

$$u \cdot \frac{\partial w}{\partial r} + w \cdot \frac{\partial w}{\partial z} = -\frac{1}{\rho} \cdot \frac{\partial p}{\partial z} + \nu \cdot \left[\frac{1}{r} \cdot \frac{\partial}{\partial r} \left(r \cdot \frac{\partial w}{\partial r} \right) + \frac{\partial^2 w}{\partial z^2} \right], \quad (4.2b)$$

$$\frac{1}{r} \cdot \frac{\partial(r \cdot u)}{\partial r} + \frac{\partial w}{\partial z} = 0, \quad (4.3)$$

as well as material balance equations

$$u \cdot \frac{\partial c_i}{\partial r} + w \cdot \frac{\partial c_i}{\partial z} = D_i \cdot \left[\frac{1}{r} \cdot \frac{\partial}{\partial r} \left(r \cdot \frac{\partial c_i}{\partial r} \right) + \frac{\partial^2 c_i}{\partial z^2} \right] + R_i \quad (10.3)$$

with boundary conditions:

$$\text{-- at the mixer axis } (r=0) \quad u=0 \quad \frac{\partial c_i}{\partial r} = 0, \quad (10.4a)$$

$$\text{-- at the mixer walls} \quad u=w=0 \quad \nabla(c_i) \cdot \hat{n} = 0, \quad (10.4b)$$

$$\text{-- at the central inlet } (0 \leq r < r_1) \quad u=0 \quad w=2 \cdot \bar{w}_1 \cdot [1 - (r/r_1)^2] \quad c_i = c_{i1}, \quad (10.4c)$$

$$\text{-- at the annular inlet } (r_1 < r \leq r_2)$$

$$u=0 \quad w=2 \cdot \bar{w}_2 \cdot \left[1 - \left(\frac{r}{r_2} \right)^2 + \frac{1 - (r_1/r_2)^2}{\ln(r_2/r_1)} \cdot \ln \left(\frac{r}{r_2} \right) \right] \left/ \left[1 + \left(\frac{r_1}{r_2} \right)^2 - \frac{1 - (r_1/r_2)^2}{\ln(r_2/r_1)} \right] \right. \quad c_i = c_{i2} \quad (10.4d)$$

were solved using the fluid dynamics analysis package FIDAP6. The finite element method was applied. The simulations were done in two stages. During the first stage the velocity field was calculated and used in the second stage to compute the species distributions.

10.2. Conversion and Selectivity Computations.

The course of chemical reactions occurring between initially unpremixed reactants is directly related to the rate of mixing of feeding streams. On the other hand, the mechanisms governing mixing are determined by the type of flow in the reactor. If the flow is purely laminar, mass transfer between liquid elements and within them depends on the rate of laminar deformation and molecular diffusion.

The most effective energetically is the longitudinal deformation [22]. Figures 10.3 and 10.4 showing streamline contours plots illustrate that this type of deformation is predominant in the flow domain close to the mixers axes. Both plots were obtained for the same values of the initial volume ratio:

$$a = Q_2/Q_1 \quad (10.5)$$

and the same values of Reynolds number:

$$Re = \frac{\bar{w} \cdot d}{\nu}, \quad \text{where} \quad \bar{w} = \frac{4 \cdot (Q_1 + Q_2)}{\pi \cdot d^2}. \quad (10.6)$$

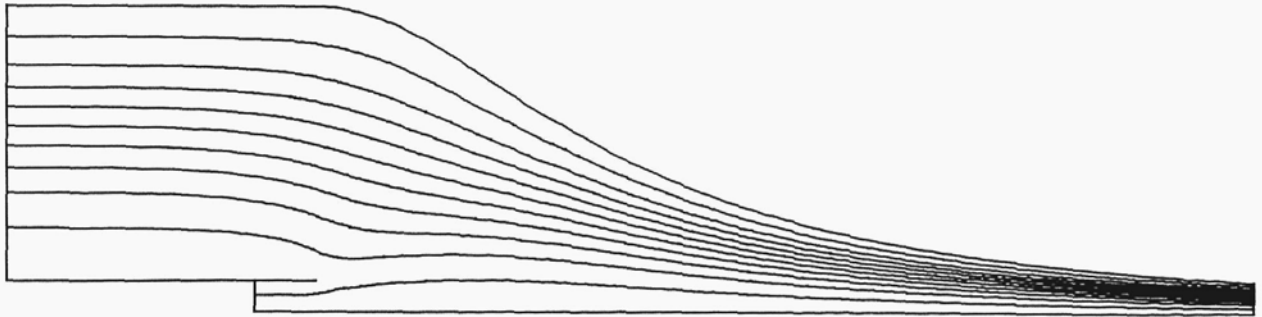


Figure 10.3. Streamlines contours - mixer I; $Re=1$, $a=9$.

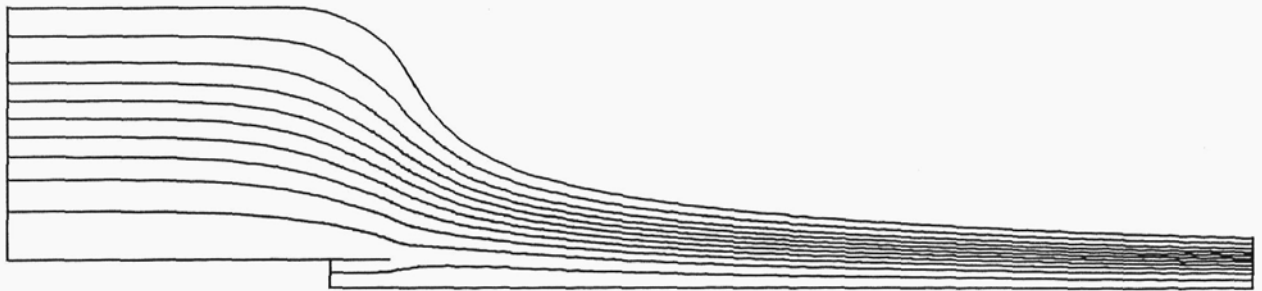


Figure 10.4. Streamline contours - mixer II; $Re=1$, $a=9$.

An evolution of the elongation rate with the age for the liquid elements flowing along the mixer axis is presented in figures 10.5 and 10.6 (age of elements at position $z=0$ equals 0). Arrows in figure 10.6 point out the exit ages of liquid elements.

Analysis of these figures reveals that in mixer I stretching takes place just before the outflow from the reactor, whereas in mixer II the rate of deformation remains constant except a small region near the central feeding pipe. It can also be seen that residence times, computed for the same inlet volumetric flows, in the second reactor are shorter than those in the first reactor.

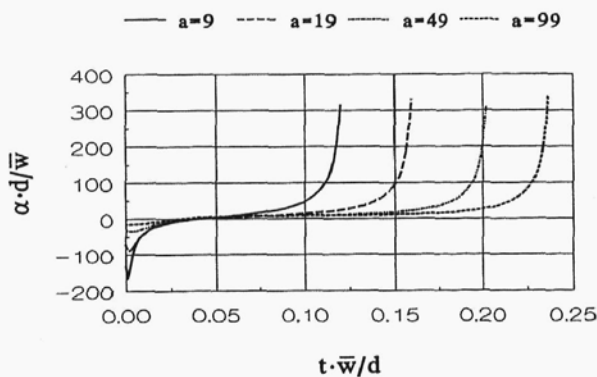


Figure 10.5. Elongation rate vs. age of liquid elements - mixer I; $Re=1$, $r=0$.

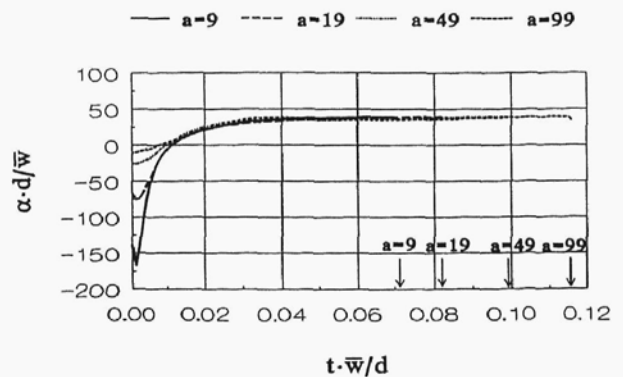


Figure 10.6. Elongation rate vs. age of liquid elements - mixer II; $Re=1$, $r=0$.

Let us now check how the differences in the flow pattern influence the courses of chemical reactions.

Three types of reaction systems which were tested as the quantitative measures of the mixing efficiency are described in table 10.I. It was assumed that all reactants have equal molecular diffusivities, which allows to replace the concentrations c_A and c_B with one composition variable $c=c_A-c_B+c_{B0}$ and replace two material balance equations (10.3) for A and B with a single equation. The concentration profiles of species reacting instantaneously can be recalculated from computed profiles of c using the following formulas:

$$c_A = \frac{|c - c_{B0}| + (c - c_{B0})}{2}, \quad (10.7a) \quad c_B = \frac{|c - c_{B0}| - (c - c_{B0})}{2}. \quad (10.7b)$$

Table 10.I. Reaction systems; reactions are irreversible.

Test system	Reactants		Reaction scheme	Reaction kinetics
	central feed	annular feed		
1	A	B	$A + B \rightarrow P$	instantaneous $R \rightarrow \infty$
2	A	B	$A + B \rightarrow P$	fast $R = -k \cdot c_A \cdot c_B$
3	A	B + C	$A + B \rightarrow P$	instantaneous $R \rightarrow \infty$
			$A + C \rightarrow Q$	fast $R = -k \cdot c_A \cdot c_B$

Conversions and selectivities are given by:

$$Y_i = 1 - \dot{N}_i / \dot{N}_{i0}, \quad (10.8) \quad X = (\dot{N}_{C0} - \dot{N}_C) / (\dot{N}_{A0} - \dot{N}_A). \quad (10.9)$$

The results of computations are presented in tables 10.II and 10.IIIabcd where

$$\overline{Da} = k \cdot \bar{c}_{A0} \cdot d^2 / D_A, \quad (10.10) \quad Sc = \nu / D_A \quad (10.11)$$

stand for Damköhler number and Schmidt number, respectively.

Data shown in table 10.II indicate that conversion of a single instantaneous reaction depends mainly on the extent of the reaction zone and is hardly affected by the residence times of the liquid elements being mixed and by the history of deforma-

Table 10.II. Conversions in instantaneous and fast reactions; $Re=1$, $Sc=1000$, $\dot{N}_{A0}=\dot{N}_{B0}$, $Da=1000$ (fast reaction).

a	Instantaneous reaction		Fast reaction	
	Mixer I	Mixer II	Mixer I	Mixer II
9	15.66	15.74	2.14	1.48
19	14.22	14.21	2.68	1.88
49	12.93	12.73	3.03	2.32
99	12.28	12.02	3.13	2.54

tion. In the axial direction the geometry of both mixers determines the extension of the reaction zone (distance from the tip of the central pipe to the outlet equals $1.5 \cdot d$), whereas the radial dimension of the reaction surface is directly dependent on the volume ratio, a , of the feeding flows. An increase of the feeding rate from the central pipe increases the length of the reaction zone and the resulting conversion; compare figures 10.7 and 10.8. The conversion of a fast reaction increases with the increasing residence time; compare table 10.II with figures 10.5 and 10.6.



Figure 10.7. Mixer I, $a=9$.

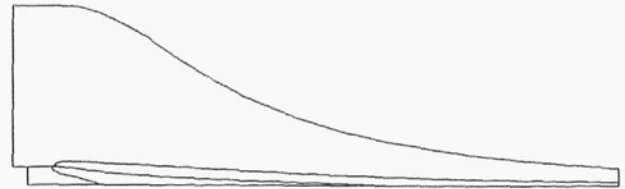


Figure 10.8. Mixer I, $a=99$.

Concentration contours of reagent A (1%, 50%, 99%); $Re=1$, $Sc=1000$, $\dot{N}_{A0}=\dot{N}_{B0}$.

Let us consider now the competitive-parallel reactions. One can see that the conversion of a single reaction does not tell much about the history of mixing. On the other hand, two parallel reactions (system 3 in table 10.I) with the first one instantaneous and the second one fast, provide a unique measure of segregation in the reactor [66].

For fast mixing the limiting substrate A is mostly consumed in the reaction with B, which decreases the selectivity. The high initial volume ratio of reactants is equivalent to the high initial segregation of the reactants, which results in slower mixing and higher selectivity - see tables 10.IIIabc.

Data presented in tables 10.IIIab, obtained for the same Reynolds number ($Re=1$), indicate that conversions of the limiting substrate, Y_A , are practically equal for both mixers and depend only on the initial volume ratio, a . In these conditions, conversions of the fast

Table 10.IIIa. Conversions and selectivities in competitive-parallel reactions; mixer I, $Re=1$, $Sc=1000$, $\bar{Da}=1000$, $\dot{N}_{A0}=\dot{N}_{B0}=\dot{N}_{C0}$.

a	Y_A [%]	Y_B [%]	Y_C [%]	X[%]
9	16.92	15.41	1.51	8.91
19	16.10	13.96	2.14	13.26
49	15.29	12.69	2.60	17.02
99	14.83	12.09	2.74	18.47

Table 10.IIIb. Conversions and selectivities in competitive-parallel reactions; mixer II, $Re=1$, $Sc=1000$, $\bar{Da}=1000$, $\dot{N}_{A0}=\dot{N}_{B0}=\dot{N}_{C0}$.

a	Y_A [%]	Y_B [%]	Y_C [%]	X[%]
9	16.76	15.64	1.11	6.64
19	15.59	14.09	1.50	9.61
49	14.69	12.62	2.08	14.12
99	14.24	11.96	2.28	16.03

reaction, Y_C , and consequently the final selectivities, X , defined by equation (10.9), are higher in the first mixer. Considering these results and the fact that the mean residence time in mixer **I** is 2.3 times longer than in mixer **II** for the same values of Re and a , one can conclude that mixture in the second mixer is more homogeneous (less segregated) than in the first one. This results from the fact that distribution of the rate of deformation of fluid elements in the system is more uniform in mixer **II** than in mixer **I**, where mixing of reactants streams takes place mainly at the end of the mixer.

Table 10.IIIc presents results of computations performed for mixer **I**, for the same value of the mean residence time as in mixer **II**. To obtain equal values of the mean residence time Reynolds number was set to 2.3 in mixer **I**. Again one can see that mixing in the second reactor is better, because for the same mean residence time the

Table 10.IIIc. Conversions and selectivities in competitive-parallel reactions; mixer **I, $Re=2.3$, $Sc=1000$, $\bar{Da}=1000$, $\dot{N}_{A0}=\dot{N}_{B0}=\dot{N}_{C0}$.**

a	$Y_A[\%]$	$Y_B[\%]$	$Y_C[\%]$	$X[\%]$
9	10.31	9.81	0.50	4.87
19	9.42	8.62	0.80	8.52
49	8.57	7.45	1.12	13.03
99	8.02	6.79	1.24	15.44

conversions of the limiting substrate, Y_A , are approximately 40% lower in mixer **I** than in mixer **II**. Smaller conversion in the first system results also in smaller selectivity than in the second system. However, a comparison of selectivities obtained in both reactors does not say much about the quality of mixing in both systems. The selectivity can be applied as a measure of mixing efficiency only for the systems with the same degree of conversion of the substrate remaining in stoichiometric deficiency.

The above results can be useful for design and determination of operating conditions of chemical reactors when one has to avoid side reactions leading to excessive consumption of the main substrate or producing impurities lowering quality of the final product.

10.3. Degrees of Segregation.

The common definition of the degree of segregation [8,9] is based on the distribution of dimensionless concentrations of non-reacting species $f_A=c_A/c_{A0}$ and $f_B=c_B/c_{B0}$ (usually $f_B \cong 1 - f_A$)

$$I_S = \frac{\overline{(f'_A)^2}}{\bar{f}_A \cdot (1 - \bar{f}_A)} = \frac{\overline{(f'_B)^2}}{\bar{f}_B \cdot (1 - \bar{f}_B)} = -\frac{\overline{f'_A \cdot f'_B}}{\bar{f}_A \cdot \bar{f}_B} = 1 - \frac{\overline{f_A \cdot f_B}}{\bar{f}_A \cdot \bar{f}_B}. \quad (10.12)$$