Two-Phase Solid Catalyzed Reaction in Microchannels

The goal of this project is to establish a suitable model to predict a production rate of a compound emerging from a two-phase solid-catalyzed reaction in a microchannel reactor. A typical disposition of reactants and catalyst in this type of chemical reaction process is illustrated in the figure below. In developing the model you may want to use any appropriate data that is available in open literature.

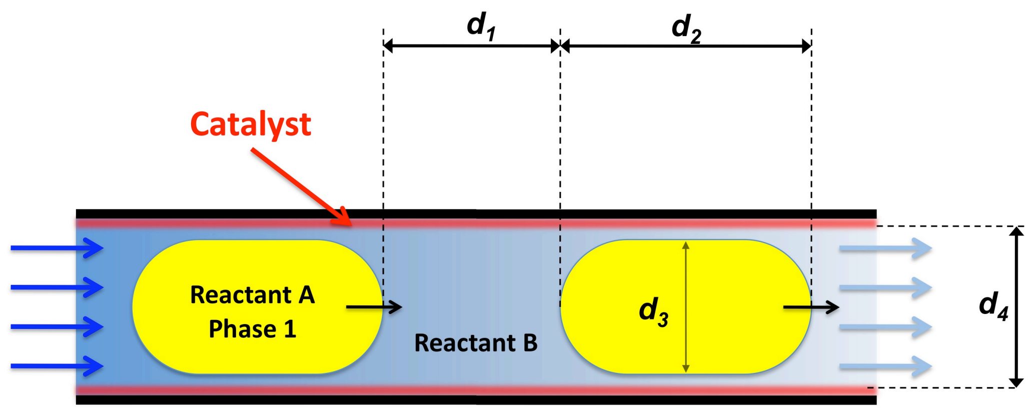

Figure 1.: Schematic representation of a two-phase flow microreactor.

$$A + B \xrightarrow{k''} products \qquad \frac{1}{S_{cat}}\frac{dN_A}{dt} = \frac{1}{S_{cat}}\frac{dN_B}{dt} = -k''C_A C_B \left[\frac{mol\ \ A}{m_{cat}^2 s}\right]$$

Simple analysis of this type of reaction processes indicates that they are mass transfer limited, i.e. the transport of reactants A and B through both phases and onto the catalyst surface presents the largest resistance to the chemical reaction process.

The above reaction process includes two phase flow contacting scheme. Limited solubility of the reactant A into Phase 2, is an additional challenge in the design of this process. It is safe to assume that reactant B does not diffuse into Phase 1. Indicate any other assumption pertinent for the consideration of this problem.

The objectives of this project are:

1. **to present background information that would justify the consideration of a microscale based chemical reactor.**

2. **to collect appropriate data - physical/chemical properties, which will help your effort in the analysis and the design of the process.**

3. **to "construct" Mathematical Model that would assist you in the numerical simulation of this process. In the realization of this objective you have to include all assumptions, differential equations, boundary and initial conditions, or any other type of correlation or simplification that makes the model workable and/or particular.**

4. **to numerically simulate envisioned process using the mathematical model developed in this project. This section should contain graphics created from the simulation (COMSOL for example) and other graphs that would illustrate the results of your work. Parametric study of the model is probably the best way to benefit from your work in modeling and simulation. We suggest that design parameters d_1, d_2, d_3, and/or d_4 be taken as parametric variables in search of an "improved" solution.**

5. **to analyze modeling results and reflect on the success of the microreactor model. We suggest that you use real physical properties of Phase 1 and Phase 2 containing reactants *A* and *B* in the modeling/designing of the microchannel reactor. You could use any data set that is available in open literature.**

6. **to prepare a power point presentation and a technical report which will follow the format that will be suggested separately.**

Assuming that the parametric study in part 4 would yield "optimal" values for d_1, d_2, d_3, and/or d_4, design a microscale-based device, which will successfully generate the two-phase flow illustrated in Figure 1 above. While you have every freedom to envision any concept and design of the two-phase flow mixer, we suggest that you consider the two concepts shown in Figure 2.

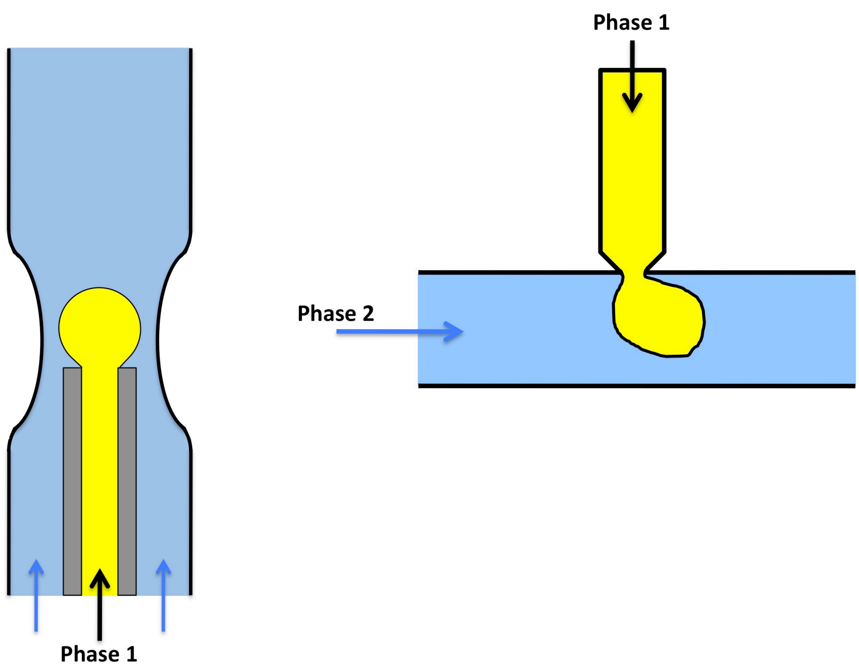

Figure 2.: Schematic representation of two conceptual designs of a two-phase flow mixer.