6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

MODELLING OF CHEMISTRY AND MASS TRANSFER IN A MONOLITHIC REACTOR WITH SINUSOIDAL CHANNEL FOR THE CATALYTIC OXIDATION OF FORMALDEHYDE

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Key Words: *Formaldehyde Oxidation, Kinetic Model, Metallic Monolith, Mass Transport Limitation, CFD.*

A comprehensive study is presented on kinetics and mass transfer in a catalytically coated metallic monolith converter with sinusoidal channels. For the description of flow field and mass transport inside the channel as well as species diffusion and chemical reaction inside the porous washcoat, a three-dimensional approach is applied and the calculations were performed, using ANSYS-FLUENT. The calculation domain of the 3D model consists of a singel channel of real corrugated metallic monolith optimized for formaldehyde oxidation applicable in after-treatment system of lean-burn gas engines. Three different computational models representing different washcoat distributions are compared. The effect of washcoat distribution and mass transfer on kinetics and catalyst activity are investigated in details and the numerically obtained results are compared with experimental data. For the modelling of the chemical reactions, an elementry-like-step surface reaction mechanism consisting of 30 reactions on platinum was applied.

All three models have shown to operate in mass transport limited regime, where the diffusion distance from bulk to catalyst surface as well as reactant concentration play a significant role. So that in spite of very high intrinsic reaction rate at operation temperature, the complete conversion of formaldehyde could not be gained. Thus, very low levels of formaldehyde emissions would be technically hard to achieve and a long catalyst is required to overcome the low diffusion rate.

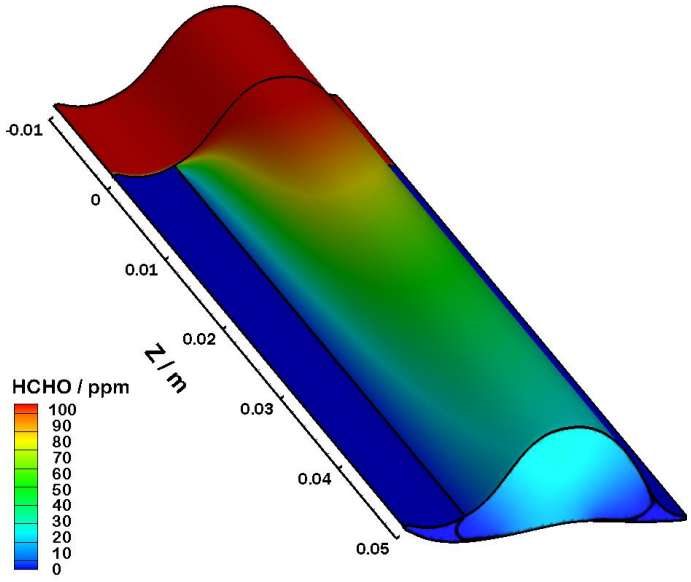

Figure 1: 3D concentration distribution of formaldehyde along z-axis. The calculation domain conists of one cm of the flow prior to the channel enterance, channel flow and non-uniform porous washcoat volume at the channel edges.