**Effects of flow structure on mixing related processes.**

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**Highlights**

* Effects of flow structure on mixing, mass transfer and emulsion behavior are considered.
* The rate-of-strain and rate-of-rotation tensors characterize flow structure.
* The invariants of the rate-of-strain and rate-of-rotation tensors are used in modeling.

**1. Introduction**

Details of micro- and meso-scale flow structures affect the course of many processes of industrial importance. Most often effects of hydrodynamics on processes and products are expressed in terms of such variables like the rate of energy dissipation or the Reynolds number.

Objectives of this work are to characterize the flow structure and show its effect on micromixing in single-phase systems and mass transfer in two-phase systems. Also effects of flow structure on drop breakup and rheolology of dense emulsion will be briefly considered.

A difference in breaking droplets in simple shear and hyperbolic flows is well known. It has been often interpreted and generalized using a simple two-dimensional linear flow approximation [1].

 (1)

where **S** and **Ω** arethe deformation and rotation tensors**,** *G* is the scalar velocity gradient, and *a* determines the flow type: *α =* 0for simple shearflow, *α =* 1 for plane hyperbolic flow and *α =* -1for pure rotation.

**2. Models for flow structure dependent processes.**

In 3D flows instead of eq.(1) one can characterize the flow using the second invariants of the rate-of-strain tensor  and the rate-of-rotation tensor , being component of vorticity vector :

 (2)

The second invariant characterizes deformation rate and is proportional to the local rate of viscous dissipation of kinetic energy. In turbulence, high values of viscous dissipation are concentrated in sheet-like and ribbon-like structures. is proportional to the enstrophy density (enstrophy is the integral of the square of vorticity). In turbulent flows regions of high enstrophy form tube-like structures. Both, deformation and rotation affect micromixing rate [2] and micromixing efficiency [3]. In Figure 1 relative energetic efficiency is presented for the flow defined as elongation in direction 1 and contraction in directions 2 and 3 and and including effect of Sc; here **represents effect of reduction of deformation due to rotation effect. In fact **is similar to the energetic efficiency by Ottino [4].



**Figure 1.** Effect of deformation rate *s* and Schmidt number on relative efficiency of mixing in 3-dimensional flow

In typical models of mass transfer between droplets and continuous phase, the Sherwood number is proportional to *Pe*1/2  with coefficients of proportionality dependent of flow structure. More universal approach, including application of the second invariant, was proposed by Polyanin [5].

 (3)

where *K* represents the viscosity ratio  and *D* is the coefficient of molecular diffusion.

However, this approach neglects effects of rotation on mass transfer coefficient. Batchelor [6] has shown that for solid particles at high *Pe* the Sherwood number depends on the ratio of extension rate to rotation rate, ; for small  it affects the Sherwood number for any value of the Péclet number and becomes asymptotically independent of at high values of this ratio. A real challenge is to generalize this effects by using the second invariants of the rate-of-strain tensor and the rate-of-rotation tensor. At present we can show that for high *Pe* and high  the region of closed streamlines around a droplet across which the transfer by molecular diffusion takes place becomes a shell of thickness proportional to . Hence, the external mass transfer coefficient can be expressed as . As the values to which the mass transfer coefficient tends are .

Application of both second invariants enables description of drop breakage in 3D laminar flows of emulsions, extension to turbulence and linking to CFD. Rheology of dense emulsions depends on the maximum packing volume fraction that increases with increased deformation of droplets.

**3. Conclusion**

It has been shown that flow structure affects several chemical engineering processes. A possible way to model these effects is to use the second invariants of the rate-of-strain tensor and the rate-of-rotation tensor. Examples of new results based on proposed approach are presented.

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