10. Numerical Simulations of Mass Transfer Process in On-Line Mixers.

10.1. Description of Investigated Systems.

The numerical experiments were conducted in two axisymmetric, on-line, steady-state flow systems shown in figures 10.1 and 10.2. The rate of deformation in these mixers depends on the shape of the mixer contraction section; the shapes are given by the following equations:

- mixer I $$\frac{r}{d}=\frac{0.125}{0.25+(z/d)^2} \quad 0\le z/d\le 1.5\ , \qquad \textbf{(10.1)}$$

- mixer II $$\frac{r}{d}=0.262+\sqrt{0.238^2-[(z/d)+0.171]^2} \quad -0.171\le z/d\le 0.042\ , \qquad \textbf{(10.2a)}$$

$$\frac{r}{d}=\frac{0.5}{\sqrt{1+20\cdot(z/d)}} \quad 0.042\le z/d\le 1.5\ . \qquad \textbf{(10.2b)}$$

Other important factors are the flow rates of two feeding flows, the central one emerging from a small pipe ($\mathbf{Q_1}$), and the annular one ($\mathbf{Q_2}$).

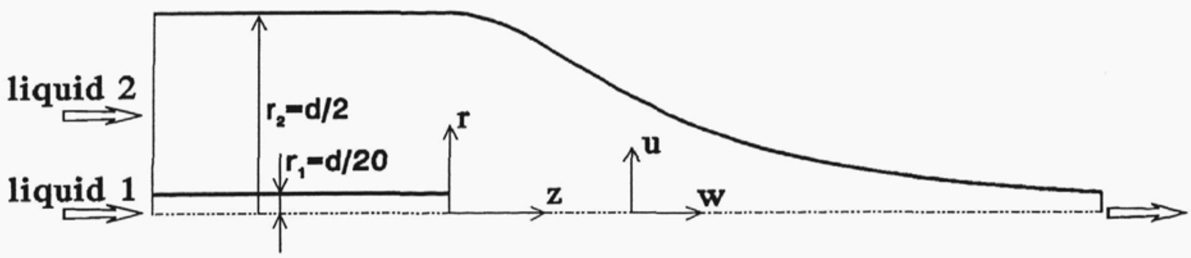

Figure 10.1. Mixer I.

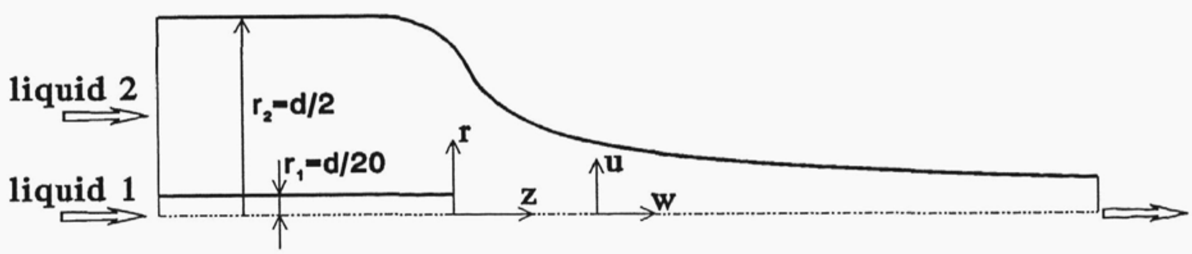

Figure 10.2. Mixer II.

Mixed liquids are incompressible, Newtonian and completely miscible. Densities, viscosities, coefficients of molecular diffusion and rate constants of chemical reactions are constant. The equations of motion and continuity for a steady-state, axisymmetric flow:

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

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

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

as well as material balance equations

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

with boundary conditions:

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

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

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

- at the annular inlet $(r_1<r\le r_2)$

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

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:

$$a = Q_2/Q_1 \tag{10.5}$$

and the same values of Reynolds number: