268d Meso-Scale Modelling of Reactions and Transport in Digitally Reconstructed Porous Catalyst: Co Oxidation on Pt/Al2o3

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In a typical monolith reactor for the conversion of automobile exhaust gases one has to consider processes on several length-scales: monolith length and diameter on the order of 10 cm, the channel diameter approx. 1 mm, the porous catalytic washcoat layer with thickness on the order of 10-100 μm, the particles forming the supporting material (typically gamma-Al2O3) – diameter on the order of 1 μm, meso- and micro-pores of the supporting material with diameter on the order of 1-10 nm, the active catalytic sites with size in nanometres, and the reacting molecules with size in angstroms. The modeling of such reactor is a multi-scale problem [1].

In this paper we focus on the length-scale of the washcoat layer and present a methodology for modelling of reaction-transport processes in a digitally reconstructed, porous heterogeneous catalyst [2]. Microkinetics of the CO oxidation on Pt/gamma-Al2O3 with an explicit consideration of the surface-deposited species has been employed in the model [3,4]. The reaction takes place on the Pt sites located on the Al2O3 surface and in the meso-pores, simultaneously with the transport of gaseous reaction components. The transport inside the meso-porous Al2O3 particles is characterised by the effective diffusivity based on Knudsen diffusion.

Several 3D porous structures have been digitally reconstructed from the typical SEM images of Pt/gamma-Al2O3 catalytic washcoats of monoliths. The dependences of overall CO reaction rate and the effectiveness factor on the temperature and properties of the Pt/Al2O3 catalytic porous structure (washcoat macro-porosity, characteristic size of the macro-pores, the size of Al2O3 particles and the noble metal loading) have been studied.

References

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