1D/3D Modeling of a Liquid-Liquid Two-Phase Flow in a Milli-Structured Heat Exchanger/Reactor

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Abstract : Milli-structured heat exchanger/reactors have been recently widely used, especially in the chemical industry, due to their enhanced performances in heat and mass transfer compared to conventional apparatuses. In our work, the 'DeanHex' heat exchanger/reactor with a 2D-meandering channel is investigated both experimentally and numerically. The square cross-sectioned channel has a hydraulic diameter of 2mm. The aim of our study is to model local physico-chemical phenomena (heat and mass transfer, axial dispersion, etc.) for a liquid-liquid two-phase flow in our lab-scale meandering channel, which represents the central part of the heat exchanger/reactor design. The numerical approach of the reactor is based on a 1D model for the flow channel encapsulated in a 3D model for the surrounding solid, using COMSOL Multiphysics V5.5. The use of the 1D approach to model the milli-channel reduces significantly the calculation time compared to 3D approaches, which are generally focused on local effects. Our 1D/3D approach intends to bridge the gap between the simulation at a small scale and the simulation at the reactor scale at a reasonable CPU cost. The heat transfer process between the 1D milli-channel and its 3D surrounding is modeled. The feasibility of this 1D/3D coupling was verified by comparing simulation results to experimental ones originated from two previous works. Temperature profiles along the channel axis obtained by simulation fit the experimental profiles for both cases. The next step is to integrate the liquid-liquid mass transfer model and to validate it with our experimental results. The hydrodynamics of the liquid-liquid two-phase system is modeled using the 'mixture model approach'. The mass transfer behavior is represented by an overall volumetric mass transfer coefficient 'kLa' correlation obtained from our experimental results in the millimetric size meandering channel. The present work is a first step towards the scale-up of our 'DeanHex' expecting future industrialization of such equipment. Therefore, a generalized scaled-up model of the reactor comprising all the transfer processes will be built in order to predict the performance of the reactor in terms of conversion rate and energy efficiency at an industrial scale.

Keywords : liquid-liquid mass transfer, milli-structured reactor, 1D/3D model, process intensification
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