5. Application of Integral Methods to Model Micromixing in Very Viscous Liquids.

Laminar mixing is a very complex process, governed by several elementary processes (as presented in chapter 3) and thus difficult to describe mathematically. The process can be observed and described from two points of view: Lagrangian and Eulerian. Modelling in Eulerian or fixed frame of reference gives at any instant of time a spatial distribution of species in the system. This requires solution of the system of differential transport equations with the appropriate initial and boundary conditions. Such a solution is generally possible, especially with the use of modern Computational Fluid Dynamics (CFD) methods [37,38] However, in the case of very complicated geometry of mixers, a full numerical simulation may be difficult due to limitation of computers and due to difficulties in imposing the boundary conditions.

The process of mixing can be also described in the frame of reference moving with a fluid element (Lagrangian approach). This allows to follow the course of the elementary processes of mixing occurring in the fluid element. The processes of deformation, molecular diffusion and chemical reaction can be simply described in a small fluid element by equations of type:

$$\frac{\partial c_i}{\partial t} - \alpha(t) \cdot x \cdot \frac{\partial c_i}{\partial x} = D_i \cdot \frac{\partial^2 c_i}{\partial x^2} + R_i \ , \qquad (5.1)$$

which with the appropriate initial and boundary conditions gives history of local concentrations. Determination of the global material balance demands in this case linking of macromixing (large scale motions) to micromixing (deformation, diffusion, reaction). This requires solution of Partial Differential Equation (PDE) of type (5.1) for each considered fluid element as well as solution of PDEs to find the position of fluid elements in the system. In many cases it may result in long computation times. To avoid these problems, one can transform equation (5.1) into a simpler form and develop in this way a mechanistic model of micromixing.

In this chapter two integral methods are presented which allow to replace PDE (5.1) with Ordinary Differential Equation (ODE). In addition, a method of linking micromixing to macromixing is formulated, different from that proposed by Ottino [23] and given by equation (2.35).

The following considerations are restricted to laminar, isothermal mixing of Newtonian, incompressible liquids not differing in viscosity. The flow is assumed to be stable, i.e. no segregated structures are formed.