Evaluation of highly viscous liquid mixing based on particle tracking

Mixing in stirred vessels is one of the basic and important requirements for most production systems in process industries. In the past, extensive experimental investigations were carried out by several researchers to realise the effect of various parameters on mixing efficiency for different mixing devices at variable process conditions and material properties. However, for small changes in the design parameters of the mixers or for the different materials to be studied in the mixer, it is too laborious and expensive to perform experiments each time. On the other hand, from past two decades computer based simulation method computational fluid dynamics (CFD) has become a widely used tool for analysing, optimising and supporting the design of mixing processes. Numerical tracer experiments, Lagrangian particle tracking and entropy based calculations are some of the widely used methods to assess the quality of mixtures.

While numerical tracer experiments are of increasing importance as a means to analyse mixing processes, there is a principle problem which becomes severe obstacle in case of highly viscous liquid mixing. In this situation, a sufficiently accurate solution of the species equation is spoiled by the effect of so-called numerical diffusion, i.e. the artificially generated smoothing of a tracer profile due to errors from the discretisation. This numerical diffusion can be some times much stronger than the true physical diffusion. A way to avoid this problem is to replace the continuous tracer concentration by a number concentration obtained from Lagrangian (i.e. inertia free) particles that are tracked during the simulation. This approach does not suffer from artificial diffusion, since the position of tracer particles can be resolved with sub-grid-scale accuracy and the velocity field at these particle positions can be obtained by interpolation from its values at grid points.

In the present work, the method of calculating intensity of segregation and hence the intensity of mixing and mixing time are discussed based on the Lagrangian particle tracking method. The total computational domain is divided into smaller compartments (sub-volumes) and particles are initially placed in one compartment, say. During the process of particle tracking the resulting number concentrations are recorded and allow for computation of the evolution of its variance. A fundamental question in this approach is how many compartments and particles are needed for a reliable assessment of the mixing quality. Based on elementary statistics, it can be shown that a reliable mixing time $t_M^{1-\varepsilon}$ for a given level $\varepsilon > 0$ requires $100/\varepsilon^2$ particles (if standard deviations instead of variances are employed) while a surprisingly small number of about 20 compartments is sufficient.

This method has been evaluated using the numerical investigation of mixing in a vessel stirred with an anchor impeller as well as a specific kneader element. Mixing in such kind of stirred vessels is due the relative movement (motion) between fixed walls (stator) and rotating impeller (rotor). To model a flow in these equipments a *single rotating reference frame method* has been used. Navier-Stokes (momentum) equations are modified by taking into account Coriolis and centrifugal force terms and are solved for laminar flow condition. The study is performed using commercial finite volume CFD software package Star-CD. Finally, a mapping matrix method is elaborated to evaluate the quality of mixing. This mapping method employs a transition matrix, which describes how many particles are advected from one compartment to the other compartment in a particular period of time. With the aid of this transition matrix one can compute variance evolutions and mixing times using vector multiplications with significantly less computational effort.