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# Mathematical models for mixing in deep jet bioreactors: analysis

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**Abstract.** A mathematical model for single and multi step deep-jet bioreactors is presented. A stagewise approach based on macroscopic mechanistic model which divides the reactor into compartments with good quality of mixing and plug flow regions (macromixer), was used. For the mathematical representation of this model a system of differential equations, describing the concentration of tracer in structural elements based on mass balance, and the Runge-Kutta-Fehlberg numerical method of integration, was applied. The mixing time in a 300 dm$^3$ tank was determined by conductivity method with NaCl as tracer.

**List of symbols**

| | | |
|---|---|---|
| $V_g$ | dm$^3$ | total volume of liquid |
| $V_1; V_6$ | dm$^3$ | volumes of ideally mixed compartments in the vessel |
| $V_2; V_7$ | dm$^3$ | volumes of macromixer in the inner circulation flows |
| $V_3; V_9$ | dm$^3$ | volumes of liquid phase in the pump |
| $V_4; V_8$ | dm$^3$ | volumes of liquid phase in the pipe between the vessel and the pump |
| $V_5; V_{10}$ | dm$^3$ | volumes of liquid phase in pipes between the pump and the air input system, including falling jet |
| $F_E; F_{E,1}; F_{E,2}$ | dm$^3$/s | the inner volumetric circulation flow rates accross the macromixers |
| $F_{E,3}; F_{E,4}$ | dm$^3$/s | exchanges volumetric flow rates between two ideally mixed compartments in the vessel |
| $F_{cir}; F_{1,cir}; F_{2,cir}$ | dm$^3$/s | external volumetric circulation flow rates (pumping capacity) |
| $t_A$ | s | time interval of puls application |
| $t_{AA}$ | s | time point of impuls application related to the free chosen point of simulation |
| $t_{end}$ | s | end time of simulation |
| $F_{qu}$ | g$^2$/dm$^6$ | sum of quadratic error |
| $C_{*,*}$ | kg/m$^3$ | concentration of the tracer in the indicated compartment |
| $C_0$ | kg/m$^3$ | concentration of the tracer before the injection |
| $C_t$ | kg/m$^3$ | concentration of the tracer at the indicated time |
| $C_\infty$ | kg/m$^3$ | theoretical concentration of full mixed tracer |
| $i$ | – | index of an arbitrary tank |
| $C_{sim}$ | kg/m$^3$ | calculated concentration of the tracer by numerical integration method |

## 1 Introduction

Mixing with microbial growth is a process that involves fluid mechanics, diffusion and kinetics. These three mechanisms govern the process in any reacting mixture. Coupling of mixing and microbial kinetics plays an important role in establishing the performance of bioreactors, and especially in the scale up of microbial processes. Deep jet bioreactors are used in the three fields of industrial bioprocesses: fodder yeast production, aeration in treatment of waste waters and baker's yeast production. Although it is possible to find in the literature a lot of mathematical models and expressions for mixing in stirred tanks with impellers [1–4], air lift reactors, [5–9] bubble columns [6, 10] and plunging jet reactors [11–13], the deep jet reactor is not often the object of mathematical modelling. The mathematical solution of mixing in bioreactors by the finite elements method needs often a long operating time of computer systems. Therefore, we have tried to use the relatively simple macroscopic mechanistic model suggested by Singh et al. [14], based on tanks-in series, for the evaluation of the measured data.

## 2 Experiment

For the modelling, the reactor (Fig. 1) was split up into five compartments (structural elements). Our model is presented in Fig. 2.

The vessel is represented by an ideally mixed volume $V_1$, by the number of completely mixed tanks in series $V_2$ (macromixer) and by the inner exchange flow $F_E$. The external circulation system of reactor consists of the external circulation flow (pumping capacity) $F_{cir}$, the compartment of the pump as ideally mixed volume $V_3$, and two pipe volumes represented by a number of completely mixed tanks in series: $V_4$ and $V_5$ (the volume of pipe connection between tank and pump including the volume under the refusing plate and the pipe connection between pump and aeration system included the volume of the falling jet in the vessel). The volumes $V_1 - V_5$ are the liquid phase volumes in related compart-

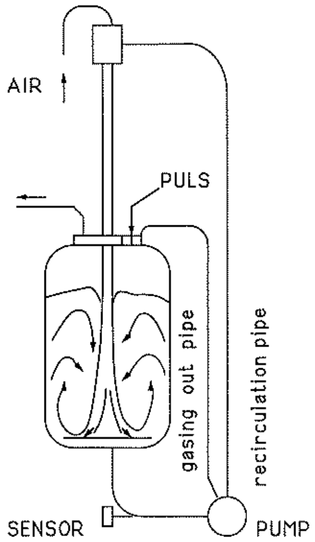

**Fig. 1.** The deep jet reactor and the inner directions of flows

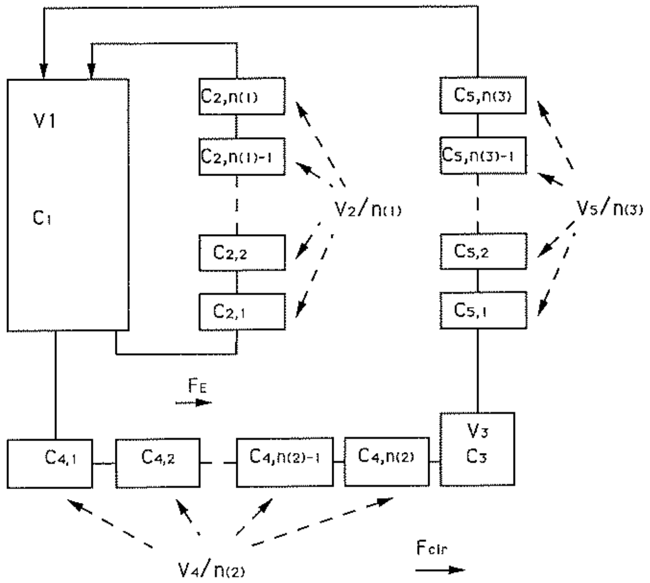

**Fig. 2.** The mechanistic model of mixing for one stage deep jet reactor

ments. For the mathematical representation of this model a system of differential equations (1.1 – 1.5), describing the concentration ($C$) in the structural elements based on mass balance, was used. The solution of this system can only be achieved with numerical method, therefore the Runge-Kutta-Fehlberg method was chosen, a method with control of the relative error and with variable step of integration [15]. In our simulations we have used a maximal integration step of 0.05 (s).

$$\frac{dC_1}{dt} = \left(\frac{F_E}{V_1}\right) C_{1,n(1)} + \left(\frac{F_{cir}}{V_1}\right) C_{4,n(2)} - \left(\frac{F_{cir}+F_E}{V_1}\right) C_1 \tag{1.1}$$

$$\frac{dC_{2,i}}{dt} = \left(\frac{F_E * n_{(1)}}{V_2}\right) C_{2,i-1} - \left(\frac{F_E * n_{(1)}}{V_2}\right) C_{2,i} \quad i \in \{1 \ldots n_{(1)}\} \tag{1.2}$$

$$\frac{dC_3}{dt} = \left(\frac{F_{cir}}{V_3}\right) C_{5,n(3)} - \left(\frac{F_{cir}}{V_3}\right) C_3 \tag{1.3}$$

$$\frac{dC_{4,i}}{dt} = \left(\frac{F_{cir} * n_{(2)}}{V_4}\right) C_{4,i-1} - \left(\frac{F_{cir} * n_{(2)}}{V_4}\right) C_{4,i} \quad i \in \{1 \ldots n_{(2)}\} \tag{1.4}$$

$$\frac{dC_{5,i}}{dt} = \left(\frac{F_{cir} * n_{(3)}}{V_5}\right) C_{5,i-1} - \left(\frac{F_{cir} * n_{(3)}}{V_5}\right) C_{5,i} \quad i \in \{1 \ldots n_{(3)}\} \tag{1.5}$$

$$F_{qu} = \sum_{t_A}^{t_{end}} (C_t - C_{sim})^2 \quad \left[\frac{kg}{m^3}\right]^2 \tag{1.6}$$

Using this relations and the measured data obtained with the tracer method in the 300 dm$^3$ VB-IZ-12 bioreactor [16] we have executed the simulations on a PC. In these simulations the experimental data obtained by two different volumes of liquid (200 dm$^3$ and 175 dm$^3$) and by the two levels of aeration (1 dm$^3$/dm$^3$ min and 4 dm$^3$/dm$^3$ min) were used. It is convenient to test the model before the simulation [4]. To make this possible, a set of data with adjustable parameters and those data which characterize the plant or the experiment (Table 1) was chosen. Then the parameters are altered according to the procedure described by Jury [6] and the effect on the quadratic error (Eq. 1.6) was registered. As reference values on the quadratic error (Eq. 1.6) was registered. As reference values for estimation of $F_{qu}$, the results obtained for 200 [dm$^3$] liquid volume and aeration level 1 [dm$^3$/dm$^3$ min] were used. In order to be able to evaluate the

**Table 1.** Parameters needed for simulation of one stage deep-jet bioreactor

| Plant and experiment characterized parameters | | | | | | | Aeration | Puls injection in compart. | Adjustable parameters | | | | | | Fig. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $V_g$ [dm$^3$] | $V_2=(V_g-V_1-V_3-V_4-V_5)$ [dm$^3$] | $V_3$ [dm$^3$] | $V_4$ [dm$^3$] | $V_5$ [dm$^3$] | $t_A$ [s] | $t_{AA}$ [s] | dm$^3$/dm$^3$ min | | $V_1/V_g$ | $n_{(1)}$ | $n_{(2)}$ | $n_{(3)}$ | $F_e$ [dm$^3$/s] | $F_{cir}$ [dm$^3$/s] | |
| 200 | 100.00 | 8.00 | 60.00 | 23.00 | 0.30 | 1.00 | 1 | $n_{(1)-1}$ | 0.045 | 3.00 | 35.00 | 20.00 | 13.75 | 13.00 | 6 |
| 200 | 100.00 | 8.00 | 60.00 | 23.00 | 0.30 | 1.00 | 1 | $n_{(1)}$ | 0.045 | 3.00 | 35.00 | 20.00 | 13.75 | 13.00 | 7 |
| 200 | 100.00 | 8.00 | 60.00 | 23.00 | 0.30 | 1.00 | 1 | $V_1$ | 0.045 | 3.00 | 35.00 | 20.00 | 13.75 | 13.00 | 8 |
| 200 | 115.72 | 4.40 | 60.00 | 10.88 | 0.30 | 1.00 | 4 | $n_{(1)-1}$ | 0.045 | 3.00 | 35.00 | 20.00 | 13.75 | 13.00 | 9 |
| 200 | 115.72 | 4.40 | 60.00 | 10.88 | 0.30 | 1.00 | 4 | $n_{(1)-1}$ | 0.045 | 4.00 | 35.00 | 20.00 | 18.50 | 12.50 | 10 |
| 175 | 82.51 | 8.00 | 60.00 | 23.00 | 0.30 | 1.00 | 1 | $n_{(1)-1}$ | 0.009 | 7.00 | 35.00 | 20.00 | 6.50 | 12.50 | 11 |

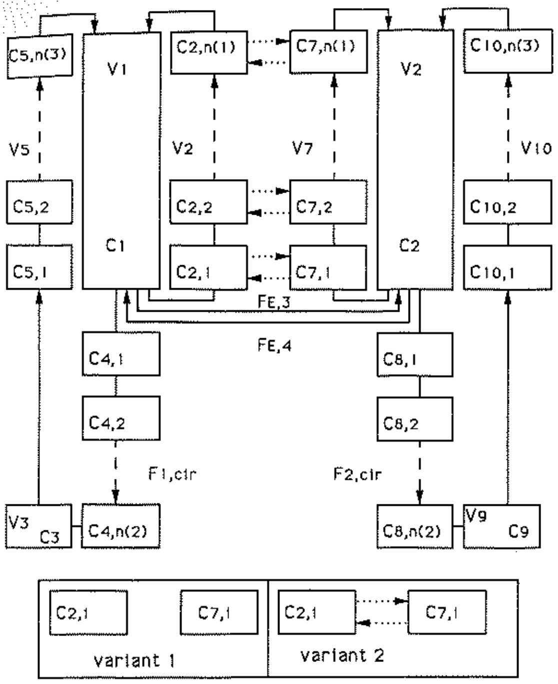

**Fig. 3.** The mechanistic model for mixing for two stage deep jet reactor

parameters of the model from measured responses to the injection of a tracer, we have simulated the tracer injection in the ideally mixed compartment $V_1$ and in the two last compartments of tank-in-series (the inner loop, volume $V_2$). As criteria for success of a simulation, the mixing time ($t_m$; with degree of mixing 90%), the circulation time ($t_c$) and the sum of quadratic error (Eq. 1.6) was used. A similar model (in two variants) for the two-stage deep jet bioreactor is proposed (Fig. 3), and used for the discussion of the validity of this model type by the calculation of flow pattern for the tracer in deep jet reactors.

## 3 Results and discussion

According to the macroscopic approach, mixing properties of bioreactors should be evaluated by simplified mathematical models. The macromixer compartment can be represented by the Bodenstein number or by the tank-in series model. In this work we have chosen a macroscopic mechanistic model. It can be seen that the model presented in Fig. 2 is completely defined with eleven parameters, seven of them are adjustable parameters ($V_1/V_g$, $V_3$, $n_{(1)}$, $n_{(2)}$, $n_{(3)}$, $F_E$ and $F_{cir}$) and four are those which characterize the plant and the operation conditions ($V_g$, $V_3$, $V_4$, $V_5$). In addition the time of puls application ($t_A$) as well as the starting point of impuls injection $t_{AA}$ are parameters which characterize the experiment. They are not included in the model, but they are included in the system of mathematical solution (as a delta Dirac function-vector inhomogenities). As in reality, and because the volumes of liquid phase in the pump and pipes ($V_3$, $V_4$, $V_5$), the total volume of liquid ($V_g$) and the capacity of pumping ($F_{cir}$) are constant for each plant or each defined experiment by the definite aeration rate, the number of adjustable parameters can be reduced to three: $V_1/V_g$, $n_{(1)}$, and $F_E$. Volume $V_2$ is not an adjustable parameter, because it is defined as the difference between total liquid volume $V_g$ and volumes of liquid phase in all others compartments (Table 1). In the case of not constant aeration rate, the capacity of pump depends on the density of biphasic system, and circulation flow $F_{cir}$ is also an adjustable parameter. Therefore, if the aeration rate is changed, the volume of liquid phase in the pump compartment and in the pipe connection between vessel and pump must also be changed. The excess of air is liberated in a special part of the pump (Fig. 1). The behaviour flow in pipe connections is practically always plug flow. These can be represented by great enough a number of tank-in-series. Therefore, the parameter $n_{(2)}$ and $n_{(3)}$ can be treated as constants, too.

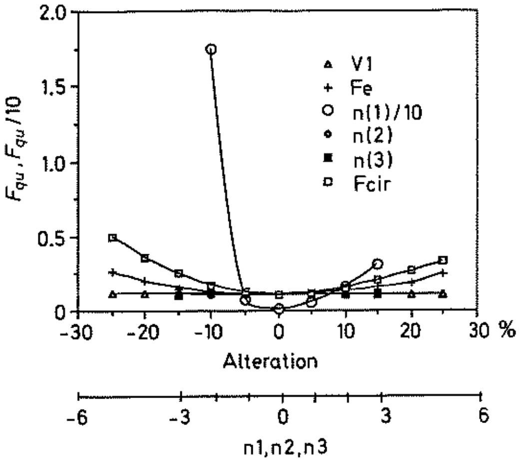

**Fig. 4.** Dependence of quadratic error on the changes (in percentage) of adjustable parameters. The number of tanks in the cascade is altered by integer numbers. Results for $n_{(2)}$ are located under results for $n_{(3)}$

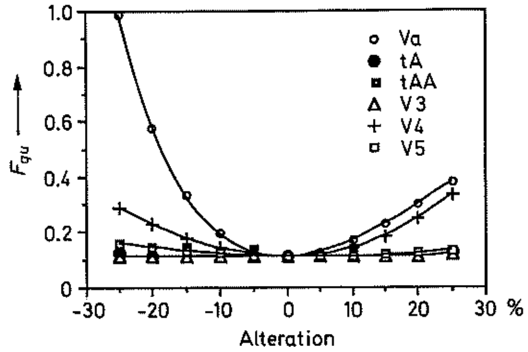

**Fig. 5.** Dependence of quadratic error on the changes (in percentage) of parameters which characterize the plant or the experiment. The number of tanks in the cascade is altered by integer numbers

The sensitivity of our model to the changes in adjustable parameters and parameters which characterized the plant (experiment) was tested [4, 6]. The results are presented in Figs. 4 and 5.

The model for one stage aeration system above described is very sensitive to the alteration of compartments number in tank-in series $n_{(1)}$, to the alteration of external circulation flow ($F_{\mathrm{cir}}$) as well as to the changes of the inner circulation flow ($F_E$) from adjustable parameters dataset (Fig. 4). Furthermore, results of the simulation procedure according to this mathematical model (Fig. 5) are strongly dependent on the the total volume of liquid ($V_g$) as well as on the volume of the liquid phase in the pipe connection ($V_4$) from the set of parameters which characterize the plant or the experiment. Also, the comparison of influence of tanks number in the tank-in-series (i.e. $n_{(1)}, n_{(2)}, n_{(3)}$) on results of simulation, expressed as the quadratic error (Figs. 4 and 5), show that the sensitivity of this model is higher when the values of $n$ are close to zero (Fig. 4). By increasing tank number in the cascade (Fig. 5), the sensitivity of model to the alteration of this parameter is lower.

The simulated and measured data of flow pattern for injected tracer by the volume of 200 dm$^3$ and 175 dm$^3$ liquid in the vessel are presented in Figs. 6–11. The set of parameters used for this simulations are listed in Table 1.

The locations of a tracer injection as well as sensors have to be chosen in a manner that identification of these points in the model is easy. Usually, it is a rule to locate the puls injection and sensors in the good mixed zone, that means, close to the stirrer. In the deep jet reactor, however, this area located over the refusing plate could not be exactly identified, because stirrers are missing. That is why the pulse injection was carried out as close as possible to the point of contact of falling jet and the liquid surface. This point cannot easily be defined in the model. Therefore, we have simulated three possibilities of pulse injection (in an ideally mixed volume $V_1$, in the compartment before the last volume in tank-in-series $V_2$ and in the last tank in this series) to acchieve a successful agreement between measured and simulated data (Figs. 6–8).

The best results were obtained by the simulated pulse injection in the compartment before the last of macromixer $V_2$ (Fig. 6). Furthermore, the simulation of the pulse injection in the last compartment of tank-in series $n_{(1)}$ (Fig. 7) leeds to the significant alteration of the circulation time and the height of the first peak. The worst result (Fig. 8) was acchieved by the simulation of pulse injection in the zone of good mixing quality (volume $V_1$). Repeated simulations (injection of pulse in the last tank of cascade and in the $V_1$), using other adjustable parameter as is indicated for Figs. 7 and 8 (Table 1), did not significantly reduced the above errors. This means, according to the above results (Fig. 6, 7 and 8), that the pulse injection on the surface of liquid in the real experiment could not be treated like the injection in the volume $V_1$ in the simulation procedure of our mathematical model.

The executed simulations by the altered aeration level (4 dm$^3$/dm$^3$ min) are presented in Fig. 9 and 10.

If we compare parameters needed to simulate the mixing of 200 dm$^3$ of liquid in the vessel by two different levels of aeration (Table 1, Figs. 6, 9 and 10), it will be seen that by

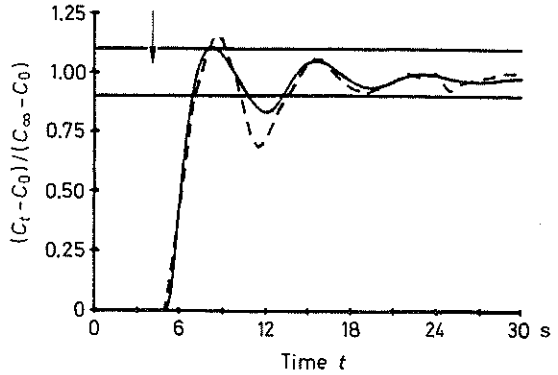

**Fig. 6.** Response for injection of the tracer (dashed line) and simulated data (plain line) achieved under the following conditions: $V_g = 200$ dm$^3$; aeration (1 dm$^3$/dm$^3$ min); simulation of tracer injection (indicated by the arrow) in the tank before the last in the cascade of $V_2$. Other parameters as indicated in Table 1

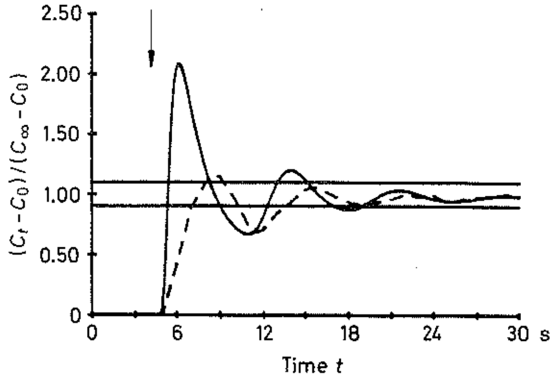

**Fig. 7.** Response for injection of the tracer (indicated by an arrow) and simulated data when injection of the tracer was considered in the last compartment of macromixer $V_2$. Other parameters are indicated in Table 1. Dashed line shows the measured data

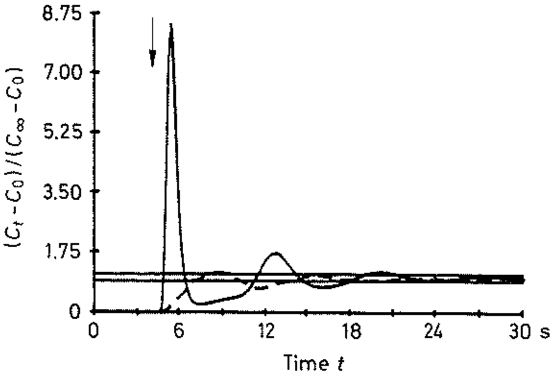

**Fig. 8.** Response for injection of the tracer (indicated by an arow) and simulated data when injection of the tracer was considered in the ideally mixed compartment $V_1$. Dashed line shows the measured data. Other parameters are indicated in Table 1

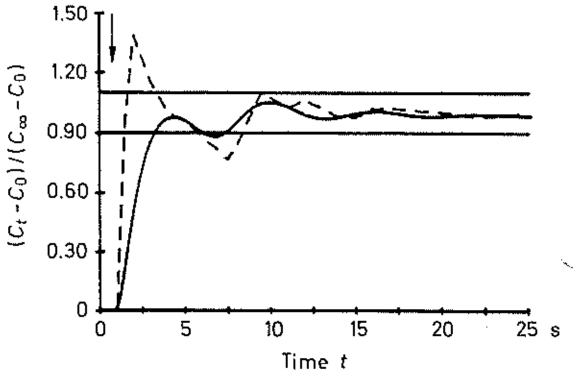

**Fig. 9.** Measured (dashed line) and simulated data for the injection of the tracer (arrow) achieved by 200 $dm^3$ liquid in vessel at an aeration level of 4 $dm^3/dm^3$ min, when in the model only the volume of liquid phase in the pump and in compartments of pipes were changed. Simulation of the pulse injection was done in the tank before the last compartment of the macromixer $V_2$

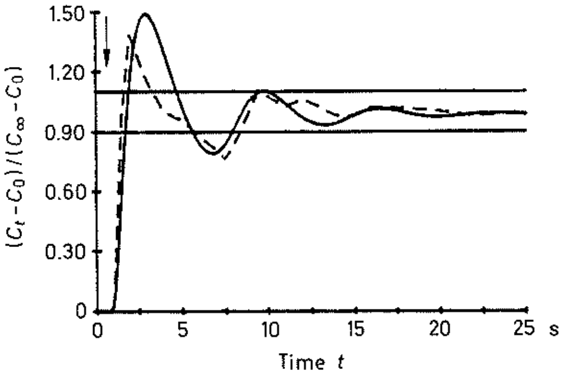

**Fig. 10.** Response for the injection of the tracer indicated by an arrow (dashed line) and simulated data achieved by experimental conditions as indicated by Fig. 9 and by parameters according to Table 1 (plain line)

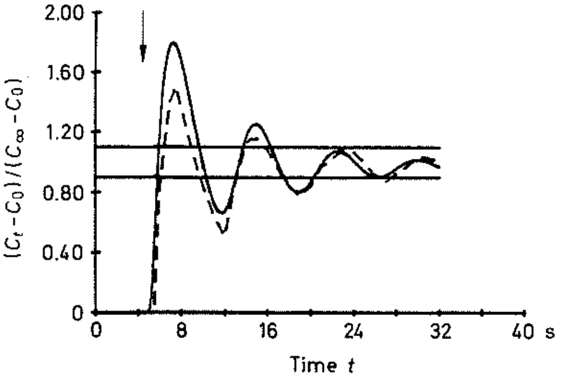

**Fig. 11.** Response for the injection of the tracer (dashed line) and simulated data (plain line) achieved by liquid volume $V_g = 175$ $dm^3$; Pulse injection (shown by an arrow) was simulated in the tank before the last compartment of macromixer $V_2$. Other parameters are indicated in Table 1

changing aeration level it is not sufficient to change only the related parameters in the model (i.e. volumes of liquid phases in pipes and in the pump which are in dependence of the air quantity in the two phase system (see Fig. 9)). In this case, to have a successful simulation (Fig. 10) it is necessary to change other adjustable parameters, too (Table 1).

According to Fig. 5, the volume of liquid in the vessel is a parameter which has a great influence on the success of simulation. Therefore, we have simulated the flow pattern of tracer using 175 $dm^3$ of liquid as the parameter. The result of this simulation is presented in Fig. 11.

Looking to the change of the aeration level, the comparison of results achieved by 200 $dm^3$ and 175 $dm^3$ liquid in the vessel (Figs. 6 and 11) and by related parameters needed for these simulations (Table 1), leeds to an interesting observation: if the volume of liquid in the reactor is changed, this is not the only parameter which should be altered in the model. This means, – similar to the fact reported earlier (17), – that it will will be necessary to find the relation between adjustable parameters and the total volume of liquid in the vessel as well as the relation between these parameters and the level of aeration. This will be our future work. Also, as before (Fig. 6), in the above experiments (Figs. 9, 10, 11) the best simulation was achieved by the pulse injection in the compartment before the last in tank-in series $n_{(1)}$.

A more complicated situation arises if we look for a model of the reactor with double aeration system (Fig. 3). This model is completely defined by 23 parameters, but this number can be reduced to twelve, as both systems (aeration and external circulation) are identical in its technical properties. Also, similar to the model for the one stage aeration system described above, further reduction of number of parameters, is possible in a real situation. The recirculation system is characterised by the plug flow, the geometrical characteristics of the plant are constants for each reactor and each experiment. Thus, this number could be reduced to four ($V_1/V_g = V_6/V_g$, $F_{E,1} = F_{E,2}$, $n_{(1)}$, $F_{E,3} = F_{E,4}$), eventually to five (additionally $F_{1,\mathrm{cir}} = F_{2,\mathrm{cir}}$). In a second variant, exchange flows in both directions could be established between two parallel compartments in tank-in-series of two inner circulation flows (between $V_{2,i}$ and $V_{7,i}$ and Fig. 3). Thereby, the number of adjustable parameters is increased by one. For multistage industrial scale reactors (three stages of aeration systems or more, 120–1000 $m^3$ of total volume), the presented model system will perhaps not easily be applicable, as the number of adjustable parameters increases with the number of aeration systems incorporated in the bioreactor. Furthermore, a complicated mathematical system needs a long operating time of the computer. In addition, mechanistic model for several types of reactors based on tank-in series contain a different number of adjustable parameters: air lift reactor, six [18]; bubble column, two [6]; three stage stirred tank reactor, four [19]. If it were be possible to measure the volume of the ideally mixed compartment $V_1$ separately, as suggested earlier [20], the number of adjustable parameter could be deminished by one.

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