Liquid-liquid flow in a corrugated channel: hydrodynamics and transfer
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- Flow patterns map and mass transfer laws are proposed for zigzag millichannel of a heat exchanger/reactor.
- The scale-up issue is addressed by studying three millichannels of increasing dimensions.
- A 1D/3D model integrating thermal-hydraulic mechanisms and mass transfer is developed.

Introduction
Milli-structured heat exchanger/reactors are promising for the implementation of chemical syntheses, especially rapid and exothermic ones. In the case of multiphase reactions, mass transfer can become the limiting step controlling the chemical reaction. Therefore, this work aims at characterizing the flow and the liquid-liquid mass transfer in the millichannel of the "DeanHex" exchanger/reactor in order to build a complete model of this device capable of predicting its performances at an industrial scale.

Methods
Experimental studies (hydrodynamics and mass transfer) are conducted in three zigzag millichannels of square cross-sections (hydraulic diameters \(d_h = 2, 3\) and \(4\) mm). Water/rhodamine B (RhB)/octanol fluid system is used. The flow is visualised for different flowrates of the phases. The transfer of RhB from water to octanol is then investigated for different total flowrates (1.5 to 6 kg h\(^{-1}\)) and flowrates ratios \(q\) (0.5 to 2). At the reactor outlet, based on the wettability of liquids to a given solid material, the organic phase is extracted and analyzed by UV-Vis spectrometry.

Results and discussion
Four types of flow regimes are observed in the three millichannels (Figure 1). A flow patterns map based on the Weber number of the dispersed phase \(\text{We}_{aq}\) and the internal Dean number of the continuous phase \(\text{De}_{org}\) is proposed, as shown in Figure 1.

![Flow patterns map separating the flow regimes.](image)

The mass transfer coefficient \(k_{l,a}\) obtained in the millichannels varies between 0.003 and 0.13 s\(^{-1}\). At iso-velocity, the flow regime is maintained regardless of channel size and similar \(k_{l,a}\) trends are observed (interesting result for scale-up procedure). A modified Sherwood correlation is established for each flow regime:

\[
\text{Sh} = \frac{k_{l,a}\cdot d_h}{D} = C_1 \cdot \text{De}_{org}^{C_2} \cdot \text{We}_{aq}^{C_3} \cdot \left(\frac{R_a}{L_a}\right)^{C_4}
\]

(\(D\) in m² s\(^{-1}\) is the diffusion coefficient of the solute in the aqueous phase, \(R_a\) and \(L_a\) in m are the internal radius of curvature and the straight length between bends; \(C_1\) to \(C_4\) are constants that depend on flow regime). These correlations are able to predict the experimental results to within \(\pm 20\%\) (Figure 2). They are then used to feed and validate the complete model (hydrodynamics and heat and mass transfer) of the "DeanHex" developed based on the 1D/3D numerical approach [1]. The latter allows to perform less resource demanding simulations for high \(L/d\) ratio channel and considers conduction effects, in particular between adjacent channels. In addition, for two-phase flow, the model takes into account the flow regime, by applying exchange surface correction factors to the Nusselt number of each phase. This allows to reproduce in the model the real flow conditions.

![Comparison between experimental and predicted \(k_{l,a}\).](image)

The heat transfer experiments in two-phase flow allowed the validation of the thermal model (relative temperature difference \(<20\%\) (Figure 3).

![Simulated and experimental outlet process temperature.](image)

The mass transfer model is validated with the experimental results of this work (relative difference \(<17\%\) while integrating the \(k_{l,a}\) experimental correlations (see Figure 4).

![Simulated and experimental outlet concentrations for the 2mm diameter channel.](image)

Conclusions
This work concerns the hydrodynamics and the mass transfer of a liquid-liquid flow in three corrugated millichannels of increasing dimensions. A flow map and mass transfer coefficient scale-up laws are established and used to feed the 1D/3D model developed for the "DeanHex" integrating thermal-hydraulic mechanisms and mass transfer. This model is validated with experimental results.

References