{L,n} + \beta s_n (m c_{G,0} - c_{L,n}) +$$

$$+ \dot{q}_L c_{L,0} \quad (16)$$

where $\beta = (K a) L/n$

$$S_k = 0 \text{ provided: } t \leq \tau_G \frac{k-1}{n}$$

$$S_k = \frac{t - \frac{\tau_G}{n}(k-1)}{\frac{\tau_G}{n}} \text{ provided: } \tau_G \frac{k-1}{n} < t < \tau_G \frac{k}{n} \quad (17)$$

$$S_k = 1 \text{ provided: } t \geq \tau_G \frac{k}{n}$$

The coefficient s_k expresses the active portion of interfacial surface in the k -th cascade member, *i. e.* through which the substance transfer proceeds.

It is very good for this model to introduce the vector of variables

$$\mathbf{X}^T = (c_{L,1} \ c_{L,2} \ \dots \ c_{L,i} \ \dots \ c_{L,n-1} \ c_{L,n}) \quad (18)$$

where n is the number of cascade members of perfectly stirred regions in the liquid phase.

Matrices **A** and **B** for eqns (2) are temporally variable (δ) and some their elements must be regenerated for each step of solution up to $t > \tau_G$ (variability — s_k).

The real forms of matrices for eqn (2) are as follows

$$\mathbf{A} = \begin{bmatrix} \lambda_{2,1} & \lambda_3 & 0 & & & 0 \\ \lambda_4 & \lambda_{5,2} & \lambda_3 & 0 & \dots & 0 \\ 0 & \lambda_4 & \lambda_{5,3} & \lambda_3 & 0 & 0 \\ 0 & & 0 & \lambda_4 & \lambda_{5,n-1} & \lambda_3 \\ 0 & & 0 & 0 & \lambda_4 & \lambda_{2,n} \\ \vdots & & & & & \end{bmatrix} \quad (19)$$

$$\mathbf{B} = \begin{bmatrix} \lambda_{1,1} & 0 \\ \lambda_{1,2} & 0 \\ \lambda_{1,3} & 0 \\ \dots & \\ \lambda_{1,k} & 0 \\ \dots & \\ \lambda_{1,n-1} & 0 \\ \lambda_{1,n} & \lambda_6 \end{bmatrix}$$

$$\mathbf{U}^T = (c_{G,0} \ c_{L,0})$$

$$\mathbf{Y} = (c_{L,1})$$

$$\mathbf{c} = (1, 0 \ \dots \ 0)$$

where

$$\lambda_{1,k} = \frac{s_k \beta}{V_L}, \quad \lambda_{2,k} = -\frac{(1+b_L) \dot{q}_L + \beta s_k}{V_L}, \quad \lambda_3 = \frac{(1+b_L) \dot{q}_L}{V_L},$$

(20)

$$\lambda_4 = \frac{b_L \dot{q}_L}{V_L}, \quad \lambda_{5,k} = -\frac{(1 + 2b_L) \dot{q}_L + \beta s_k}{V_L}, \quad \lambda_6 = \frac{\dot{q}_L}{V_L}$$

We used again the semiimplicit Euler method for solving the system of differential equations and the method of factorization [5] for solving the system of linear algebraic equations with tridiagonal matrix.

2. Identification of parameters of the model of laboratory countercurrent absorber

In this chapter we are concerned with the determination of parameters of the described models of absorbers on the basis of experimental measurements performed by *Linek et al.* [4]. The aim was to estimate the suitability of the models proposed by us and to confirm or find out further relationships between the models involving a cascade of perfectly stirred regions with countercurrent and the models involving axial dispersion flow.

The desorption of air oxygen from distilled water into a flow of nitrogen proceeded in a laboratory countercurrent absorber. The above authors measured jump responses in the liquid and gaseous phase to jump change in concentration in the gaseous phase. The advantage of this experiment consisted in the fact that the change in concentration in the gaseous phase by the effect of absorption or desorption was practically negligible, which made possible to identify individual parameters of the model of flow of the gaseous phase. After ascertaining the parameters τ_G , n_G , and b_G , the parameters characterizing the flow of the liquid phase and the value of $(K a)$ were sought for. The procedure of seeking of individual parameters is described in more detail in paper [6].

According to expectation, the model with different number of cascade members proved to be the best. The values of the Peclét numbers calculated according to eqn (1)

$$Pe^x = \frac{2n}{1 + 2b} \quad (21)$$

were in very good agreement with the values obtained by the authors of this experiment for the axial dispersion model. A good consistence was also in the values of other parameters (τ_G , τ_L , $(K a)$), the average deviation being 10–15% of the value found for the axial dispersion model.

The inadequacy of the model with equal number of the cascade members especially manifested itself in very different axial stirring. For instance, provided $n_G = 40$ and $n_L = 10$, it was necessary to use about 40 cascade members for the model with equal number of cascade members, which resulted in the fact that the

coefficient of countercurrent for the liquid phase b_L was $\in (2.3)$. In these cases, the determination of the coefficient of countercurrent was very inaccurate owing to low parametric sensitivity and the value of the coefficient b_L itself was practically unreal in the physical sense (it is difficult to imagine an absorber in which the axial stirring proceeds with such high countercurrent).

For low stirring of the gaseous phase the model with piston flow proved to be very good. The values of n_L and b_L obtained for model 1.3 of this study were very near to the values obtained for different number of cascade members. These values were used as starting basis for the model with different number of cascade members.

3. Comparison of the models of absorbers

A comparison of the models of absorbers with an axial dispersion flow with the models containing a cascade of perfectly stirred regions with countercurrent can be also performed on the basis of the relations

$$(K a)_P : (K a)_D; \quad (K a)_P : (K a)_K \quad (22)$$

$(K a)_P$ is the value of the product of the overall coefficient of substance transfer and interfacial surface on the assumption that the flow in the liquid as well as gaseous phase is piston flow; $(K a)_D$ is the same value as $(K a)_P$ but for dispersion flow in the liquid phase and piston flow in the gaseous phase; $(K a)_K$ is the same value as $(K a)_D$ but for a cascade of perfectly stirred regions with countercurrent.

The purpose of this comparison was a quantitative evaluation of deviations of the models with equal axial stirring in the sense of eqn (21).

Let us assume that we examine absorption or desorption of very poorly soluble gas so that the concentration of the investigated component in the gaseous phase does not practically depend on the course of absorption or desorption.

The ratio $(K a)_P : (K a)_D$ was computed by means of the equation put forward by *Miyauchi* [7]

$$\exp(-N_{LP}) = \frac{4s \exp(Pe_L/2)}{(1+s)^2 \exp(Pe_L s/2) - (1-s)^2 \exp(-Pe_L s/2)} \quad (23)$$

where

$$s = (1 + 4N_L/Pe_L)^{1/2}$$

$$N_{LP} = (K a)_P L / \dot{q}_L; \quad N_L = (K a)_D L / \dot{q}_L$$

For Pe_L we substituted the values according to eqn (15).

The ratio $(K a)_p : (K a)_k$ was computed by means of the equation

$$(K a)_p = \frac{-\dot{q}_L \ln(1 - c_{L, st})}{L} \tag{24}$$

where $c_{L, st}$ is the normed value of steady state which was obtained by numerical solution of the system of differential equations for given $(K a)_k$, τ_L , n_L , and b_L .

Fig. 4 represents the course of deviations

$$\alpha = \frac{(K a)_p / (K a)_D - (K a)_p / (K a)_k}{(K a)_p / (K a)_D} \tag{25}$$

for conditions $(K a)_D = (K a)_k = 10^{-4} \text{ m}^2 \text{ s}^{-1}$, $L = 1 \text{ m}$, $\tau_L = \tau_G = 10$, $N_L = 1$. It results from this figure in conformity with expectation that the model with axial

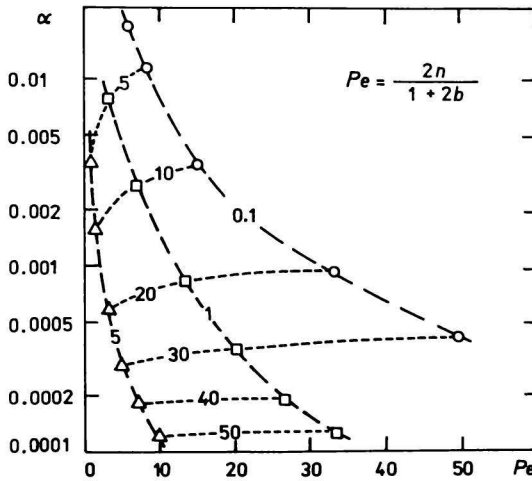


Fig. 4. Graphical representation of the deviations of the model of absorber with a cascade and countercurrent from the model of absorber with axial dispersion flow evaluated on the basis of differences in steady state.

--- n is constant; — — — b is constant.

dispersion flow and the model with a cascade of perfectly stirred regions approach to each other with increasing value of n , h . This figure also illustrates the statement alleged by *Lapidus* [8] that the model with a cascade of perfectly stirred regions and the axial dispersion model [3] are equally adequate provided the countercurrent is significant.

Conclusion

This paper is further contribution to the use of linear models for simulating the dynamics of real systems. On the basis of the processed experimental data we may state that the models of absorbers with cascade of ideally stirred regions with countercurrent are more adequate for significant axial stirring ($n \leq 20$) from the view-point of intricacy of calculation than the models of absorbers with axial dispersion flow. If the stirring is poor ($n \geq 50$), the system of linear differential equations expands very much so that the model of absorber with axial dispersion flow may become more convenient.

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Symbols

A	matrix in the system of differential equations	
<i>b</i>	coefficient of countercurrent	
B	matrix in the system of differential equations	
C	matrix in the system of differential equations	
E	unit matrix	
\dot{f}	rate of substance transfer by interfacial transfer	[kmol s ⁻¹]
<i>c</i>	concentration	[kmol m ⁻³]
<i>h</i>	integration step of differential equations	
<i>K a</i>	product of the overall coefficient of substance transfer and interfacial surface referred to unit length of absorption column	[m ² s ⁻¹]
<i>L</i>	length of absorption column	[m]
<i>m</i>	coefficient of equilibrium	
<i>n</i>	number of cascade members	
$N = (K a) L / \dot{q}_L$	number of transformation units	
P	auxiliary vector	
$Pe = u L / \varepsilon$	Peclet number	
Q	auxiliary vector	
\dot{q}	volume flow	[m ³ s ⁻¹]
$Re = du / \mu$	Reynolds number	
<i>t</i>	time	[s]
<i>S</i>	cross section of column	[m ²]
$u = q_0 / S$	axial velocity	[m s ⁻¹]
U	input vector	
<i>V</i>	volume	[m ³]
<i>w</i>	weight for the implicit Euler method	

X	vector of variables in the system of differential equations	
Y	vector of outputs from the systems	
Z	auxiliary vector	
α	quantity defined by eqn (25)	
β	quantity defined by eqn (6)	
ε	coefficient of axial stirring	$[\text{m}^2 \text{s}^{-1}]$
μ	dynamic viscosity	$[\text{kg m s}^{-1}]$
τ	mean retention time	

Indices

G	gaseous phase
L	liquid phase
P	piston flow
D	dispersion flow
K	cascade of ideally stirred regions with countercurrent
k, i, j	the k -th, i -th, and j -th

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