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Simulation of stirred tank reactors using a dynamic model based on flow characteristics

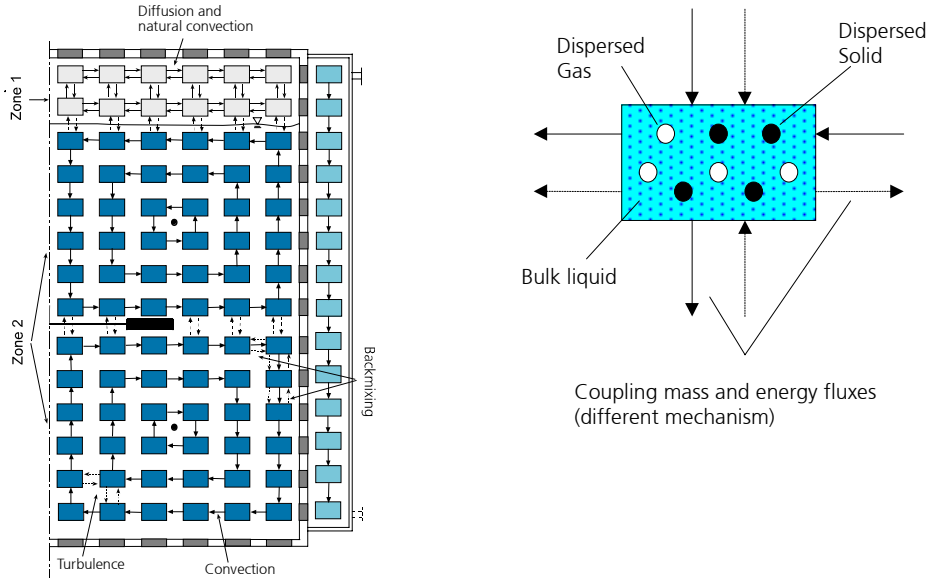
Stirred tank reactors are widely used in process industries due to their flexible mode of operation. In batch or semi-batch processes this type of reactor is often used to produce high value products (fine chemicals or pharmaceuticals) whereas large-scale production is done continuously (i. e. polymerization). The correct design of these reactors can be crucial to the profitability of the process by virtue of its influence on reaction yield or product quality. Traditionally the design of the reactors is based on empirical correlations describing macroscopic properties such as power demand, mass transfer coefficient or gas hold-up or on models assuming perfect mixing.

The present work deals with a dynamic reactor model based on flow characteristics including empirical knowledge of the above-mentioned parameters.

The basic idea of the model is to divide the reactor into two zones, one representing the gas phase (zone 1) at the top of the apparatus and one zone describing the fluid below the free liquid surface (zone 2). Each zone consists of a network of cells, which are connected corresponding to the flow characteristics.

Figure 1:

Structure of the reactor model and its basic element



Analysing the distribution of local velocities, the turbulent dissipation rate and the turbulent kinetic energy in zone 2, one can identify regions of negligible convection and turbulence. Just as in zone 1, these regions are dominated by diffusion and natural convection, appearing at the bottom of the tank or close to the free liquid surface. The other parts of zone 2 are characterized by convection and turbulence.

The cells are perfectly backmixed. In case of multiphase flow they consist of dispersed gas, solid and the liquid bulk phase (Figure 1). It is assumed that the temperature and pressure in each cell is constant and therefore the thermodynamic phases are in a state of equilibrium. The model consists of the balance equations for mass in every phase and energy in every cell forming a system of differential- algebraic equations, which is solved numerically.

Evaluation of the state variables, e. g. temperature and concentration, in each cell provides information about the direction of mass and energy fluxes connecting two adjacent cells. To quantify the fluxes one additionally has to calculate transport parameters (diffusion, mass or heat transfer coefficient). The model makes it possible to include the computation of these quantities using different published correlations.

The present contribution shows various strategies to model the convective and turbulent motion in stirred tank reactors emphasising the representation of different impellers. There are different levels of modeling concerning the required parameters. The simplest model is based on the circulation flow number, the most detailed method evaluates the distribution of measured or calculated local velocities. There are examples of one-phase mixing and chemical reactions that serve to compare the different methods and underline the influence of imperfect mixing. Simulation results will be compared with regard to model parameters. There will be a survey of those empirical equations concerning the parameters, that have significant influence on these results.