MICROTOMOGRAPHY-BASED NUMERICAL SIMULATIONS OF HEAT TRANSFER AND FLUID FLOW THROUGH SIC OPEN-CELL FOAMS FOR CATALYSIS

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Abstract

β-SiC open-cell foams are novel carriers for intensifying catalytic reactions. Realistic 3D models of *β*-SiC foams were generated using X-ray microtomography data obtained by computed tomography. The foam models were used for pore-scale FEA and CFD simulations of heat transfer and fluid flow. The thermal conductivity predicted by FEA simulation is comparable to the experimental result. The microscopic characteristics of laminar flows through open-cell foams are revealed by direct CFD simulations.

Keywords

β-SiC open-cell foam, X-ray microtomography (μ-CT), Realistic models, direct numerical simulation.

Introduction

Porous SiC-based cellular materials (*i.e.* open-cell foams) stimulated novel ideas of designing multi-scale porous structured reactors for intensified catalytic/chemical applications, *e.g.* Fischer-Tropsch synthesis (Liu et al. 2013) and photocatalytic wastewater treatment (Kouamé et al. 2012), due to their interesting combinations of mechanical and physical properties (such as enhanced transport phenomena and superior chemical resistance).

To develop full understanding of behaviour of materials in complex processes such as catalytic reactors it is desirable to complete experimental studies with modelling, including in particular momentum-transfer problems that are difficult to interpret without visualisation of internal flow structure that can be achieved either experimentally by *e.g.*, MRI imaging, or through numerical simulation. In this work, the microscopic approach based on μ-CT is used to generate models with the preservation of geometrical features. μ-CT data are processed using new advanced algorithms and exported in relevant mesh formats for direct numerical analyses.

Experimental

Method, image processing and mesh generation

β-SiC open-cell foams (30 ppi) were from SICAT SARL (France) and were scanned with a Metris XT H 320 LC Micro-Focus CT system (Nikon Metrology). Necessary image processing were performed using SIMPLEWARE ScanIP to reduce the number of pixels of original models resulting in 10 × 10 × 10 mm models with 75 micron pixel spacing and geometrical features preservation. +FE Free meshing algorithm in SIMPLEWARE $^{+}$FE was used for mesh generation. The lowest in-out aspect ratio was kept smaller than 0.20 for all the meshes.

Numerical modeling

FEA simulation of uncoupled heat transfer analysis through *β*-SiC foam models (*i.e.* thermal and mechanical problems are uncoupled) was conducted using ABAQUS

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FEA. CFD simulation of laminar flows through β-SiC foams was performed using ANSYS FLUENT.

Results and Discussion

FEA analysis of heat conduction through β-SiC foams

Variations of the effective static thermal conductivity (λ_{eff}) values along different space directions were noticed for all foam models, ranging from 4 to 23% (Figure 1a). Such anisotropic feature of heat conduction through porous media can be attributed to the difference in strut paths and numbers of pores along different directions within the computational domain. The overall effective thermal conductivity from the direct FEA simulations is comparable to the result estimated by the experimental measurement, and are in the order of 10^{-1} W m^{-1} K^{-1}, see Figure 1b (Edouard et al. 2010). Thermal transport through fluid-saturated β-SiC foams was found to depend on the solid-to-fluid conductivity ratio.

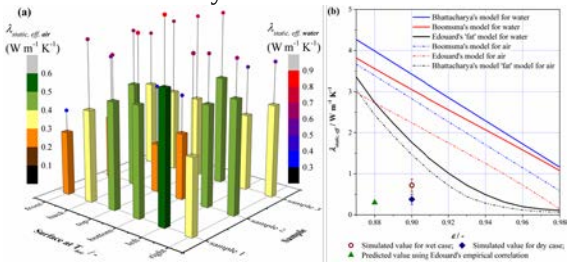

Figure 1. (a) Computed λ_{eff} for β-SiC foam models with air or water as saturating fluids. (b) Comparison of calculated bulk thermal property of a β-SiC foam with literatures.

CFD simulation of laminar flows through β-SiC foams

Steady-state laminar flow simulation showed that the flow fields within open-cell foams are in the Darcy-Forchheimer regime (pore-scale Re number < 40). The velocity fields are featured with uninform distribution of velocity across the pores of foams due to mixing of high inertia flow streams coming from adjacent pores and vicious flows in the stagnation regions (pore walls). Such flow features cannot be observed in the CFD simulation of idealised periodic structures, such as Kelvin cells.

Circulation of fluids in the downstream regions (after foams) was represented by the CFD simulation of realistic foam models, as seen in Figure 2. This phenomenon can be attributed to the negative pressure at the exit of foam models, which increases the adverse pressure gradient on the leeward side, slow down the outgoing fluid and eventually cause deformation of flow after foams.

Diffusion and dispersion of species within the flow through open-cell foams are evaluated by tracking the fluid particles as a function of time, as seen in Figure 3 (Red markers – the tracked particle position at 0.03 second later). Diffusion constant and thermal diffusivity within a foam model at Re = 40 were estimated as in the magnitude of 10^{-4} m^2 s^{-1} which exceeds the values of molecular diffusion (10^{-5} m^2 s^{-1}).

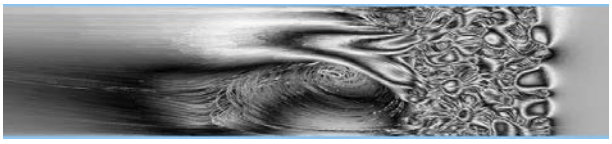

Figure 2. Streamlines on yz plane (Re = 2)

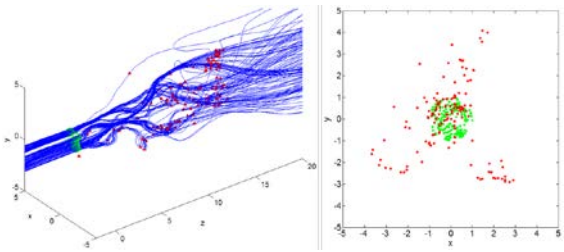

Figure 3. Axial and radial dispersion of tracked particles on streamlines

Conclusions

Microtomography-based modelling of β-SiC open-cell foams was performed in this work. The structural features of foams have been preserved in the realistic 3D geometrical models through high-resolution μ-CT. Accurate pore-scale simulations (FEA and CFD) were carried out to evaluate the heat transfer and fluid flow characteristics through β-SiC foams. 3D approach (model generation, meshing and simulation) based on the X-ray microtomography technique, although challenging, was demonstrated as a promising approach for desiginf and optimising novel catalytic processes based on open-cell foams.

Acknowledgments

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