Modelling of the liquid flow in the microreactor

Yuliia Miroshnychenko, Author 1
National Technical University of Ukraine "Kiev Polytechnic Institute"
Kyiv, Ukraine
e-mail: Ju1ianna@ukr.net

Yu. Beznocyk, Author 2
National Technical University of Ukraine "Kiev Polytechnic Institute"
Kyiv, Ukraine

***Abstract*—Microstructured reactors (MSR) open a new perspective to chemical technology and reaction engineering offering high surface-to-volume ratio, very efficient heat and mass transfer, intrinsic safety because of the small channel dimensions, which gives reliability, and last but not least, a better process control. With microreactors, fine chemicals can be produced in a continuous mode, thus enabling stable operation conditions and a high product quality. Different MSR have been successfully used to carry out fluid-fluid reactions, namely: emulsion polymerization, phase transfer catalysis, homogenous, catalyst screening, enzymatic reactions, extraction, precipitation, crystallization and cell separation. Based on various operating conditions and flow properties a detailed investigation of flow regimes, such as drop, slug, slug-drop, deformed interface, annular, parallel and dispersed flow, can be conducted by means of modelling of reaction systems in the specialized software environment. A complete model gives a clear picture of the fluid dynamics, heat and mass transfer in MSR thereby helping to improve the performance of the reactors in general. Computational fluid dynamic simulations also provide insight into liquid-phase systems. Microreactors can be used both as research instruments in laboratory scale to enhance the development and optimization of the processes and as real production units in large to improve the economic benefits. In the present work, processes and products implemented for commercial production with the help of MSR is presented. The practical examples confirmed an economic potential of a microreactor scaling-up strategy.**

***Keywords*—microstructured reactor; computational fluid dynamics; volume-of-fluid approach; liquid-phase system; microchannel.**

References

[1] H. Löwe, W. Ehrfeld, "State-of-the-art in microreaction technology: concepts, manufacturing and applications", Electrochimica Acta 44, 1999, pp. 3679-3689.

[2] M.N. Kashid, A. Gupta, A. Renken, L. Kiwi-Minsker, "Numbering-up and mass transfer studies of liquid–liquid two-phase microstructured reactors", Chem. Eng. Journal. 158, 2010, pp. 233-240.

[3] King Lun Yeung, Xiongfu Zhang, Wai Ngar Lau, Rosa Martin-Aranda, "Experiments and modeling of membrane microreactors", Catalysis Today 110, 2005, pp. 26-37.

[4] J.R. Hernandez Carucci, K. Eränen, D.Yu. Murzin, T.O. Salmi, "Experimental and modelling aspects in microstructured reactors applied to environmental catalysis", Catalysis Today 110, 2009, pp. 149-150.

[5] B. Yang, T. Yuschak, T. Mazanec, A. Lee Tonkovich, S. Perry, "Multi-scale modeling of microstructured reactors for the oxidative dehydrogenation of ethane to ethylene", Chem. Eng. Journal. 135, 2008, pp. 147-152.

[6] M.N. Kashid, D.W. Agar, S. Turek, "CFD modelling of mass transfer with and without chemical reaction in the liquid–liquid slug flow microreactor", Chemical Engineering Science, 62, 2007, pp. 5102–5109.

[7] D. Qian, D., A. Lawal, "Numerical study on gas and liquid slugs for Taylor flow in a T-junction microchannel", Chemical Engineering Science 61(23), 2006, pp. 7609–7625.

[8] V. Kumar, S. Vashisth, Y. Hoarau, K.D.P. Nigam, "Slug flow in curved microreactors: hydrodynamic study", Chemical Engineering Science 62(24), 2007, pp. 7494–7504.

[9] R. Gupta, D.F. Fletcher, B.S. Haynes, "On the CFD modelling of Taylor flow in microchannels", Chemical Engineering Science 64(12), 2009, pp. 2941–2950.

[10] M.N. Kashid, A. Renken, L. Kiwi-Minsker, "CFD modelling of liquid–liquid multiphase microstructured reactor: Slug flow generation", Chem. Eng. Research and Design. 88, 2010, pp. 362-368.

[11] V.Chokkalingam, "A droplet-based microfluidic scheme for complex chemical reactions", dissertation, Saarbrücken, 2010.

[12] M.N. Kashid, A. Renken, L. Kiwi-Minsker, "Gas–liquid and liquid–liquid mass transfer in microstructured reactors", Chem. Eng. Science. 66, 2011, pp. 3876-3897.

[13] J.M. Bolivar, J. Wiesbauer, B. Nidetzky, “Biotransformations in microstructured reactors: more than flowing with the stream”, Trends in Biotechnology 29 (7), 2011, pp. 333-342.

[14] Paul D. I. Fletcher, Stephen J. Haswell, Esteban Pombo-Villar, Brian H. Warrington, Paul Watts, Stephanie Y. F. Wong, X. Zhang, “Microreactors: principles and applications in organic sythesis”, Tetrahedron 58, 2002, pp. 4735-4757.

[15] Klavs F. Jensen, “Microreaction engineering - is small better”, Chem. Eng. Science 56, 2001, pp. 293-303.

[16] Patrick L. Mills, David J. Quiram, James F. Ryley, “Microreactor technology and process miniaturization for catalytic reactions—A perspective on recentdevelopments and emerging technologies”, Chem. Eng. Science 62, 2007, pp. 6992-7010.

[17] A.A. Kulkarni, A.K. Gorasia, V.V. Ranade, “Hydrodynamics and liquid phase residence time distribution in mesh microreactor”, Chem. Eng. Science 62, 2007, pp. 7484-7493.

[18] A. Karim, J. Bravo, D. Gorm, T. Conant, A. Datye, “Comparison of wall-coated and packed-bed reactors for steam reforming of methanol”, Catalysis Today 110, 2005, pp. 86-91.

[19] Yu. Miroshnychenko, Yu. Beznocyk, “Modelling of processes of chemical technology in microreactor”, 4th Int. Scientific Conference “Computer simulation in chemistry, technology and systems for sustainable development CSCT-2014”, 2014, pp. 151-157.

[20] Yu. Miroshnychenko, Yu. Beznocyk, “Simulation of the process of silica functionalization in the microreactor”, Eastern-European Journal of Enterprise Technologies, №2/5 (22) 2015, pp. 46-53.

[21] S. Buchholz, “Future manufacturing approaches in the chemical and pharmaceutical industry”, Chemical Engineering and Processing 49, 2010, pp. 993–995.