

## **9. Methodology of Determination of Energetic Efficiency of Mixing.**

Mixing of very viscous liquids requires high power inputs or long mixing times, which means that the cost of this operation mainly depends on the total energy input. Thus in the industrial practice, when choosing a new reactor or modifying an existing mixing device, one usually faces one of the following problems:

- 1) how to minimize the energetic cost of mixing without affecting the product quality or the product output,
- 2) how to maximize the product output without affecting its quality or increasing the energy input for mixing,
- 3) how to improve the product quality for the same energy input and a product output.

In all these situations, one needs a rigorous procedure allowing to compare the performance of mixing devices of a different geometry and a different mode of operation (e.g. continuous or batch). To develop such a procedure one has to define a parameter quantifying energetic performance of a mixer and to find a way of evaluating this parameter for a given system.

As it was shown in the literature review, a consistent method of quantifying mixer performance is based on the interpretation of mixing as a generation of intermaterial area per unit volume. Using this approach Ottino and co-workers [45,46,47] formulated a universal measure of energetic efficiency of mixing of Newtonian fluids as:

$$eff(\vec{X}, t) = -\frac{\overline{\overline{D}} : \hat{n} \hat{n}}{\sqrt{\overline{\overline{D}} : \overline{\overline{D}}}} = \frac{d \ln a_v(\vec{X}, t)}{dt} \bigg/ \sqrt{\frac{\epsilon}{2 \cdot \mu}}, \quad (9.1)$$

The main problem in applying this definition is associated with the fact that it requires a complete knowledge of the fluid motion in time and space, including information on the distribution and orientation of all the interfaces in the system. Thus, direct computation of  $eff(\vec{X}, t)$  from expression (9.1) is unpractical for complex flows present in industrial mixers. Another way to estimate efficiency of mixing is to recalculate it, using a verified model of micromixing, from the results of the experiments with test reactions (e.g. conversion or selectivity).

As pointed out by Ranz [21] and Ottino et. al [22], the rate of generation of intermaterial area is related to the local rate of stretch:

$$\alpha(\vec{X}, t) = \frac{1}{a_v} \cdot \frac{da_v}{dt}, \quad (9.2)$$

which in turn appears in a local material balance of a reactant:

$$\frac{\partial c_i}{\partial t} - \alpha(\vec{X}, t) \cdot \vec{x}' \cdot \frac{\partial c_i}{\partial x'} = D_i \cdot \frac{\partial^2 c_i}{\partial x'^2} + R_i . \quad (9.3)$$

A comparison of expressions (9.1)÷(9.3) indicates that the energetic efficiency of mixing is directly related to mixing on the molecular level, so its value must affect the reactant conversion or product distribution. There is no similar direct relation between the mixing time, determined using classical methods, e.g. a decolouration reaction, thermal or conductivity methods [40,41,43], and the course of the processes which influence mixing on the micro scale. The value of the mixing time is usually dominated by large scale fluid motions.

If equation of type (9.3) is a starting point in formulation of a mathematical description of mixing with deformation, molecular diffusion and chemical reaction (micromixing models presented in chapter 5 were developed in this manner), then the rate of stretch will be one of the most important model parameters.

Having the test reactions the course of which can be influenced by micromixing (see conditions outlined in chapter 2.6), one can carry out these reactions in a mixer or in a reactor and measure conversion (a single test reaction) or selectivity (complex test reactions). The experiments should be conducted in such a way as to maximize the influence of micromixing, and consequently the influence of the efficiency, on conversion or product distribution. This can be done by slow feeding of one substrate solution into the reactor containing a solution of other substrates. Then, knowing the reaction kinetics and diffusion coefficients of the reactants, one can find the average value of stretching rate in the reaction zone by fitting the results of model computations to experimentally determined conversion or selectivity values. One should remember at this point that the model used to interpret the experimental results should be adequate to the experimental conditions, e.g. one should not use the first model of concentration moments (see chapter 5.1) to describe batch mixing of comparable volumes of substrates solutions.

According to equations (9.1) and (9.2) the energetic efficiency of mixing is related to the rate of stretch,  $\alpha$ , the rate of energy dissipation per unit volume,  $\epsilon$ , and fluid viscosity,  $\mu$ :

$$eff(\vec{X}, t) = \alpha \cdot \sqrt{2 \cdot \mu / \epsilon} . \quad (9.4)$$

The last expression allows to estimate, the average value of  $eff(\vec{X}, t)$  from:

$$\overline{eff} = \overline{\alpha} \cdot \sqrt{\frac{2 \cdot \mu}{\phi \cdot \langle \epsilon \rangle_V}} , \quad (9.5)$$

where factor  $\phi$  determines the ratio of the local value of  $\epsilon$  characteristic for the reaction zone to the mean power input per unit volume in the reactor,  $\langle \epsilon \rangle_V$ . Thus the energetic efficiency of mixing calculated from expression (9.5) refers only to that region of a reactor where mixing proceeds by chemical reaction. This means that changing the position of a feeding point or modifying these experimental conditions that may influence the shape of the reaction zone (e.g. agitation speed or initial volume ratio) one can determine the energetic efficiency in several different regions of a mixer. To do this one needs to know the exact distribution of  $\phi$  in the investigated reactor. Values of the local rate of energy dissipation per unit volume and consequently values of  $\phi$  can be determined directly from the velocity field in the mixer; the fluid velocity can be either measured using for example Laser Doppler Anemometry or computed with the use of CFD methods. In this way, basing on  $\overline{eff}$  computed from expression (9.5), one can create a hierarchy of systems from the point of view of energetic efficiency, differing not only in geometry but also in the mode of operation - a way of contacting mixed liquids.

However, from the point of view of the energetical cost of mixing, much more important is the local efficiency of mixing related not to the local value of the rate of energy dissipation but to the total power consumption in the mixer:

$$\overline{eff}_V = \overline{eff} \cdot \sqrt{\phi} = \bar{\alpha} \cdot \sqrt{2 \cdot \mu \cdot V / P} . \quad (9.6)$$

In other words, one does not need to know the exact distribution of  $\phi$  in the reactor to find a solution to one of three problems outlined at the beginning of this chapter. In such a case it suffices to compare  $\overline{eff}_V$  for different mixers.

Let us illustrate the role which  $\overline{eff}_V$  plays in evaluating the energetic cost of mixing. For this purpose we shall consider a simple case of continuous blending of two non-diffusive, non-reacting and Newtonian liquids. The striation thickness ( $s=1/a_V$ ) at the outlet of a continuous mixer can be computed from the following equation:

$$s_f = s_0 \cdot \exp(-\bar{\alpha} \cdot t_{res}) = \exp\left[-\overline{eff}_V \cdot \sqrt{P/(2 \cdot \mu \cdot V)} \cdot t_{res}\right] , \quad (9.7)$$

where  $t_{res}$  is the residence time in the mixer of volume  $V$ . The energetic cost of producing a unit volume of the mixture in the mixer equals:

$$C_E = P \cdot t_{res} / V = P / Q , \quad (9.8)$$

where  $Q$  is the total flow rate through the mixer. The rate of product output per unit volume of the mixer equals:

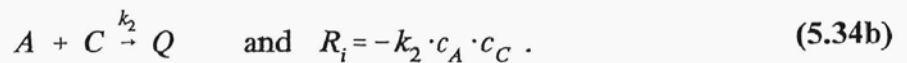
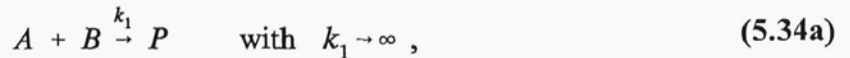
$$Q_V = 1/t_{res} = Q/V . \quad (9.9)$$

Thus, if a desired product quality, given in this case by the ratio  $s_f/s_0$ , is to be maintained one finds from equation (9.7) the relation between the efficiency, the energetic cost and the product output in the following from:

$$\overline{eff}_V \cdot \sqrt{C_E/Q_V} = \text{const} . \quad (9.10)$$

As it can be seen, the energetic cost of mixing is inversely proportional to the square of the efficiency. On the other hand, the rate of the product output per unit volume of the mixer is directly proportional to the square of the efficiency. Ottino [48] estimated that the average efficiency of mixing of Newtonian liquids in Kenics static mixer is almost twice as high as in ISG Ross static mixer. Thus, replacing ISG Ross mixer with Kenics mixer one can either decrease four times the energetic cost of mixing without changing  $s_f/s_0$  and  $Q_V$  or increase four times the product output per unit volume of the mixer while preserving the product quality and  $C_E$  at the same level.

Let us apply now the effectiveness factor  $\overline{eff}_V$ , equation (9.6) and a model of micromixing to show how the product output and the product quality are related to the energy input into the system in the case of competitive-parallel reactions considered in chapter 5.1:



The reactions are carried out in a semi-batch reactor between chemically equivalent amounts of reactants: **A**, **B** and **C**. The total amount of substrates introduced into the system (the average initial concentration) is kept constant in each realization. The concentrated solution of **A** is fed slowly into the premixture of **B** and **C**. The product quality (selectivity) defined by equation (5.36) depends on such parameters as: the average rate of stretching in the reaction zone, the initial size and shape of the feeding stream and the initial volume ratio of the mixed solutions - see chapter 5.1. According to expression (9.6) the average rate of stretching is related to the power input and the volume of the mixture through the efficiency of mixing. If the feeding stream has a shape of a slab then its initial size,  $s_0$ , and consequently the initial penetration distance of the limiting reactant,  $\delta_0$ , can be found from expressions (5.44) and (7.3):

$$\delta_0 = s_0 / \sqrt{12} = Q_f / (\sqrt{12} \cdot l \cdot v) , \quad (9.11)$$

where  $Q_f$  is the volumetric feeding rate,  $v$  stands for bulk liquid velocity in the region of the feeding point and  $l$  is the width of the feeding stream. The volumetric feeding rate is related to the feeding time,  $t_{fd}$ , and the volume of solution A through:

$$Q_f = \frac{V_{A0}}{t_{fd}} = \frac{V}{(1+a) \cdot t_{fd}} . \quad (9.12)$$

where  $a$  is the initial volume ratio  $V_{(B,C)0}/V_{A0} = V/V_{A0} - 1$ .

Let us now consider a system with well developed axial flow throughout the reactor and let the feeding point be localized in the axial flow stream approaching the impeller. In such a case the velocity,  $v$ , is directly proportional to the volumetric circulation flow,  $Q_c$ , in the mixer and, consequently, inversely proportional to the circulation time,  $t_c$ :

$$v = Q_c/A_c = V/(A_c \cdot t_c) , \quad (9.13)$$

where  $A_c$  is the cross-flow area. Moreover, in the creeping flow regime the circulation time and the power input on mixing should be given by the following correlations [40,86]:

$$n \cdot t_c = const_1 , \quad (9.14)$$

$$Po \cdot Re = \frac{P}{n^3 \cdot d^5 \cdot \rho} \cdot \frac{n \cdot d^2 \rho}{\mu} = const_2 \quad (9.15)$$

Combining expressions (9.11)÷(9.15) one receives:

$$\delta_0 = \frac{A_c}{l} \cdot \frac{const_3 \cdot \sqrt{\mu}}{1+a} \cdot \sqrt{\frac{V}{t_{fd}^2 \cdot P}} , \quad (9.16)$$

where

$$const_3 = const_1 \cdot \sqrt{\frac{const_2}{12} \cdot \frac{d^3}{V}} . \quad (9.17)$$

depends on the system geometry.

The energetic cost of producing a unit volume of the product equals:

$$C_E = P \cdot t_{fd} / V , \quad (9.18)$$

whereas the product output per unit volume of the mixer is given by:

$$Q_V = 1/t_{fd} . \quad (9.19)$$

Introduction of  $C_E$  and  $Q_V$  into expressions (9.6) and (9.16) yields:

$$\bar{\alpha} = \overline{eff}_V \cdot \sqrt{\frac{C_E \cdot Q_V}{2 \cdot \mu}}, \quad (9.20a)$$

$$\delta_0 = \frac{const_3}{1+a} \cdot \frac{A_c}{l} \cdot \sqrt{\frac{\mu \cdot Q_V}{C_E}}. \quad (9.20b)$$

The model of concentration moments, introduced in chapter 5.1, gives the relation between the product quality and the operating conditions:

$$X = f(a, \theta, \overline{Da}), \quad (9.21)$$

where:

$$\theta = \bar{\alpha} \cdot \delta_0^2 / D_A, \quad (9.22a)$$

$$\overline{Da} = k_2 \cdot \overline{c_{A0}} \cdot \delta_0^2 / D_A. \quad (9.22b)$$

Knowing the values of parameters: **a**,  $\overline{Da}$  and  $\theta$  required to achieve the desired product quality and using equations (9.20) and (9.22) one can correlate the efficiency of mixing with the energetic cost of mixing,  $C_E$ , and the product output,  $Q_V$ :

$$Q_V = \frac{\sqrt{2 \cdot D_A \cdot k_2 \cdot \overline{c_{A0}}}}{const_3} \cdot \frac{l}{A_c} \cdot \frac{1+a}{\overline{eff}_V} \cdot \frac{\theta}{\sqrt{\overline{Da}}} = \kappa_Q \cdot \frac{1+a}{\overline{eff}_V} \cdot \frac{\theta}{\sqrt{\overline{Da}}}, \quad (9.23)$$

$$C_E = \sqrt{\frac{2}{D_A} \cdot (k_2 \cdot \overline{c_{A0}})^{3/2} \cdot \frac{A_c}{l} \cdot \frac{\mu}{1+a} \cdot \frac{const_3}{\overline{eff}_V} \cdot \frac{\theta}{\overline{Da}^{3/2}}} = \frac{\kappa_C}{(1+a) \cdot \overline{eff}_V} \cdot \frac{\theta}{\overline{Da}^{3/2}} \quad (9.24)$$

Figure 9.1 presents four examples of such correlations obtained for two initial volume ratios and two values of selectivity.

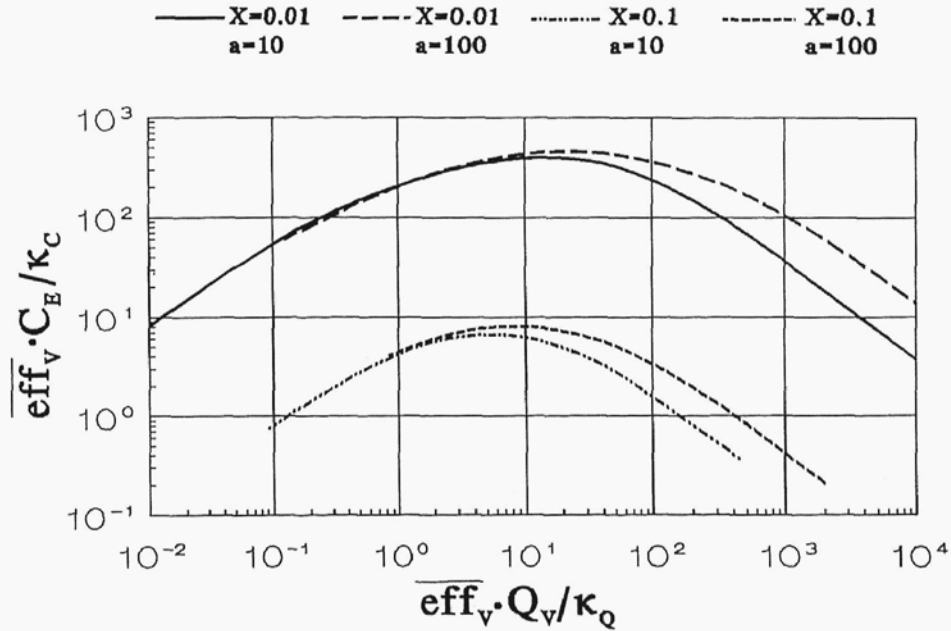


Figure 9.1. Effect of the selectivity,  $X$ , and the initial volume ratio,  $a$ , on the relation between the efficiency,  $\overline{eff}_V$ , the energetic cost,  $C_E$ , and the product output,  $Q_V$ .

As it can be seen, increasing product quality equivalent to decreasing the final selectivity results in higher energetic costs of mixing,  $C_E$ . Comparing curves obtained for different values of the initial volume ratio,  $a$ , shows that decreasing this ratio may lower the energetic cost of mixing. The curves exhibit a maximum of the energetic cost. For small  $Q_V$  increasing  $Q_V$  rises  $C_E$  due to increase of  $\delta_0$ . The points on the right side of the maximum were obtained for still larger values of the initial size of the feeding stream. According to the model of concentration moments, the final selectivity does not depend on the initial size of the feeding stream when  $\delta_0$  is large enough -see figures 5.5 and 5.6 in chapter 5.1. Thus for high enough  $Q_V$  decreasing the feeding time and consequently increasing the product output one can lower down the energetic costs of mixing, provided that one operates in the micromixing controlled regime. Short feeding time may, however, lead to the influence of macromixing on the product distribution, not considered in this work. Slow mixing on the macro scale always raises the energetic cost of mixing.

In the region where selectivity depends on  $\delta_0$  - the points on the left hand side of the maximum -rising  $Q_V$  increases  $C_E$ , provided that the efficiency of mixing is unchanged. The only possibility to improve the process in this case is to increase the efficiency of mixing, e.g. by replacing the existing impeller with another one or to change the position of the feeding point, in order to achieve one of three goals outlined at the beginning of this chapter. Figure 9.1 shows that keeping  $Q_V$  constant but increasing  $\overline{\text{eff}}_V$  always decreases  $C_E$ . The influence of  $\overline{\text{eff}}_V$  on the relation between  $C_E$  and  $Q_V$  is better observed in figure 9.2.

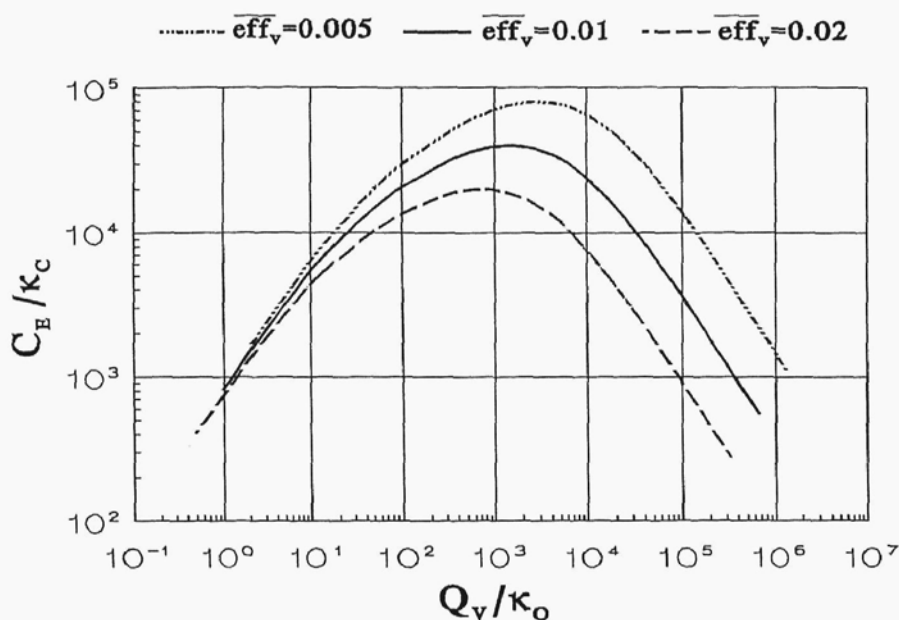


Figure 9.2. Effect of the efficiency of mixing on the relation between the energetic cost of mixing and the product output;  $X=0.01$ ,  $a=10$ .



Analysis of this figure confirms that increasing of  $\overline{\text{eff}}_v$  always lowers the energetic cost of mixing. It is also shown that keeping  $C_E$  constant but increasing  $Q_v$  requires increase of  $\overline{\text{eff}}_v$  for small values of  $Q_v$  and decrease of  $\overline{\text{eff}}_v$  in the region of large  $Q_v$  (provided that macromixing is fast enough).

Recapitulating the above considerations, it has been shown that the knowledge of efficiency of mixing facilitates the selection of a proper mixing device in view of the energetic cost of mixing. In order to find the efficiency of mixing in a mixer one needs two things: the test reactions the course of which can be influenced by micromixing and a model of micromixing. A scheme of the procedures leading to the determination of the efficiency, proposed in this chapter, is shown in figure 9.3.

#### EXPERIMENTAL

##### SYSTEM:

- flow field
- kinetics of test reactions
- diffusivity of reactants
- conversion or selectivity of test reactions

+

MODEL

$\Rightarrow$

ENERGETIC  
EFFICIENCY  
eq.(9.5)

$\Rightarrow$

HIERARCHY  
OF SYSTEMS

##### EXPERIMENTAL SYSTEM OR ITS MATHEMATICAL EQUIVALENCE:

- kinetics of test reactions
- diffusivity of reactants
- conversion or selectivity of test reactions

+

MODEL

$\Rightarrow$

EFFICIENCY  
eq.(9.6)

$\Rightarrow$

HIERARCHY  
OF MIXERS  
ENERGETICAL  
COSTS OF  
MIXING  
IMPROVEMENT



**Figure 9.3. A scheme of the methodology of determining the efficiency of mixing.**