**Structured multiphase reactors for electrocatalytic conversions**

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**Highlights**

* Millichannel reactors are an attractive choice for CO2 conversion.
* Dimensionless numbers show that millichannels have clear advantages over microchannels.
* The channel walls can act as electrodes; the channel flow prevents stagnant bubbles.

**1. Introduction**

There is a broad consensus that the chemical industry will have to make a transition to renewable feedstocks. An important route will be to use electrochemical processes, driven by electricity from sustainable sources, to produce hydrogen from water, hydrocarbons from CO2 and water, and ammonia from nitrogen and water. This will require novel reactor designs, with special attention to the structured design of electrodes. Although there is progress in electrochemical flow reactors, scalable macro- and micro-reaction environments need to be developed involving e.g. gas-liquid electrolyte flow [1].

**2. Methods**

We examine the use of millichannels in designing multiphase reactors for electrocatalytic applications. We give a general analysis based on dimensionless numbers, followed by an illustration of this approach to catalytic packed-bed reactors. Finally, we discuss how such reactors can play an important role of increasing the number of electrocatalytic processes in the chemical industry.

**3. Results and discussion**

Although the electrocatalysts required for CO2 reduction receive substantial research interest, the research efforts devoted to the design of electrocatalytic reactors remains behind. Traditionally electrochemical reactors are designed as semi-2D geometries (one dimension much smaller than the other two) because of the use of plate electrodes. However, when gas bubbles are involved (e.g., due to hydrogen formation), the use of small channels might be attractive. Here we study the influence of channel size (hydraulic diameter *dh* and length *L*), possibly filled with particles of diameter *dp*, at porosity ε. We consider flow at superficial velocity *U* of two types of fluids through these reactors, one gas-like and one liquid-like, for which we will use the physical properties of air and water at 20 0C temperature and 1 atm pressure.

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| **Figure 1.** Pressure drop needed to reach Re=100 as a function of hydraulic or particle diameter. Blue: microchannel, yellow: millichannel. |

The differential pressure drop necessary to reach significant convective improvement of mixing and heat and mass transfer (typically Re>100) becomes prohibitive for small channels. For example, for an empty structured channel of hydraulic diameter *dh*, the pressure drop associated with wall friction can be described by the Darcy-Weisbach equation [2]. Fig. 1 shows Δ*p*/*L* as a function of *dh* for liquid-like (black solid line) and gas-like (black dashed line) fluids at Re = 100, assuming *f* = 64/Re. At this *fixed* Re, *U* decreases like 1/*dh,* leading to 1/*dh*3 scaling of the required pressure drop: for *dh* = 0.1 mm, the pressure drop to reach Re=100 is already substantial, approximately 10 bar/m, while for *dh* = 1 mm the necessary pressure drop is a more manageable: 0.01 bar/m.

For a channel filled with catalytic particles of diameter *dp*, the differential pressure drop can be described by the Ergun equation [3]. Figure 1 shows Δ*p*/*L* as a function of *dp* for liquid-like (red solid line) and gas-like (red dashed line) fluids at Re = 100 and ε=0.5. For the Ergun equation, *both* laminar and turbulent terms scale like 1/*dp*3 at fixed Reynolds number. Under these conditions, for *dp* = 0.1 mm, the pressure drop necessary to reach Re=100 is enormous, approximately 1000 bar/m, while for *dp* = 1 mm, the necessary pressure drop is much more reasonable, approximately 1 bar/m.

Pressure drop and mass and heat transfer are not the only important consideration. We also need to consider that smaller reactors are also more prone to contaminants and agglomerates getting stuck in corners of the channel or pore space. Moreover, it is important to tune the residence time in the channel to optimize reaction yield or selectivity. The average residence time is τ = ε*L*/*U*. At fixed Re, this leads to τ/*L* = ρ*dh*/(μRe) or τ/*L* = ρε*dp*/(μRe), for the two respective systems. In the regime where inertial flow enhancement becomes relevant (Re>100), reaching sufficiently *long* residence times requires sufficiently wide channels or sufficiently large particles.

**4. Conclusions**

Millichannels have clear advantages over traditional, non-structured reactors, in electrocatalytic processes. Analysis based on dimensionless numbers shows that the use of millichannels has important advantages over microchannels. The walls can act as electrode, while the channel configuration prevents problems with gas bubbles encountered in other types of electrocatalytic reactors.

**References**

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