Simulation of mixing in a flow reactor with jet and regulating partition

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Received 27 February 1975

Accepted for publication 12 May 1975

The paper is concerned with the simulation of mixing in a flow reactor with jet and regulating partition. The distribution of residence time measured by the method of stimulus and response was compared with the distribution of residence time for some models of non-ideal mixing. It is shown which of the models considered complied best with the given experimental conditions in the considered type of reactor.

Цель настоящей работы — моделировка мешания в проточном реакторе с соплом и с направляющей перегородкой. Методом возмужения и реакции измеренное распределение времени пребывания сравнивалось с распределением времени пребывания для нескольких моделей неидеального мешания. Было показано, которая из предлагаемых моделей лучше всего подходит для данных условий эксперимента в приведенном типе реактора.

The simulation of non-ideal mixing in flow reactors was studied by several authors. For instance, the models of *Gianetto* and *Cazzulo* [1], *Van de Vusse* [2], *Rippin* [3], *Hochman* and *McCord* [4], *Gibilaro* [5], and others [8, 9] are well known. In all these cases the so-called combined models, non-ideal due to the presence of stagnant zone, by-pass flow recirculation, cross-flow, *etc.*, are involved.

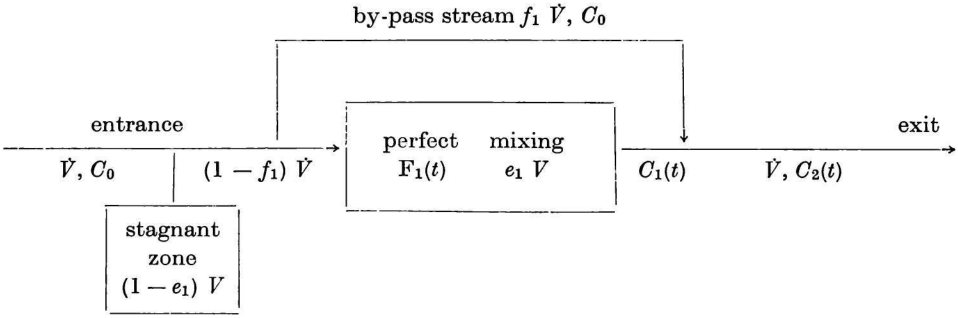

Fig. 1. Diagram of model *1.*

At the simulation of non-ideal mixing we started from some of the above models. We considered a system comprising a perfectly mixed region of the volume $e_1 V$, stagnant zone of the volume $(1 - e_1) V$, and by-pass stream of the volumetric rate $f_1 \dot{V}$ (Fig. 1) to be the simplest model. The cumulative residence time distribution function [6] is

$$F(t) = f_1 + (1 - f_1)(1 - e^{-at}), \tag{1}$$

where

$$a = \frac{(1 - f_1)\dot{V}}{e_1 V}. \tag{2}$$

As another model we used the *Gibilaro* [5] recirculation model consisting of a perfectly mixed region of the volume $e_2 V$ and volumetric rate $(1 + f_2)\dot{V}$, and of a recirculation stream for which we assumed a piston flow [7]. The volume of this recirculation stream was $(1 - e_2) V$, the volumetric rate being $f_2 \dot{V}$ (Fig. 2).

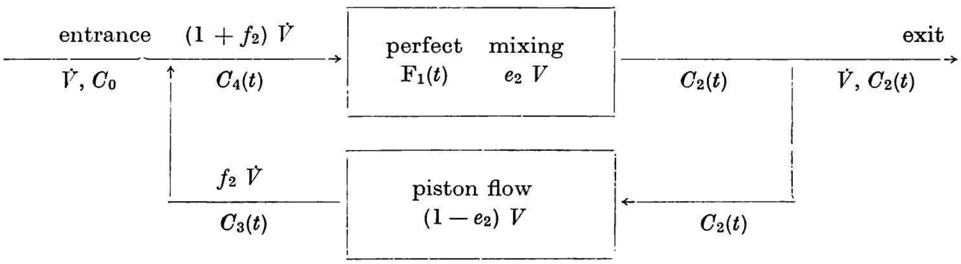

Fig. 2. Diagram of model 2.

The concentration of the tracer at the exit from the perfectly mixed region $C_2(t)$ fulfils the relationship

$$C_2(t) = \int_0^t C_4(s)\dot{F}_1(t - s)\,ds, \tag{3}$$

where $\dot{F}_1(t)$ is the derivative with respect to the time of the cumulative residence time distribution function $F_1(t)$ in the perfectly mixed region

$$F_1(t) = 1 - e^{-at} \tag{4}$$

and

$$a = \frac{(1 + f_2)\dot{V}}{e_2 V}. \tag{5}$$

The material balance obeys the following equation

$$\dot{V} C_0 + f_2 \dot{V} C_3(t) = (1 + f_2)\dot{V} C_4(t) \tag{6}$$

and for the concentration $C_3(t)$ it holds

$$C_3(t) = C_2(t - \bar{t}_m), \tag{7}$$

where $\bar{t}_m$ is the mean residence time in the recirculation stream

$$\bar{t}_m = \frac{(1 - e_2)\,V}{f_2\,\dot{V}}. \tag{8}$$

By inserting eqns (*6*) and (*7*) into eqn (*3*) we obtain the following relationship for the cumulative residence time distribution function $\mathrm{F}(t)$ for this model

$$\mathrm{F}(t) = \frac{C_2(t)}{C_0} = \frac{1}{1 + f_2}\,\mathrm{F}_1(t) + \frac{f_2}{1 + f_2}\int_0^t \frac{C_2(s - \bar{t}_m)}{C_0}\,\dot{\mathrm{F}}_1(t - s)\,\mathrm{d}s. \tag{9}$$

The third model used was the model proposed by *Gianetto* and *Cazzulo* [1]. It is a combination of the two preceding models (Fig. 3). It comprises a region of perfect mixing (volume $e_1 e_2 V$, volumetric rate $(1 - f_1)(1 + f_2)\dot{V}$), recirculation in which

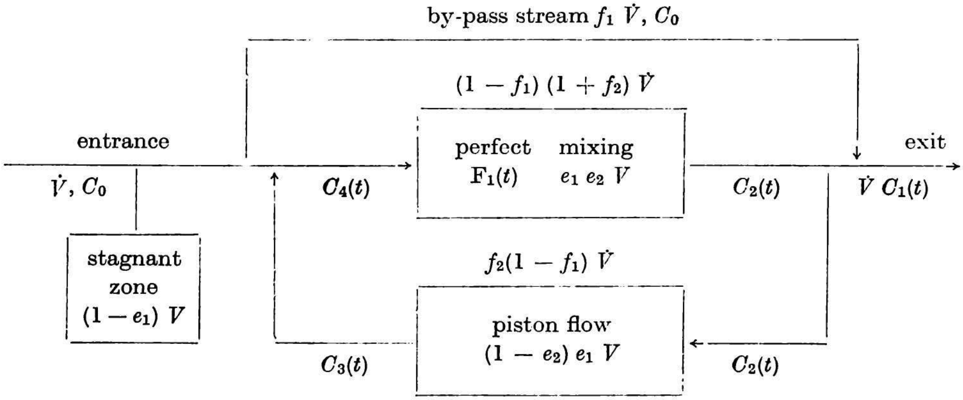

Fig. 3. Diagram of model *3*.

a piston flow is assumed (volume $(1 - e_2)\,e_1 V$, volumetric rate $f_2(1 - f_1)\,\dot{V}$), stagnant zone (volume $(1 - e_1)\,V$), and by-pass stream (volume flow $f_1\,\dot{V}$).

For the concentration at the exit from the perfectly mixed region $C_2(t)$ it holds

$$C_2(t) = \int_0^t C_4(s)\,\dot{\mathrm{F}}_1(t - s)\,\mathrm{d}s, \tag{10}$$

where $\mathrm{F}_1(t)$ is given by eqn (*4*) and

$$a = \frac{(1 - f_1)(1 + f_2)\,\dot{V}}{e_1 e_2 V} \tag{11}$$

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The material balance may be expressed by the following equation

$$\dot{V} C_0 + \dot{V} f_2 C_3(t) = \dot{V}(1 + f_2) C_4(t) \tag{12}$$

and for the concentration $C_3(t)$ it holds

$$C_3(t) = C_2(t - \bar{t}_m), \tag{13}$$

where

$$\bar{t}_m = \frac{(1 - e_2) e_1 V}{(1 - f_1) f_2 \dot{V}} \tag{14}$$

By substituting eqns (*12*) and (*13*) into eqn (*10*) we obtain

$$\frac{C_2(t)}{C_0} = \frac{1}{1 + f_2} F_1(t) + \frac{f_2}{1 + f_2} \int_0^t \frac{C_2(s - \bar{t}_m)}{C_0} \dot{F}_1(t - s)\, ds. \tag{15}$$

The cumulative residence time distribution function for the given model is

$$F(t) = \frac{C_1(t)}{C_0} = f_1 + (1 - f_1) \frac{C_2(t)}{C_0}. \tag{16}$$

In order to smooth the function $F(t)$ found experimentally we also used our model presented in Fig. 4. This model consists of a perfectly mixed region (volume $e_4 V$,

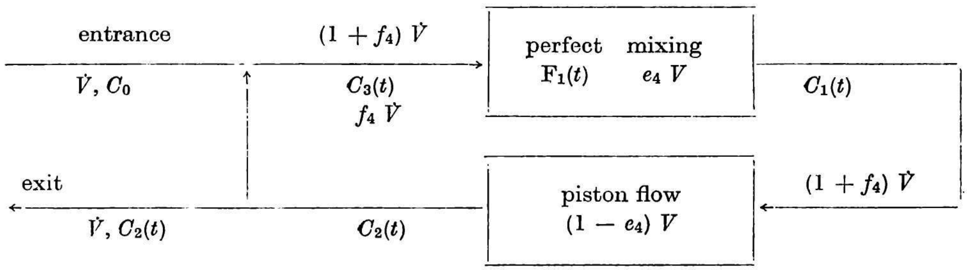

Fig. 4. Diagram of model *4*.

volumetric rate $(1 + f_4)\dot{V}$) and recirculation stream for which a piston flow is assumed (volume $(1 - e_4) V$, volumetric rate $(1 + f_4)\dot{V}$). This model corresponds to the streaming in circulation loops with equal mean residence time. The feed gets into the perfectly mixed core and the outlet stream leaves one circulation loop at the bottom of the reactor before the inlet into the perfectly mixed core.

The concentration at the exit from the perfectly mixed region is governed by the relationship

$$C_1(t) = \int_0^t C_3(s) \dot{F}_1(t - s)\, ds, \tag{17}$$

where

$$a = \frac{(1 + f_4)\,\dot{V}}{e_4\,V} \tag{18}$$

and

$$\bar{t}_{\mathrm{m}} = \frac{(1 - e_4)\,V}{(1 + f_4)\,\dot{V}}. \tag{19}$$

The material balance obeys the equation

$$f_4\,\dot{V}\,C_2(t) + \dot{V}\,C_0 = (1 + f_4)\,\dot{V}\,C_3(t) \tag{20}$$

and the subsequent equation holds for the concentration at the exit from the piston flow

$$C_2(t) = C_1(t - \bar{t}_{\mathrm{m}}) = \int_0^{t-\bar{t}_{\mathrm{m}}} C_3(s)\,\dot{\mathrm{F}}_1(t - \bar{t}_{\mathrm{m}} - s)\,\mathrm{d}s. \tag{21}$$

By inserting eqn (*20*) into eqn (*21*) we obtain for the function $\mathrm{F}(t)$

$$\mathrm{F}(t) = \frac{C_2(t)}{C_0} = \frac{1}{1 + f_4}\,\mathrm{F}_1(t - \bar{t}_{\mathrm{m}}) + \frac{f_4}{1 + f_4}\int_0^{t-\bar{t}_{\mathrm{m}}} \frac{C_2(s)}{C_0}\,\dot{\mathrm{F}}_1(t - \bar{t}_{\mathrm{m}} - s)\,\mathrm{d}s. \tag{22}$$

The models hitherto described characterize the mixing inside a reactor. If the reactor should work with an external recirculation if a more intensive stirring is required or a heat exchanger is to be attached, the residence time distribution function may be calculated from the function $\mathrm{F}(t)$ found experimentally for a stirred reactor provided the flow in the recirculating stream is a piston flow (Fig. 5). The function $\mathrm{F}(t)$ which is derived analogously to that used for model *2* is

$$\mathrm{F}(t) = \frac{C_2(t)}{C_0} = \frac{1}{1 + f}\,\mathrm{F_e}(t) + \frac{f}{1 + f}\int_0^{t} \frac{C_2(s - \bar{t}_{\mathrm{m}})}{C_0}\,\dot{\mathrm{F}}_{\mathrm{e}}(t - s)\,\mathrm{d}s, \tag{23}$$

where $\mathrm{F_e}(t)$ is the cumulative residence time distribution function of a stirred reactor obtained experimentally and $\bar{t}_{\mathrm{m}}$ is the mean residence time in the recirculating stream.

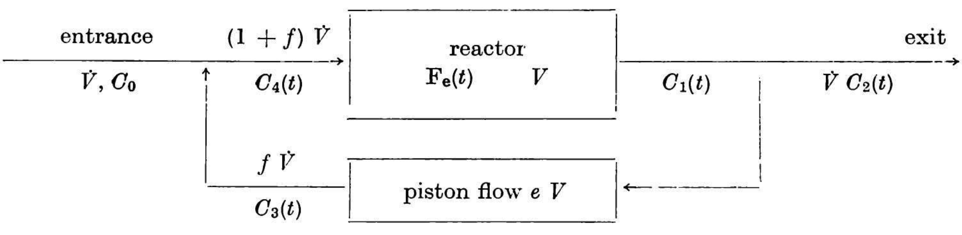

Fig. 5. Diagram of the reactor with external recirculation.

Experimental

The reactor in which the mixing was simulated is presented in Fig. 6. The liquid (water) entered the reactor through a jet of the diameter of 2.17 mm. The volume of the reactor was 2.79 l (diameter 137 mm, height 189 mm), the diameter of the regulating partition was 80 mm and its height 50 mm. The volumetric rate through the reactor was chosen within the range from 0.30 to 2.80 l min^{-1}. The measurements were carried out either without or with the regulating partition the position of which was adjustable in the range from 30 to 90 mm from the bottom.

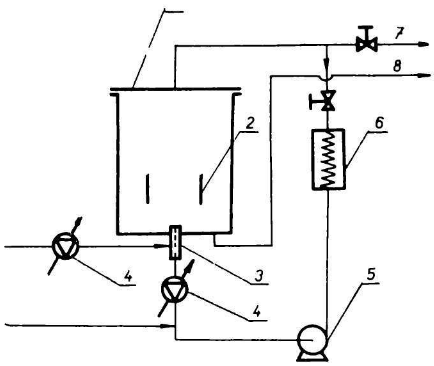

Fig. 6. Diagram of the reactor and its connection.
1. Reactor; *2.* regulating partition; *3.* jet; *4.* rotameters; *5.* centrifugal pump; *6.* heat exchanger; *7.* exit from the reaction system with recirculation; *8.* exit from the reaction system without recirculation.

The cumulative residence time distribution function F(t) was measured by the method of stimulus and response (into the entering stream an aqueous solution of methylene blue was injected and the samples in which the content of methylene blue was determined colorimetrically were taken from the exit stream in short time intervals). Altogether, 30 measurements were performed at three different positions of the regulating partition and four volumetric rates.

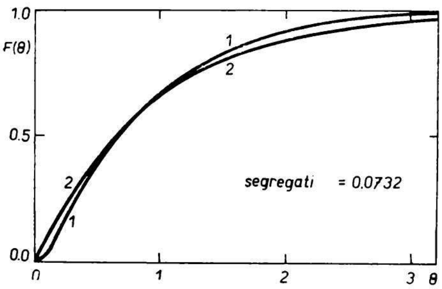

Fig. Function F(t) for the reactor without regulating partition and volumetric rate 0.98 l min^{-1}.
1. Experimental; *2.* smoothed for model *1.*

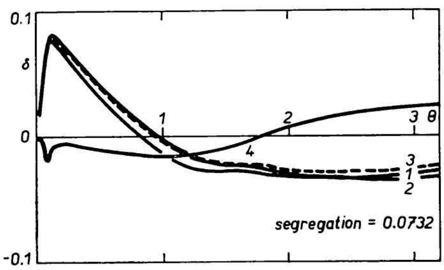

Fig. 8. Absolute deviations of the functions F(t) for individual models (reactor without regulating partition, volumetric rate 0.98 l min^{-1}).
Parameter of each line corresponds to the number of model.

A programme in the Fortran language was elaborated. It consisted of the following subroutines:

1. Subroutine involving the calculation of the function F(t) from the experimental relationship between the concentration of tracer and time in the exit stream at the impulse signal on the inlet and the calculation of the deviation of this function from the cumulative residence time distribution function for a perfectly mixed system (the so-called segregation defined by *Danckwerts* [7]).
2. Subroutine for smoothing the experimental function F(t) into eqn (*1*) — model *1*.
3. Subroutine for smoothing the experimental function F(t) into eqn (*9*) — model *2*.
4. Subroutine for smoothing the experimental function F(t) into eqn (*16*) — model *3*.
5. Subroutine for smoothing the experimental function F(t) into eqn (*22*) — model *4*.
6. Subroutine involving the calculation of the function F(t) at the attachment of external recirculation for different values of the recirculation ratio.

In subroutines 2—5, the values of parameters were found by scanning so that the sum of squared deviations between the measured and calculated function F(t) should reach the minimum.

With respect to a large extent of experimental results we present only two measurements performed at volumetric rates 0.98 and 0.37 l min^{-1} (without regulating partition). Fig. 7 shows the experimental function F(t) smoothed into the form F(t) for model *1* at volumetric rate 0.98 l min^{-1}. Since all functions F(t) for further models are situated between these two curves, for illustration we present Fig. 8 with the values of absolute

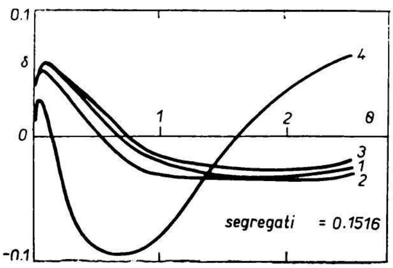

Fig. 9. Absolute deviations of the functions F(t) for individual models (reactor without regulating partition, volumetric rate 0.37 l min^{-1}).
Parameter of each line corresponds to the number of model.

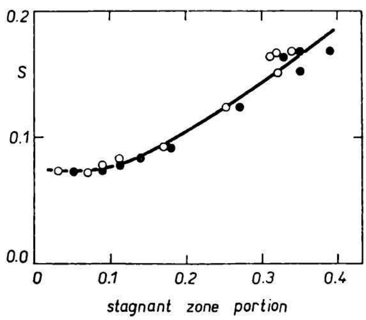

Fig. 10. Portion of stagnant zone as a function of segregation for model *1* and *3*. ○ Model *1*; ● model *3*.

deviations for individual models. In Fig. 9 the values of absolute deviations are presented for the measurements at volumetric rate 0.37 l min^{-1}.

Provided the segregation was less than 0.05, the measurements were not smoothed into the form of F(t) functions for individual models.

Discussion

If the segregation took place in the interval between 0.05 and 0.10, model *4* was evidently the best to depict the mixing in reactor (circulation in loops) which is demonstrated by Fig. 8. For a segregation exceeding 0.10 model *3* is more suited (Fig. 9). Models *1*, *2*, and *3* show no fundamental difference. All these models suggest the presence of a stagnant zone (for model *2* the stagnant zone is represented by a piston flow with relatively considerable volume and slight volumetric rate). No by-pass flow occurred in the reactor. The size of the stagnant zone for models *1* and *3* (Fig. 10) as well as the mean residence time in the region with piston flow for models *2* and *4* (Figs. 11 and 12) depends on the magnitude of segregation.

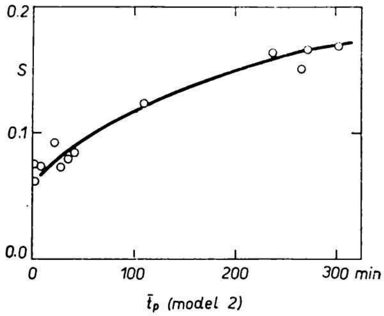

Fig. 11. Dependence on segregation of the mean residence time in the region of piston flow for model *2*.

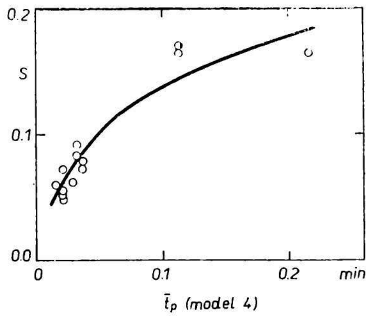

Fig. 12. Dependence on segregation of the mean residence time in the region of piston flow for model *4*.

Some measurements were carried out with external recirculation. As the measured function was in a good agreement with the calculated function F(t), we did not consider it necessary to continue measuring. For illustration, we present the measurements with volumetric rate 0.2 l min^{-1} for the recirculation ratio of 12.8 (Fig. 13).

Fig. 14 shows the function F(t) at different recirculation ratios when compared with a perfect mixing. The volumetric rate through the stirred reactor was 0.98 l min^{-1} (measurements without regulating partition) while the segregation without external recirculation equaled 0.073. It is obvious from this figure (and it may be also proved

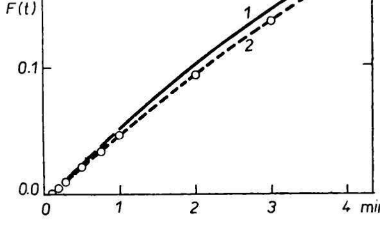

Fig. 13. Function F(t) at external recirculation for the volumetric rate through reaction system equal to 0.2 l min^{-1} and the recirculation ratio 12.8.
1. Calculated; *2.* experimental.

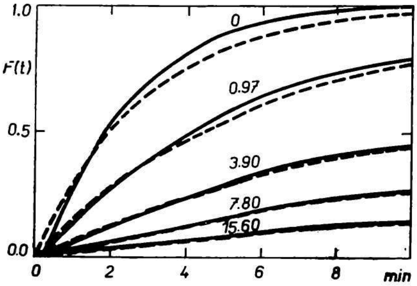

Fig. 14. Function F(t) at external recirculation for different recirculation ratios (parameter of lines).
——— Function F(t) of the reaction system (reactor without regulating partition, volumetric rate through reactor 0.98 l min^{-1}).
- - - - Function F(t) of perfectly mixed system.

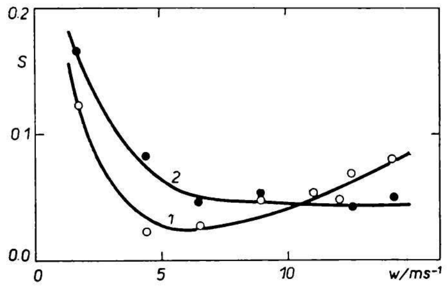

Fig. 15. Dependence of segregation on velocity in the jet.
1. Reactor without regulating partition;
2. reactor with regulating partition situated 6 cm from the bottom.

theoretically) that the mixing approaches to perfect mixing with an increasing recirculation ratio. The value of the necessary recirculation ratio depends on segregation in the stirred reactor.

The dependence of segregation on the velocity in the jet (Fig. 15) shows that the mixing is very sensitive to this velocity. At first, with increasing velocity in the jet the segregation decreases and afterwards it starts to increase. Though the regulating partitions has no any great influence on segregation at lower velocities in the jet, its influence is evident at higher velocities (the segregation changes very little with increasing velocity).

Symbols

a	ratio of the volumetric rate to the volume of perfectly mixed region
C	concentration of tracer
e_i	volume fraction
f_i	fraction of volumetric rate
F(t)	cumulative residence time distribution function
s	variable of integration
S	segregation
t	time
$\bar{t}$	mean residence time
V	volume of reactor
$\dot{V}$	volumetric rate through reactor
w	velocity in the jet
Θ	dimensionless time ($= (\dot{V}/V)\ t$)
δ	deviation of the calculated function F(t) from the experimental function

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Translated by R. Domanský