Pressure drop in microfluidic reactor

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ABSTRACT

Microfluidic reactors are devices of internal volume in few microliters, which can be exploited to conduct complex reactions in a continuous mode. In this study, the Labtrix START (Chemtrix, NL) platform with a glass microfluidic reactor was examined from the hydrodynamics point of view for planned reaction – a stereoselective hydrogenation.

The comparison of the measured and predicted pressure drop in the microfluidic reactor indicated that the measured pressure drop was about two times higher than the theoretical prediction.

INTRODUCTION

Microfluidic reactors can be advantageously used in specific reactions, e.g. for the preparation of fine chemicals in pharmaceutical industry or in the case of handling of dangerous or toxic compounds.

In this study the Labtrix START (Chemtrix, NL) platform with a glass microfluidic reactor 3222 (Fig. 1) was tested from the hydrodynamic point of view to validate its functionality for a stereoselective hydrogenation. The stereoselective hydrogenation will be enabled by a stereoselective catalyst, Ruthenium BINAP complex (2,2'-bis(diphenyl-phosphino)-1,1'-binaphtyl), in a mixture of reactants, methanol and water[1]. A presence of ionic liquid $[N_{R,222}][Tf_2N]$, namely n-alkyl-triethylammonium bis(trifluoromethane-sulfonyl)imide, allows for an easy separation of this stereoselective catalyst via its pseudo-immobilisation[2].

The testing of the microfluidic reactor lied in inquiring of measured pressure drops in dependence on the flow rates of the reaction mixture in the micro reactor channel. Comparative measurements in a straight capillary of a well-defined geometry were also carried out. The testing measurements were performed without reactants, i.e. only with methanol, a binary mixture (ionic liquid and methanol), and a ternary mixture (ionic liquid, methanol and water).

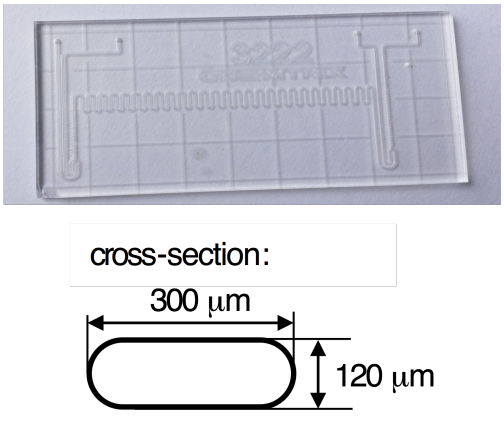

Figure 1. Microfluidic reactor 3222.

EXPERIMENTAL

Viscosity measurement

Viscosities of the studied liquids were measured using a Brookfield LVDV-II+Pro

Extra viscometer. The viscometer was equipped with a small sample adapter containing the chamber SC4-13RPY and the spindle SC4-18. Measurements were carried out in the range of shear rates from 132 to 264 s^{-1}.

Experimental arrangement

The experimental arrangement including the Labtrix START (Chemtrix, NL) platform with a glass microfluidic reactor 3222 is schematically shown in Fig. 2.

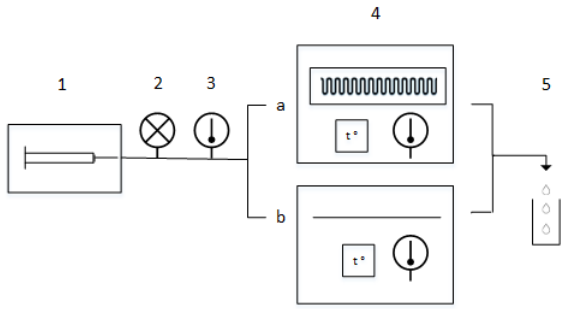

Figure 2. The experimental arrangement: 1 – linear pump, 2 – pressure sensor, 3 – temperature sensor, 4a – microfluidic reactor, 4b – capillary, 5 – product collection and sampling.

Microfluidic reactor geometry

The channel length in the microfluidic reactor 3222, see Fig. 1, was of 151.9 mm. The channel cross-section A was 32910 μm^2, and its circumference P was 737 μm. The hydraulic equivalent radius of the channel $R_H = 2A/P$ was 89.3 μm.

Capillary geometry

The capillary from the PEEK® material (VICI) of the inner diameter 125 μm and the length 410 mm was used. The internal volume of the capillary was the same as that of microfluidic reactor (5 μl).

Pressure drop measurement

The pressure drop measurements were carried out at three temperatures of 25°C, 35°C and 50°C.

In order to determine the pressure drop solely for the key element of interest (capillary or microfluidic reactor) the contribution of the surrounding flow infrastructure (capillaries, fittings etc.) on total pressure drop was examined. This contribution was measured in separate experiments under identical flow and temperature conditions. The contribution of the flow infrastructure was subtracted from the total pressure drop and the information about correct pressure drop in the key element was determined.

RESULTS

The pressure drop in the microfluidic reactor of non-trivial geometry (Fig. 1) cannot be predicted by means of the Hagen-Poiseuille equation (HP), because the overall pressure drop is increased due to the flow separation and recirculations caused by curvature of reactor space. The pressure drop in the microfluidic reactor should be predicted in terms of an empirical correction of HP prediction on the curvature.

Firstly, measurement in a straight capillary of a well-defined geometry (and the same volume as microfluidic reactor) was performed with the aim to verify the correctness of the pressure drop measurements (including the subtraction of pressure drop due to surrounding flow infrastructure). The measured pressure drop ΔP_{exp} was compared with the predicted one ΔP_{HP} using Hagen-Poiseuille equation:

$$\frac{\Delta P_{HP}}{\Delta L} = \frac{8\eta Q}{\pi R^4}, \qquad (1)$$

where η corresponds to viscosity, Q is flow rate, and R and ΔL stand for the capillary radius and length. Measurements were carried out with methanol, a binary mixture of $[N_{8,222}][Tf_2N]$/methanol (molar fractions 0.13/0.87 respectively) and a ternary mixture of $[N_{8,222}][Tf_2N]$/methanol/water (molar fractions 0.11/0.67/0.22 respectively). Viscosities of binary and ternary mixtures shown in Fig. 3 were used as input data to the HP equation. The viscosity data of methanol were taken from the literature[3].

The comparison of the predicted ΔP_{HP} vs. measured ΔP_{exp} pressure drop in a straight capillary is presented in Fig. 4. Very good agreement between the measured and predicted pressure drop confirmed the correctness of pressure drop measurement.

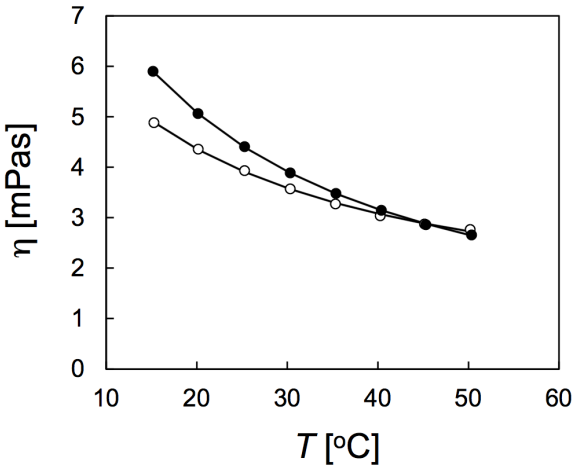

Figure 3. Temperature dependencies of viscosity of binary (o) and ternary (•) mixtures.

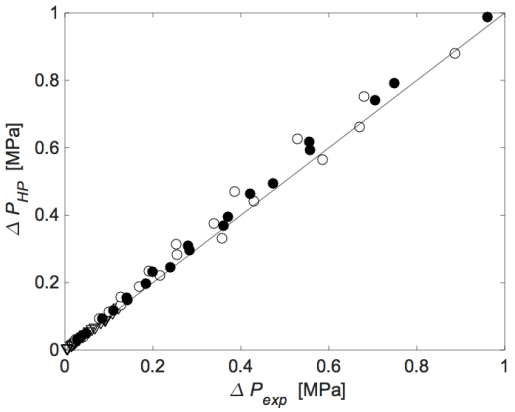

Figure 4. Predicted vs. measured pressure drop in capillary: methanol (▼), binary (o) and ternary (•) mixtures. A diagonal guides eyes to $\Delta P_{HP} = \Delta P_{exp}$.

Secondly, the measurement of the pressure drop in the microfluidic reactor 3222 was performed, and results were compared again to the prediction of pressure drop. Two different approximations of the microreactor channel cross-section were used for the pressure drop calculation:

(i) HP equation included the classical hydraulic radius R_H:

$$\frac{\Delta P_{HP,R_H}}{\Delta L} = \frac{8\eta Q}{\pi R_H^4}. \qquad (2)$$

(ii) the analytical solution[4] for the elliptical cross-section of semi-axis b and c, where c < b, which is similar to our cross-section, see Fig. 1:

$$\frac{\Delta P_{HP,elliptical}}{\Delta L} = \eta \frac{Q}{A} \frac{4\left(1+(c/b)^2\right)}{c^2}. \qquad (3)$$

These approximations differ only in a geometrical parameter and gave very close results $\Delta P_{HP,elliptical} = 0.98\ \Delta P_{HP,R_H}$. The elliptical shape is only an approximation of our cross-section shape (see Fig. 1), therefore we present the prediction in terms of the hydraulic radius in Fig. 5, where the comparison of predicted ΔP_{HP} vs. measured ΔP_{exp} pressure drop in the microfluidic reactor is shown.

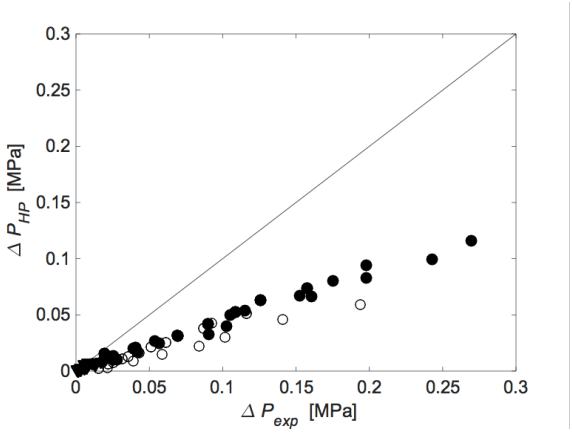

Figure 5. Predicted vs. measured pressure drop in microreactor: methanol (▼), binary (o) and ternary (•) mixtures. A diagonal guides eyes to $\Delta P_{HP} = \Delta P_{exp}$.

The comparison of the measured and predicted pressure drop in the microfluidic

reactor 3222 (Fig. 5) indicates that the measured pressure drop is about two times higher than the predicted one. It means that the empirical correction factor, which should be included to the HP equation is about 2:

$$\Delta P_{\text{exp}} \approx 2\ \Delta P_{HP}. \qquad (4)$$

Note that this correction factor is valid for the specific geometry of microfluidic reactor 3222 and all used liquids. For a different geometry of microfluidic reactor or markedly more viscous liquids another validation process should be carried out.

CONCLUSIONS

In this experimental study the microfluidic reactor 3222 was tested from the hydrodynamic point of view. The measured pressure drops of microfluidic reactor in dependence on flow rates of the reaction mixture was inspected.

The correctness of pressure drop measurement was verified via comparative measurements with a straight capillary. In the case of the straight capillary very good agreement with prediction via Hagen-Poiseuille equation was found.

The measured pressure drop in microfluidic reactor was higher than the predicted one using Hagen-Poiseuille equation due to flow irregularities in non-trivial geometry of reactor. The measured pressure drop was found two times higher than predicted one for the used microfluidic reactor 3222 and used liquids of viscosities in range from 0.5 to 6 mPas. The difference between measured and predicted pressure drop will be else for another microfluidic reactor of different geometry, therefore it is suitable to test a microfluidic reactor from hydrodynamic point of view before using it for a specific reaction.

ACKNOWLEDGMENTS

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