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Comparison of Experiments, CFD and Laminar Flow Model.**

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Evaluation of residence time distribution in millireactor with laminar flow: comparison of experiments, CFD and laminar flow model

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Knowledge about the residence time distribution (RTD) of a reactor is essential to the assessment of its performance. For an optimal control of the chemical reactions, one key parameter for the design of such reactors is just the RTD of the fluid. Many models have been suggested to characterize the RTD through pipes, one of the most commonly known being the axial dispersed plug flow developed by Taylor in 1953.

We present a study of RTD in the case of small straight channels. RTD measurements in liquid phase were performed by a dye injection and its absorbance measurements with a spectrometer at the inlet and the outlet of the reactor (Figure 1). The method consistency was confirmed by a dye mass balance between inlet and outlet which was satisfied with an error of 5% rel. The RTD in the measured section was characterized by so called e-curve $E(t)$, mean residence time and Peclet number for different flow conditions (Reynold's numbers). The RTD data for various channel lengths and liquid flow rates were compared.

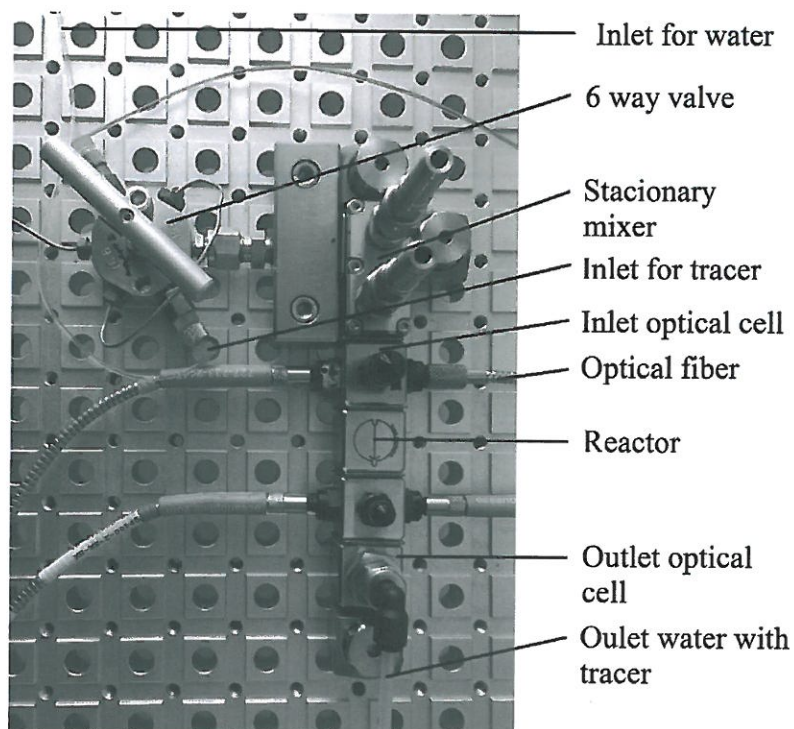


Fig.1 Exploded view of the equipment

To evaluate a contribution of a laminar flow with a parabolic profile to overall back-mixing in the channel, we have formulated a model for a general dye impulse deviation under the conditions of pure laminar flow.

The final formula of the model predicts a mean outlet concentration profile of the tracer C_{mean}^{outlet} for generally variable inlet tracer concentration profile:

$$C_{mean}^{outlet} = \int_0^1 f\left(t - \frac{L}{v}\right) \left[1 - \left(\frac{r}{R}\right)^2\right] 4 \left(\frac{r}{R}\right) d\left(\frac{r}{R}\right) \quad (1)$$

In this formula $f(t)$ designates the concentration of the tracer at the inlet as a function of time, L is long of inner radius R fed at the inlet by liquid carrying a tracer, v is flow velocity and r is radial coordination. For a simple inlet concentration functions the outlet concentration may be obtained analytically.

In the last step, CFD simulations were conducted. At the inlet of the reactor a pulse of the tracer was generated, its deviation was then simulated along the whole reactor.

The experimental data and model results from purely laminar model and CFD simulations were compared in terms of E-curves, mean residence time and Peclet number.

Thorough evaluation of laminar flow experiments and application of mathematical models and CFD simulation brings new insight to individual flow phenomena contributions to back-mixing in small channels.

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