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ABSTRACT

A turbulent reactive process is a function of two different simultaneous phenomena: the chemical reaction and the transport process, the rates of them can be evaluated by means of the characteristic times of the phenomena. The definition of a characteristic mixing time is difficult because turbulence is a phenomenon that occurs on a large range of scales from that of the characteristic length of the reactor to that of the dissipation range. In the literature a great number of models have been proposed to correlate the mixing time to a specific region of the spectrum. The models based on the Kolmogorov time scale assume that the main contribute to mixing is given by the high wavenumber region of the spectrum; others consider the contribution of the whole range of wavenumbers, thus assuming the scale of the energy containing eddies as the characteristic one for the mixing process.

To validate one of these models the authors are performing a simulation of the local concentration field generated by a fast chemical reaction in a tubular reactor with two coaxial flows in which unpremixed reactants are fed (non-homogeneous turbulence). The neutralization of NaOH with HCl is considered. The numerical results are compared with the experimental data relative to the axial concentration profiles of the key reactant, determined by spectrophotometrical analysis with a fiber-optic probe. By choosing properly the mixing constants it is possible to fit experimental data. A good agreement can be obtained not only taking into account the combined effects of both the previously defined scales, but also using a macro-mixing scale, related to the characteristic size of the reactor.

But the choice of the fitting constants, functions of reactor geometry, operative conditions, etc., to describe the experimental data, is really science or only empiricism? Is it a scientific work or only a numerical calculation exercise?