
CALCULATION OF THE DYNAMICS OF CONCENTRATION PROFILE IN A REACTOR SIMULATED BY A STAGewise MODEL

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Dynamics has been examined of the concentration profile in a reactor simulated by the stage-wise model under the isothermal conditions. Appropriate set of nonlinear differential equations has been solved iteratively using the Newton-Raphson method. Computed results have been compared with experimental data.

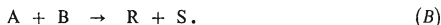
The behaviour of liquid flow in a rotating disc reactor (RD reactor) may be simulated by several models¹⁻³. A very frequently used model is the dispersion model and the model of a cascade of N perfect mixers with back flow. The dispersion models, used predominantly in connection with packed bed reactors, describe the behaviour of the reactor by partial differential equations^{1,3}. In contrast, reactors simulated by the cascade of N perfect mixers with back flow may be described by ordinary differential equations.

In this paper attention shall be paid to the transient state of the reactor simulated by N perfect mixers with back flow. This model, equally as some other models, permits simulation of the reactor behaviour over a relatively wide interval. Provided that the number of reactors in the cascade, N , equals unity, the model reduces to a perfectly stirred reactor, while for N growing to infinity with the back flow remaining finite, the model represents the plug flow. In practice it is often important to know concentration and/or temperature variations in response to a step change of the properties of the inlet stream. In order to predict these variations, one must have an adequate model and solve corresponding equations based on this model. In case that the reaction taking place in the reactor cannot be described by a linear reaction rate equation, the transient development of the concentration and/or temperature profile cannot be obtained in the closed form. For this reason this paper presents numerical solution by the Newton-Raphson method. As to the convergence this is a second order method. The computational procedure utilizing the Newton-Raphson method may be summarized in three steps. In the first step, the nonlinear terms are linearized by the quasi-linearization technique. Next, the linear equations are written in the form of the finite difference method and, finally, the obtained difference equations are solved iteratively.

THE MODEL OF THE CASCADE OF N PERFECT MIXERS WITH BACK FLOW*Isothermal Conditions*

In this part the Newton–Raphson method is applied to the set of equations describing the transient state of an isothermal continuous reactor.

Consider the cascade of N perfect mixers with back flow as sketched in Fig. 1 and the reaction



This reaction has been known as saponification of ethyl acetate. It is a second-order irreversible reaction with no side products. The kinetics of the reaction (A) may be expressed by an elementary bimolecular irreversible reaction rate equation for which we may write (A designates sodium hydroxide, B ethyl acetate)

$$\xi_v = \frac{dc_A}{v_A dt} = \frac{dc_B}{v_B dt} = k_v c_A c_B. \quad (1)$$

The effect of temperature on the reaction rate constant has been studied by Warder²⁵; who recommends the following numerical constants for the Arrhenius equation

$$\ln k_v = 16.47 - (5636.63/T). \quad (2)$$

The set of equations describing the response to a step change at the reactor inlet for the reactant A (the concentrations of reactants A and B need not be generally

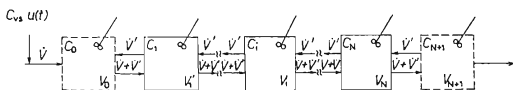


FIG. 1

Scheme of a Cascade of N Perfectly Mixed Cells with Back Flow

the same) in the dimensionless form reads as follows

$$j = 0$$

$$U(\theta) = (1 + \beta) C_{A0} - C_{A1} \quad (3)$$

$$1 \leq j \leq N$$

$$(1 + \beta) C_{A_{j-1}} - (1 + 2\beta) C_{A_j} - D_a C_{A_j} C_{B_j} + \beta C_{A_{j+1}} = \frac{1}{N} \frac{dC_{A_j}}{d\theta} \quad (4)$$

$$j = N + 1$$

$$0 = C_{AN+1} - C_{AN}, \quad (5)$$

where

$$\beta = \dot{V}'/\dot{V} \quad D_a = \tau k_v c_{A_{vs}}/N,$$

$$\tau = V/\dot{V} \quad \theta = t/\tau,$$

$$U(\theta) \begin{cases} < 1 & \text{when } \theta \geq 0, \\ < 0 & \text{when } \theta < 0. \end{cases} \quad (6)$$

Both end, so-called fictious, stages account for the concentration steps at the reactor inlet and the outlet, for they represent mixing of the feed stream with the internal back flow and their volume is negligible. On expressing the relationship between the dimensionless concentration of species A and B using

$$c_{Bvs} - c_B = c_{Avs} - c_A \quad (7)$$

by the relationship

$$C_B = c_B/c_{Avs} = C_A - 1 + (c_{Bvs}/c_{Avs}) \quad (8)$$

the set of Eqs (3)–(5) may be simplified and rewritten into the form

$$j = 1$$

$$1 - (1 + \beta) C_{A1} - D_a C_{A1}(C_{A1} - 1 + c_{Bvs}/c_{Avs}) + \beta C_{A2} = \frac{1}{N} \frac{dC_{A1}}{d\theta} \quad (9)$$

$$2 \leq j \leq N - 1$$

$$(1 + \beta) C_{A_{j-1}} - (1 + 2\beta) C_{A_j} - D_a C_{A_j}(C_{A_j} - 1 + c_{Bvs}/c_{Avs}) + \beta C_{A_{j+1}} = \frac{1}{N} \frac{dC_{A_j}}{d\theta} \quad (10)$$

$$j = N$$

$$(1 + \beta) C_{AN-1} - (1 + \beta) C_{AN} - D_a C_{AN}(C_{AN} - 1 + c_{Bvs}/c_{Avs}) = \frac{1}{N} \frac{dC_{AN}}{d\Theta} \quad (11)$$

Let us assume that the initial concentration profile of species A in the cascade at the time $t = 0$ is $c_{A\text{init}j} = 0$, $j = 1, 2, \dots, N$. The initial condition in the dimensionless form may then be written as

$$C_{Aj} = C_{A\text{init}j} = 0 \quad \text{when} \quad \Theta = 0 \quad \text{for} \quad 1 \leq j \leq N. \quad (12)$$

The set of Eqs (9)–(11) represents a nonlinear set of differential equations whose nonlinear terms may be represented by the expression

$$F(C_A^{k+1}) = F(C_A^k) + [C_A^{k+1} - C_A^k] \left[\frac{dF}{dC_A} \right]_{C_A^k} \quad (13)$$

obtained as a Taylor expansion after neglecting the terms of the order higher than the first.

Let the derivatives be replaced by the difference operator as follows

$$dC_A/d\Theta = [C_A^{k+1}(n+1) - C_A^k(n)]/\Delta\Theta, \quad (14)$$

where $C_A(n)$ designates the values of the vector C_A at the time instant $n \Delta\Theta$. The symbol k refers to the iterative step and $\Delta\Theta$ stands for the length of the time step.

The vector C_A^k may be replaced by one of the two following relationships

$$C_A^k = \frac{1}{2}[C_A^k(n+1) + C_A^k(n)] \quad (15)$$

$$C_A^k = C_A^k(n+1). \quad (16)$$

After substituting Eqs (12)–(15) into (9)–(11), a set of N linear simultaneous equations is obtained

$$\mathbf{A} \cdot C_A^{k+1}(n+1) = \mathbf{B} - \frac{1}{N \Delta\Theta} C_A^k(n) \quad (17)$$

$$\mathbf{A} = \begin{bmatrix} a_1 & \beta & & 0 & \dots & 0 \\ 1 + \beta & b_2 & \beta & & & \\ 0 & 1 + \beta & b_3 & \beta & & 0 \\ \vdots & & \dots & \dots & \dots & \dots \\ & & & 1 + \beta & b_{N-1} & \beta \\ 0 & \dots & 0 & 1 + \beta & a_N & \end{bmatrix} \quad (18)$$

$$\mathbf{B} = \begin{bmatrix} D_a[-\frac{1}{4}[C_{A1}^k(n+1) + C_{A1}(n)]^2] - 1 \\ D_a[-\frac{1}{4}[C_{A2}^k(n+1) + C_{A2}(n)]^2] \\ \vdots \\ D_a[-\frac{1}{4}C_{AN}(n+1) + C_{AN}(n)]^2 \end{bmatrix} \quad (19)$$

$$\mathbf{C}_A^{k+1}(n+1) = \begin{bmatrix} C_{A1}^{k+1}(n+1) \\ \vdots \\ C_{AN}^{k+1}(n+1) \end{bmatrix} \quad (20)$$

$$\mathbf{C}_A(n) = \begin{bmatrix} C_{A1}(n) \\ \vdots \\ C_{AN}(n) \end{bmatrix} \quad (21)$$

$$a_j = - \left\{ 1 + \beta + D_a[C_{Aj}^k(n+1) + C_{Aj}(n) + c_{Bvs}/c_{Avs} - 1] + \frac{1}{N \Delta \Theta} \right\} \\ j = 1, N \quad (22)$$

$$b_j = - \left\{ 1 + 2\beta + D_a[C_{Aj}^k(n+1) + C_{Aj}(n) + c_{Bvs}/c_{Avs} - 1] + \frac{1}{N \Delta \Theta} \right\} \\ j = 2, 3, \dots, N-1. \quad (23)$$

In the above Eq. (17), $C_{Aj}^{k+1}(n+1)$ for $j = 1, 2, \dots, N$ is an unknown variable. If it is assumed that values of $C_{Aj}(n)$ for $j = 1, 2, \dots, N$ at the n -th time step are known then its values at the $(n+1)$ -th step may be computed as follows:

- 1) estimate values $C_{Aj}^{k=0}(n+1)$, $j = 1, 2, \dots, N$
- 2) calculate $C_{Aj}^{k+1}(n+1)$, $j = 1, 2, \dots, N$ from Eq. (17)
- 3) if the following condition

$$|C_{Aj}^{k+1}(n+1) - C_{Aj}^k(n+1)| \leq \varepsilon \quad \text{for } j = 1, 2, \dots, N \quad (24)$$

is fulfilled, terminate the calculation. If the inequality (24) is false put $k = k+1$ and return to 2).

In the first time step we used a following starting values $C_A^{k=0}(n+1) = 0.001$. For time steps other than 1-st ($n = 2, 3, \dots$), the starting values of the concentration were those found in the previous time step, $C_A(n)$. For convergence reasons the value taken in the k -th iteration was the mean given by Eq. (15).

The computation of the dynamics of the concentration profile has been performed on a SIMENS 4004/150 computer for the following input data:

$$\begin{array}{ll}
 N & = 40 & c_{A_{vs}} & = 0.01965 \quad [\text{mol/l}] \\
 \beta & = 0.281 & c_{B_{vs}} & = 0.01973 \quad [\text{mol/l}] \\
 \Delta\theta & = 0.05 & \dot{V} & = 0.80 \quad [\text{l/min}] \\
 c_{A_{initj}} & = 0; \quad \theta = 0, \quad 1 \leq j \leq N & V & = 1.698 \quad [\text{l}] \\
 \varepsilon & = 10^{-6} & T & = 312.0 \quad [\text{K}] \\
 c_p & = 4144.93 \quad [\text{J kg}^{-1} \text{K}^{-1}] & k_v^0 & = 8.531 \cdot 10^8 \quad [\text{l mol}^{-1} \text{min}^{-1}]
 \end{array}$$

The results are shown in Fig. 2.

Adiabatic Conditions

Let us assume that the conditions summarized in the above paragraphs have been fulfilled and that there is an elementary irreversible second-order reaction (Eq. (A)) taking place in the reactor under the adiabatic regime. At the time instant $t = 0$ the reactor is at the initial temperature profile, T_{initj} for $j = 1, 2, \dots, N$, and for the subsequent time instants the inlet temperature is maintained at T_{vs} .

Under these assumptions the mass and energy balance of the reactor in the transient state simulated by the stagewise model with back flow, Fig. 1, may be written as:

$j = 1$

$$\begin{aligned}
 1 - (1 + \beta) C_{A1} - D_a^0 C_{A1} (C_{A1} - 1 + c_{B_{vs}}/c_{A_{vs}}) \exp(-E/RT_1) + \\
 + \beta C_{A2} = \frac{1}{N} \frac{dC_{A1}}{d\theta}
 \end{aligned} \quad (25)$$

$2 \leq j \leq N - 1$

$$\begin{aligned}
 (1 + \beta) C_{A_{j-1}} - (1 + 2\beta) C_{Aj} - D_a^0 C_{Aj} (C_{Aj} - 1 + c_{B_{vs}}/c_{A_{vs}}) \exp(-E/RT_j) + \\
 + \beta C_{A_{j+1}} = \frac{1}{N} \frac{dC_{Aj}}{d\theta}
 \end{aligned} \quad (26)$$

$j = N$

$$\begin{aligned}
 (1 + \beta) C_{A_{N-1}} - (1 + \beta) C_{AN} - D_a^0 C_{AN} (C_{AN} - 1 + c_{B_{vs}}/c_{A_{vs}}) \exp(-E/RT_j) = \\
 = \frac{1}{N} \frac{dC_{AN}}{d\theta}
 \end{aligned} \quad (27)$$

$j = 1$

$$T_{vs} - (1 + \beta) T_1 - Q C_{A1}(C_{A1} - 1 + c_{Bvs}/c_{Avs}) \exp(-E/RT_1) + \\ + \beta T_2 = \frac{1}{N} \frac{dT_1}{d\theta} \quad (28)$$

$$2 \leq j \leq N - 1$$

$$(1 + \beta) T_{j-1} - (1 + 2\beta) T_j - Q C_{Aj}(C_{Aj} - 1 + c_{Bvs}/c_{Avs}) \exp(-E/RT_j) + \\ + \beta T_{j+1} = \frac{1}{N} \frac{dT_j}{d\theta} \quad (29)$$

$$j = N$$

$$(1 + \beta) T_{N-1} - (1 + \beta) T_N - Q C_{AN}(C_{AN} - 1 + c_{Bvs}/c_{Avs}) \exp(-E/RT_N) = \\ = \frac{1}{N} \frac{dT_N}{d\theta}, \quad (30)$$

where

$$D_a^0 = \tau k_v^0 c_{Avs}/N,$$

$$Q = \Delta H(c_{Avs})^2 k_v^0 / N \rho c_p.$$

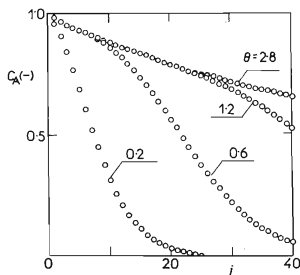


FIG. 2
Dynamics of the Concentration Profile — Isothermal Conditions

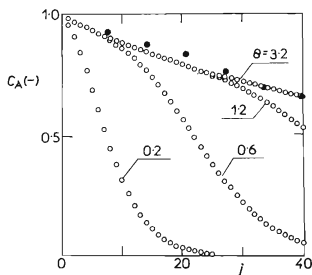


FIG. 3
Dynamics of the Concentration Profile — Adiabatic Conditions and Experimental Concentration Profile
○ Model, ● experiment.

The symbols E and R designate the activation energy and the universal gas constant. The initial conditions read:

$$C_{Aj} = C_{A \text{ init}j} \quad \text{when } \Theta = 0 \quad \text{for } 1 \leq j \leq N, \quad (31a)$$

$$T_j = T_{\text{init}j} \quad \text{when } \Theta = 0 \quad \text{for } 1 \leq j \leq N. \quad (31b)$$

The nonlinear terms in Eqs (25)–(30) may be linearized summarily

$$\begin{bmatrix} F_1(\mathbf{C}_A^{k+1}, \mathbf{T}^{k+1}) \\ F_2(\mathbf{C}_A^{k+1}, \mathbf{T}^{k+1}) \end{bmatrix} = \begin{bmatrix} F_1(\mathbf{C}_A^k, \mathbf{T}^k) \\ F_2(\mathbf{C}_A^k, \mathbf{T}^k) \end{bmatrix} + \begin{bmatrix} \frac{\partial F_1}{\partial C_A} & \frac{\partial F_1}{\partial T} \\ \frac{\partial F_2}{\partial C_A} & \frac{\partial F_2}{\partial T} \end{bmatrix}_{\mathbf{C}_A^k, \mathbf{T}^k} \cdot \begin{bmatrix} \mathbf{C}_A^{k+1} - \mathbf{C}_A^k \\ \mathbf{T}^{k+1} - \mathbf{T}^k \end{bmatrix}, \quad (32)$$

where

$$F_1(\mathbf{C}_A, \mathbf{T}) = D_a^0 C_A (C_A - 1 + c_{Bvs}/c_{Avs}) \exp(-E/RT), \quad (33)$$

$$F_2(\mathbf{C}_A, \mathbf{T}) = Q C_A (C_A - 1 + c_{Bvs}/c_{Avs}) \exp(-E/RT). \quad (34)$$

The vector \mathbf{T}^k is replaced by the relationship

$$\mathbf{T}^k = \frac{1}{2}[\mathbf{T}^k(n+1) + \mathbf{T}^k(n)]. \quad (35)$$

On replacing the derivatives by the difference operators of the type (14) and on substituting from Eqs (15)–(35) into (25)–(30) the following iteration formulas result:

$$\mathbf{A}_1 \mathbf{C}_A^{k+1}(n+1) = \mathbf{V}_1 \mathbf{T}^{k+1}(n+1) + \mathbf{E}_1 - \frac{1}{N \Delta \Theta} \mathbf{C}_A(n), \quad (36)$$

$$\mathbf{A}_2 \mathbf{T}^{k+1}(n+1) = \mathbf{V}_2 \mathbf{C}_A^{k+1}(n+1) + \mathbf{E}_2 - \frac{1}{N \Delta \Theta} \mathbf{T}(n) \quad (37)$$

in which the matrices \mathbf{A}_1 , \mathbf{A}_2 are tridiagonal ones and take identical form as the matrix \mathbf{A} with the elements

$$a_{1j} = - \left\{ 1 + \beta + D_a^0 \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot [C_{Aj}^k(n+1) + C_{Aj}(n) + c_{Bvs}/c_{Avs} - 1] + \frac{1}{N \Delta \Theta} \right\} \quad (38)$$

$j = 1, N$

$$b_{1j} = - \left\{ 1 + 2\beta + D_a^0 \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot \right. \\ \left. \cdot [C_{A_j}^k(n+1) + C_{A_j}(n) + c_{Bvs}/c_{Avs} - 1] + \frac{1}{N \Delta \Theta} \right\} \quad (39)$$

$$j = 2, 3, \dots, N-1$$

$$a_{2j} = - \left\{ 1 + \beta + Q \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot \right. \\ \left. \cdot \frac{2E [C_{A_j}^k(n+1) + C_{A_j}(n)]}{R [T_j^k(n+1) + T_j(n)]^2} \cdot \left([C_{A_j}^k(n+1) + C_{A_j}(n)]/2 + (c_{Bvs}/c_{Avs}) - 1 \right) + \frac{1}{N \Delta \Theta} \right\} \quad (40)$$

$$j = 1, N$$

$$b_{2j} = - \left\{ 1 + 2\beta + Q \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot \right. \\ \left. \cdot \frac{2E [C_{A_j}^k(n+1) + C_{A_j}(n)]}{R [T_j^k(n+1) + T_j(n)]^2} \cdot \left([C_{A_j}^k(n+1) + C_{A_j}(n)]/2 + (c_{Bvs}/c_{Avs}) - 1 \right) + \frac{1}{N \Delta \Theta} \right\} \quad (41)$$

$$j = 2, 3, \dots, N-1$$

and matrices \mathbf{V}_1 , \mathbf{V}_2 , \mathbf{E}_1 , \mathbf{E}_2 contain the elements on the main diagonal only

$$v_{1j} = D_a^0 \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot \\ \cdot \frac{2E [C_{A_j}^k(n+1) + C_{A_j}(n)]}{R [T_j^k(n+1) + T_j(n)]^2} \cdot \\ \cdot ([C_{A_j}^k(n+1) + C_{A_j}(n)]/2 + c_{Bvs}/c_{Avs} - 1) \quad j = 1, 2, \dots, N \quad (42)$$

$$v_{2j} = Q \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot \\ \cdot (C_{A_j}^k(n+1) + C_{A_j}(n) + c_{Bvs}/c_{Avs} - 1) \quad j = 1, 2, \dots, N \quad (43)$$

$$e_{1j} = -D_a^0 \exp \{ -2E/R [T_j^k(n+1) + T_j(n)] \} \cdot \\ \cdot \left\{ \frac{1}{4} [C_{A_j}^k(n+1) + C_{A_j}(n)]^2 + \frac{E [C_{A_j}^k(n+1) + C_{A_j}(n)]}{R [T_j^k(n+1) + T_j(n)]} \right\}$$

$$\cdot \left\{ [C_{A_j}^k(n+1) + C_{A_j}(n)]/2 + (c_{B_{vs}}/c_{A_{vs}})_{-1} \right\}, \quad j = 2, \dots, N \quad (44)$$

For $e_{1j=1}$ we may write

$$e_{1j=1} = e_{1j=2} - 1.$$

The elements e_{2j} , $j = 2, \dots, N$ are the same as e_{1j} , $j = 2, \dots, N$ except that instead of D_a^0 there is a symbol Q and for $e_{2j=1}$ we write

$$e_{2j=1} = e_{1j=2} - T_{vs}.$$

Let there be a functional

$$\mathbf{T}^{k+1}(n+1) = \mathbf{T}^k(n+1), \quad (45)$$

$$\mathbf{C}_\lambda^{k+1}(n+1) = \mathbf{C}_\lambda^k(n+1). \quad (46)$$

The set of Eqs (36) and (37) may then be rewritten into the form

$$\mathbf{A}_1 \mathbf{C}_\lambda^{k+1}(n+1) = \mathbf{V}_1 \mathbf{T}^k(n+1) + \mathbf{E}_1 - \frac{1}{N \Delta \Theta} \mathbf{C}_\lambda(n), \quad (47)$$

$$\mathbf{A}_2 \mathbf{T}^{k+1}(n+1) = \mathbf{V}_2 \mathbf{C}_\lambda^k(n+1) + \mathbf{E}_2 - \frac{1}{N \Delta \Theta} \mathbf{T}(n), \quad (48)$$

while each of the set of Eqs (47) and (48) may be solved separately. The computational procedure is analogous as in the previous case and it was performed on the Siemens 4004/150 computer. For the initial temperature profile we took the temperature of the feed reactants, $T_{vs} = 312.0$ K. As inputs we took the following numerical values

N	$= 40$	$c_{A_{vs}}$	$= 0.01965$ [mol/l]
β	$= 0.281$	$c_{B_{vs}}$	$= 0.01973$ [mol/l]
$\Delta \Theta$	$= 0.05$	\dot{V}	$= 0.80$ [l/min]
$c_{A_{initj}}$	$= 0; \quad \Theta = 0, \quad 1 \leq j \leq N$	V	$= 1.698$ [l]
ε	$= 10^{-6}$	T_{vs}	$= 312.0$ [K]
T_{initj}	$= T_{vs}; \quad \Theta = 0, \quad 1 \leq j \leq N$	k_v^0	$= 8.531 \cdot 10^8$ [l mol ⁻¹ min ⁻¹]
c_p	$= 4144.93$ [J kg ⁻¹ K ⁻¹]	ϱ	$= 0.993$ [kg l ⁻¹]

The results of the calculated concentration and temperature profile under the adiabatic conditions are shown in Fig. 3 and 4.

On the model RD reactor, described in detail in ref.⁴, we obtained experimentally the steady state residence time distribution function, the so-called E -curve, and the concentration profile of sodium hydroxide. Values of model parameters of the cascade of N perfectly mixed reactors $N = 40$ and $\beta = 0.281$, which had been used in the computational runs, were identified on the basis of comparison of the experimental and theoretical E -curves. The method used has been described in ref.⁴. Graphical illustration of both the experimental and theoretical E -curves is furnished in Fig. 5; the experimentally found concentration profiles together with the dynamics of the concentration profile under the adiabatic conditions is shown in Fig. 3.

From comparison of the experimentally obtained functions with the computed ones in Figs 3 and 5 there follows that the applied model of the cascade of N perfectly mixed reactors with back flow provides excellent description of the reactor response to an impulse. Moreover, it yields good results even in terms of reactor productivity and this is so even when the undergoing reaction exhibits nonlinear kinetics. The above model has been used for the calculation of the dynamics of the concentration and temperature profiles under isothermal and adiabatic conditions.

Steady state under the isothermal conditions was reached at the time $\theta = 2.8$, (Fig. 2). In ref.⁴ equations have been also solved describing the steady state under

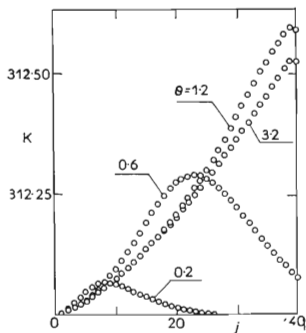


FIG. 4

Dynamics of the Temperature Profile —
Adiabatic Conditions

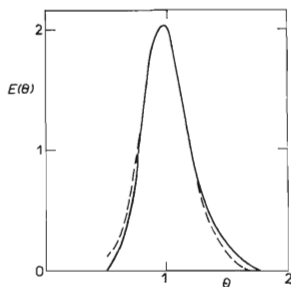


FIG. 5

Experimental and Model Residence Time
Distribution Function
— — — Model, ——— experiment.

the isothermal conditions of the reactor simulated by the cascade of N perfect mixers with back flow and the obtained results are identical those presented in Fig. 2 for $\Theta = 2.8$. This confirms correctness of the present solution of the underlying equations describing the transient state of the reactor.

As expected, under the adiabatic conditions the reactor reaches steady state later, namely at the time $\Theta = 3.2$, see Fig. 3. Fig. 4 confirms the well-known fact that in the transient state a greater temperature variations may occur in the reactor in comparison with the steady state. A comparison of Figs 2 and 3 indicates that the temperature changes, occurring during adiabatic operation, $T_{\max} = 0.5^\circ\text{C}$, have a negligible effect. For this case, which though is not typical, the problem of the dynamics of the concentration profile simplifies and one may consider only isothermal conditions.

The Newton-Raphson technique as a second-order method, in its application to solving sets of nonlinear differential equations, offers considerable advantages. It yields accurate results while it does not require excessive computer time. The first time step required 18 iterations and this number rapidly decreased to 4–6 iterations.

With these advantages it may be stated that this method may find wide use in solving equations describing the simulated reactor in the transient state for control purposes or reactor start-up.

LIST OF SYMBOLS

a, a_1, a_2	elements of matrices
A	reactant
$\mathbf{A}, \mathbf{A}_1, \mathbf{A}_2$	matrices
b	element of matrix
B	reactant
\mathbf{B}	vector
c_p	specific heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$)
c	concentration (mol/l)
$C = c/c_{vs}$	relative concentration
\mathbf{C}	vector of concentrations
D_a, D_a^0	Damkoehler number
e_1, e_2	elements of matrices
$E = 46892$	activation energy (J/mol)
$\mathbf{E}_1, \mathbf{E}_2$	matrices
k_v^0	frequency factor ($\text{l mol}^{-1} \text{min}^{-1}$)
k_v	reaction rate constant under isochoric conditions ($\text{l mol}^{-1} \text{min}^{-1}$)
n	time step
N	number of mixers
Q	a quantity characterizing reaction rate
R	gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
t	time (min)
T	absolute temperature (K)
\mathbf{T}	temperature vector

$U(\theta)$	unit function
v_1, v_2	elements of matrices
V	reactor volume (l)
\dot{V}	volume flow rate (l/min)
\dot{V}'	back flow volume rate (l/min)
$\mathbf{V}_1, \mathbf{V}_2$	matrices
$\beta = \dot{V}'/\dot{V}$	ratio of back flow to forward flow
$\Delta H = -71176$	reaction heat (J/mol)
$\Delta \theta$	time step
ε	accuracy of calculation
ρ	density (kg/l)
τ	time constant (min)
θ	dimensionless time
ν	stoichiometric coefficient
$\dot{\xi}_v$	reaction rate, (Eq.3)

Subscripts

A	reactant A
j	<i>j</i> -th stage
k	<i>k</i> -th iteration
init	at time $t = 0$
vs	inlet stream

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