Chemical Engineering Journal 215–216 (2013) 449–460

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Measuring and modeling the residence time distribution of gas flows in multichannel microreactors

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HIGHLIGHTS

- ▶ Impact factors for the residence time behaviour of gas flows in microstructured reactors (including a suggestion for an extended model).
- ▶ CFD simulations of the residence time behaviour of micro structured devices.
- ▶ Experimental data for the residence time behaviour of microstructured reactors.

ARTICLE INFO

Article history:
Available online 26 October 2012

Keywords:
Microchannel
Gas
Residence time distribution
Dispersion model
Extended correlation
Microreactor
Thermal conductivity sensor

ABSTRACT

The optimization of microreactor designs for applications in chemical process engineering usually requires knowledge of the residence time distribution (RTD). The applicability of established models to microstructured reactors is currently under debate [1–4]. This work presents investigations of the RTD behaviour for gas flows in microstructured devices by CFD (computational fluid dynamics) simulations and new experimental data for the RTD of different microstructured reactors (some provided by industrial partners). Influence of the in- and outlet regions of the devices and uneven flow distribution inside the microstructure on the RTD are discussed. Hereby, boundary conditions for the applicability of commonly used dispersion model and the correlation proposed by Taylor and Aris for the model parameter Bodenstein number *Bo* are explained. The experimental data for the RTD of the microreactors investigated are analysed, whereby a good agreement of simplified models for the RTD of the complete devices (including- in and outlet regions) is found. The determination of the model parameter may be difficult as several factors have to be considered. Here, an extended correlation based on experimental data is suggested.

1. Introduction

For real reactors the residence time (the time interval of a molecule between entering and exiting the reactor) is not the same for each molecule. The resulting residence time distribution (RTD) of these molecules in the reactor is a characteristic feature for the chemical reactions to take place inside the reactor.

A narrow RTD for microreactors is assumed by [1,4] due to the small channel dimensions of microstructured devices compared to typical channel length and short lateral diffusion times. A comparison of microchannels to conventional fixed-bed reactors [5] indicates that microchannel reactors do indeed offer the potential for narrower RTDs compared to fixed-bed reactors.

Knowledge of the RTD is essential for the prediction of reactor behaviour. Reactor modelling is very often based on simplified models (dispersion model, series of perfectly mixed cells, or other empirical models [6]) as a substitute for time-consuming computational fluid dynamics (CFD) simulations. However, the applicability of established correlations for microstructured reactors has been questioned and is the subject of on-going scientific discussion [1–3,7].

In this work the dispersion model and the correlation by Taylor and Aris [8,9] for the calculation of the axial dispersion coefficient D_{ax} are used to describe the residence time behaviour of microstructured devices consisting of parallel microchannels. Hereby, the model is applied to each channel of the microstructure and a cumulated residence time of the total device is determined. By comparing this total residence time with the correlation for one single channel limitations for the correlation and model extensions are discussed.

These considerations are compared to the results of CFD simulations. Beside this, also new experimental data for the residence

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http://dx.doi.org/10.1016/j.cej.2012.10.011