receives $\mathbf{D_A}$=5.02·10^{-10} m^2/s. The value of $\overline{s}$ at the beginning of the process was estimated from the following expression:

$$\overline{s_0} = \frac{1}{2}\cdot\frac{1}{\pi\cdot\left(R_2^2 - R_1^2\right)}\cdot\int_{R_1}^{R_2}(2\cdot\pi\cdot r)^2 dr = \frac{2\cdot\pi}{3}\cdot\frac{R_1^2 + R_1\cdot R_2 + R_2^2}{R_1 + R_2} \quad \textbf{(8.18)}$$

Figure 8.10 presents the final selectivities obtained in the first, fourth and fifth series of experiments plotted versus $\overline{\mathbf{Da_S}}$. Analysis of this figure shows considerable gain in mixing efficiency, due to the presence of the baffle in the annular gap, only for the lowest revolution speed (highest $\overline{\mathbf{Da_S}}$). A better improvement of mixing can be noticed in the case when the rotating turbine was used.

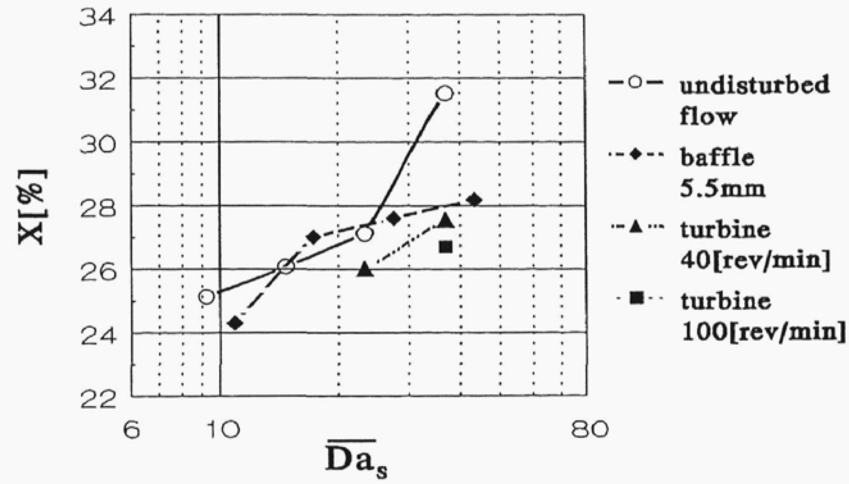

Figure 8.10. Effect of a flow disturbance on the product distribution in the batch reactor; first, fourth and fifth series.

8.2.5. Effect of a Local Disturbance of a Periodic Couette Flow on the Product Distribution.

A better improvement of mixing was achieved by means of motionless baffles for a periodic Couette flow. In this case the inner cylinder, instead of rotating in one direction, was oscillating with a constant frequency and amplitude. Experiments were conducted in three different ways:

1) without a baffle inserted in the annular gap between the cylinders,
2) with 5.5 mm wide and 2 mm thick baffle inserted in the middle of the gap,
3) with 18 mm wide and 2 mm thick baffle inserted in the middle of the gap.

The baffles were separated 67.5 degrees from the center of a zone initially occupied by the base solution, exactly as it is shown in figure 8.8. The lower edge of a baffle was fixed the reactor bottom, whereas the upper edge was fixed to the top cover of the reactor. The baffles were made of stainless steel. The initial position of the slider crank mechanism (figure 8.3) was set in such a way as to rotate the inner cylinder 180 degrees in one direction to the first turning point and then rotate it back 360 degrees to the second turning point, and so on. During the first half of a cycle, the base solution was always moved by the shear flow towards a baffle, if present. In all the experiments the initial volume of the base solution was equal to one eighth of the total liquid volume in the gap. Duration of the tests ranged from 40 minutes to 4 hours depending on oscillation frequency and geometrical configuration. Temperature of the mixer content was equal to 20°C. Tables 8.VIabc show amounts, compositions, densities and viscosities of solutions, widths of baffles, oscillation frequencies, final selectivities and approximate times of decolouration of phenolphthalein added to the substrates solutions.

Table 8.VIa. Sixth series of tests - the acid and ester solutions; w_P=42%.

Exp.no.	HCl [mol/dm^3]	Ester [mol/dm^3]	V [dm^3]	ρ [g/cm^3]	μ [Pa·s]	KCl [g/kg]
1	0.01423	0.01349	1.748	1.0704	0.4737	5.543
2	0.01411	0.01346	1.728	1.0705	0.4719	5.543
3	0.01439	0.01356	1.727	1.0705	0.4740	5.543
4	0.01476	0.01386	1.733	1.0707	0.4765	5.543
5	0.01392	0.01373	1.214	1.0704	0.4693	5.540
6	0.01392	0.01356	1.233	1.0705	0.4705	5.540
7	0.01382	0.01380	1.212	1.0704	0.4701	5.540

Table 8.VIb. Sixth series of tests - the base solutions; w_P=42%.

Exp.no.	NaOH [mol/dm^3]	V [dm^3]	ρ [g/cm^3]	μ [Pa·s]	t_f [min]
1	0.09773	0.2519	1.0705	0.4970	210
2	0.1031	0.2458	1.0704	0.4878	240
3	0.09782	0.2489	1.0706	0.4966	120
4	0.09756	0.2418	1.0705	0.5016	80
5	0.09781	0.1726	1.0705	0.4902	80
6	0.09881	0.1785	1.0705	0.4924	60
7	0.09918	0.1710	1.0704	0.4881	40

Table 8.VIc. Sixth series of tests - the final solutions after experiment; w_P=42%.

Exp. no.	f [Hz]	baffle width[mm]	Ester [mol/dm^3]	X [%]	V [dm^3]	ρ [g/cm^3]	μ [Pa·s]
1	0.333	-	0.006625	41.96	2.000	1.0703	0.4736
2	0.0833	5.5	0.006854	38.39	1.974	1.0702	0.4722
3	0.167	5.5	0.007216	37.62	1.977	1.0703	0.4770
4	0.333	5.5	0.007811	36.41	1.975	1.0703	0.4777
5	0.0833	18.0	0.07867	34.10	1.387	1.0702	0.4694
6	0.167	18.0	0.007893	31.62	1.412	1.0702	0.4682
7	0.333	18.0	0.008538	29.00	1.383	1.0703	0.4716

Results of the experiments shown in figure 8.11 indicate that mixing in a periodic shear flow can be significantly improved by motionless baffles disturbing the flow.

In order to explain the experimental results let us consider how mixing proceeds when no baffle is mounted in the annular gap and the movement of the inner cylinder is very slow.

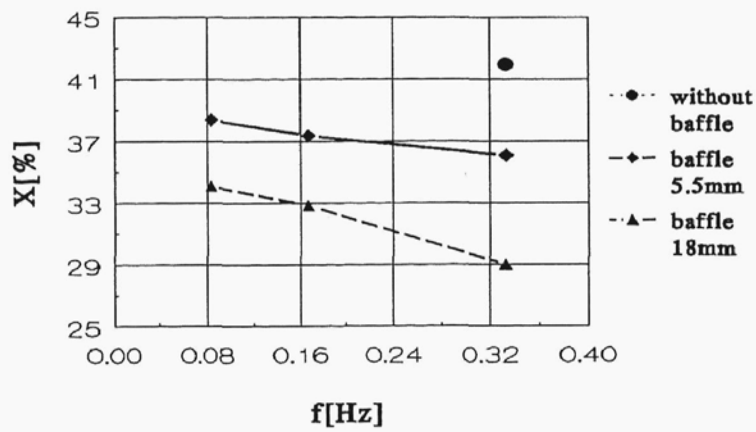

Figure 8.11. Effect of disturbance of periodic Couette flow on the final selectivity for the batch reactor; experimental results.

When the inner cylinder starts to rotate the thickness of the base zone decreases rapidly and reaches its minimum value at the first turning point. At this moment (**$\theta=\pi$**), the average thickness of the base layer

$$\bar{\delta} = \bar{\delta}_0 \Bigg/ \sqrt{1+\left(4\cdot\theta\cdot\left(\frac{R_1\cdot R_2}{R_2^2-R_1^2}\right)^2\cdot\ln\left(\frac{R_2}{R_1}\right)\right)^2} \tag{8.19}$$

is 12.5 times smaller than its initial value. When the cylinder rotates backwards the base zone regains its initial shape and so on. Thus, for low oscillation frequencies one should observe periodic decrease and increase of the segregation scales, while the average value of the segregation scale in one oscillation cycle will remain constant. Such a phenomenon was observed in the experimental system when oscillation frequency was equal or lower than 0.167 Hz. In such a case attempts to achieve a complete consumption of the limiting reactant (complete decolouration of phenolphthalein) in a reasonable time (4÷5 hours) failed.

For higher oscillation frequencies, when inert forces become comparable with viscous forces, one should observe gradually increasing differences in the shape of the base zone after a few oscillation cycles; as it took place in the experimental system when oscillation frequency was equal to 0.333 Hz. Introduction of any obstacles in the flow domain may considerably amplify the action of the inert forces and accelerate convective mixing. This thesis was fully confirmed by the experimental results; compare 42% selectivity obtained when no baffle was mounted in the reactor with 36.4% and 29.0% selectivity achieved when respectively 5.5 mm and 18 mm baffle was inserted in the gap. Analysis of figure 8.11 shows additionally, that decreasing of the oscillation frequency not only elevates the final selectivites but also decreases differences between the selectivities obtained for two different baffle widths.

8.3. Modelling of Micromixing in the Batch Reactor.

The differential material balances of the substrates of competitive-parallel reactions:

$$A + B \overset{k_1}{\rightarrow} P \qquad \text{with} \qquad k_1 \rightarrow \infty \ , \tag{5.34a}$$

$$A + C \overset{k_2}{\rightarrow} Q \qquad \text{and} \qquad R_i = -k_2 \cdot c_A \cdot c_C \tag{5.34b}$$

in a local coordinate system, attached to the symmetry plane of a layer containing reactant **A**, with the boundary and initial conditions have the following form:

$$\frac{\partial c_i}{\partial t} + \frac{x}{s} \cdot \frac{ds}{dt} \cdot \frac{\partial c_i}{\partial x} = D_i \cdot \frac{\partial^2 c_i}{\partial x^2} - k_2 \cdot c_A \cdot c_C \ , \qquad \text{where} \qquad i = A, C \ , \tag{8.20a}$$

$$\frac{\partial c_B}{\partial t} + \frac{x}{s} \cdot \frac{ds}{dt} \cdot \frac{\partial c_B}{\partial x} = D_B \cdot \frac{\partial^2 c_B}{\partial x^2} \ , \tag{8.20b}$$

- at plane $x = 0$

$$\frac{\partial c_A}{\partial x} = \frac{\partial c_C}{\partial x} = 0 \ , \tag{8.20c}$$

- at plane $x = s$

$$\frac{\partial c_B}{\partial x} = \frac{\partial c_C}{\partial x} = 0 \ , \tag{8.20d}$$

- at instantaneous reaction plane $x = x_R$

$$c_A = c_B = 0 \ , \qquad D_A \cdot \frac{\partial c_A}{\partial x} + D_B \cdot \frac{\partial c_B}{\partial x} = 0 \ , \tag{8.20e}$$