Pore-size distribution of cordierite monolith substrate experiments and digital reconstruction methods

V. Novák [a,*], P. Kočí [a], F. Štěpánek [a,b], M. Marek [a], M. Kubíček [c]

[a]Department of Chemical Engineering

[b]Chemical Robotics Laboratory

[c]Department of Mathematics

Institute of Chemical Technology Prague, Technická 5, 166 28 Prague, Czech Republic

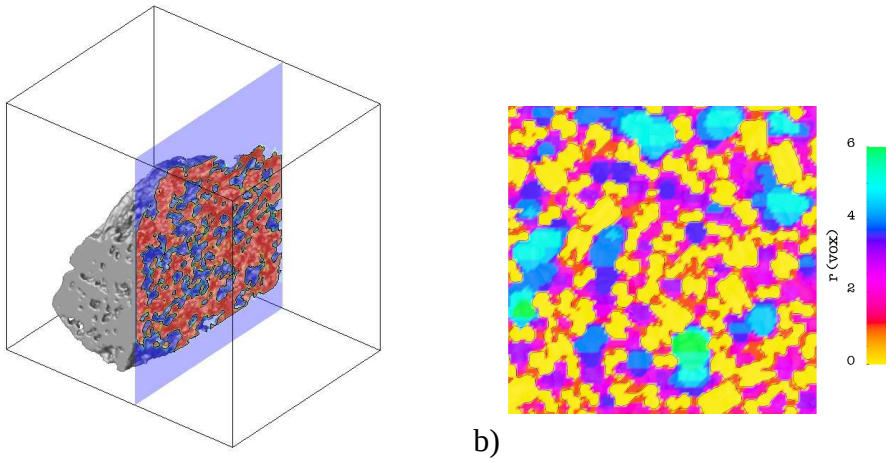
1 Introduction

Digital reconstruction methods can be used for coding of experimentally determined porous structures. The coded structures are then often used for extensive computations of transport and reaction processes (Kosek et al., 2005).

2 The studied system

In this paper porous structure of cordierite monolith substrate is investigated by means of experiment (standard mercury porosimetry, X-ray microtomography) and computer simulation (3D reconstruction of porous structure). Example of the 3D porous structure reconstructed on the basis of X-ray microtomography is given in Fig 1a. The pore-size distribution (PSD) of the computer-reconstructed medium is evaluated by virtual capillary condensation and by a newly proposed method of maximum sphere inscription. The first method is based on the solution of Kelvin equation (Štěpánek et al., 1999, 2007) and the other method follows this process: in each spatial node inside the pore a virtual sphere is expanded until it reaches the pore wall. All the spatial nodes inside this sphere belong to the pore with the diameter equal to that one of the sphere, unless another sphere with

* Corresponding author, tel: +420 22044 3293, fax: +420 22044 4320.
Email address: vladimir.novak@vscht.cz (V. Novák).
URL: http://www.vscht.cz/monolith (V. Novák).



a) b)

Fig. 1. (a) Example of 3D reconstructed cordierite structure obtained from X-ray microtomography. (b) Example of local pore sizes evaluated by the maximum sphere inscription method.

a larger size covers the node, too, Fig 1b. For common pore shapes this approximate determination of local diameter gives similar pore-size distribution as the method of virtual capillary condensation. Pore size distribution obtained by the two methods are then compared with experimentally measured PSD determined by mercury intrusion porosimetry (Starý et al., 2006), Fig 2.

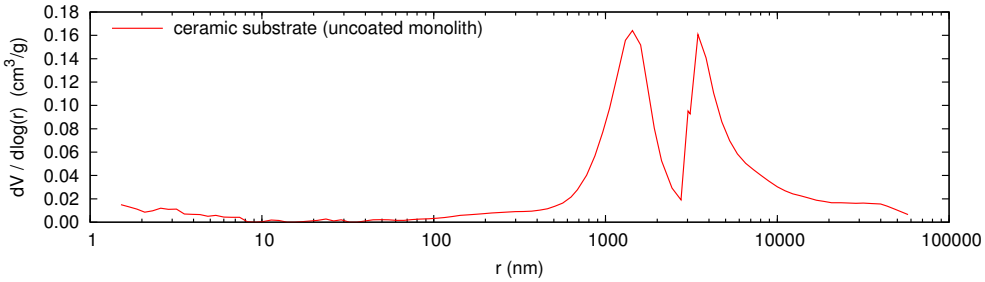


Fig. 2. Pore size distribution of cordierite from mercury intrusion porosimetry.

Computer-reconstructed porous 3D structure can be obtained directly from the X-ray microtomography reconstruction algorithms, Fig 1b, or by the virtual particle packing of primary particles (Štěpánek and Ansari, 2005; Kočí et al., 2007, 2008) . The reconstructed porous medium can be then used for simulation of transport and reaction inside the pores (Kočí et al., 2006, 2007, 2008). This 3D reaction-diffusion system is described by components mass balances in the form of the following partial differential equation. For the components $k = 1 \ldots K$:

$$\varepsilon^{\mu} \frac{\partial c Y_k(x,y,z,t)}{\partial t} = D_k^{\mathrm{eff}} c \left(\frac{\partial^2 Y_k}{\partial x^2} + \frac{\partial^2 Y_k}{\partial y^2} + \frac{\partial^2 Y_k}{\partial z^2} \right) + \sum_{j=1}^{J} \nu_{k,j} \cdot r_j \qquad (1)$$

Mass transport in small pores is governed by Knudsen diffusion (2).

$$D_k^{\mathrm{eff}} = \frac{\varepsilon^{\mu}}{\gamma^{\mu}} \frac{d^{\mu}}{3} \sqrt{\frac{8 R^{\mathrm{g}} T}{10^3 W_k \pi}} \tag{2}$$

3 Conclusion

The pore size distributions obtained by the two computional methods in the reconstructed medium were confronted with experimentally measured PSD determined by mercury intrusion porosimetry. The computationally and experimentally obtained pore size distributions were found to be comparable. The local radius evaluated from the maximum sphere inscription method can be used for approximation of local diffusivities. Results of the reaction-diffusion simulations in the reconstructed porous structure will be presented.

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