Accuracy of 2D modeling approach for performance simulation of noncircular single- and dual-layer monolithic catalysts

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Abstract

This study aims to evaluate the accuracy of widely applied approach of modeling noncircular channels and washcoats of monolithic catalysts with equivalent circular geometrical shapes. For this purpose, catalytic performance of equivalent circular and square channel cross-sectional shapes with single-layer Pt/Al₂O₃ and dual-layer Fe-ZSM-5+Pt/Al₂O₃ washcoats are investigated. For the noncircular cross-sections, three-dimensional computational fluid dynamics models that consider species gases convection inside the channel bulk flow region, and reaction and diffusion of species inside the washcoat layer(s) are utilized to simulate the performance of one channel of the monolithic catalytic converters. In addition, in order to investigate the amount of inaccuracy of 2D modeling approach for noncircular channels, 2D models are applied to simulate the equivalent monolithic catalysts with circular cross-sections, and the results of the 2D and 3D models are compared together, and also, with the experimental and 1D+1D modeling technique results available in the literature.

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