Coated wall reactor modelling - Criteria for neglecting radial concentration gradients. 1. Empty reactor tubes

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Abstract

The influence of radial mass transport on the conversion in a coated wall reactor was investigated in a modeling study. Criteria based on the observed conversion are developed to allow neglecting radial concentration gradients, and to be able to use the simple plug-flow model to describe the reactor performance and to determine reaction kinetics. The simulations were carried out using Athena Visual Studio 10.0 and Comsol Multiphysics 3.2 for several reactor geometries (round, square, annular, rectangular and triangular channels) and reaction orders. It was verified that the entrance effects, that enhance the radial mass transfer, can be neglected in most typical situations.

The criterion for the maximum allowable conversion with a less than 5% deviation in the rate constant is a function of the modified Péclet number (Pe'), the reaction order (n), and two constants a and b that depend on the reactor geometry.

$$X_{CWR} < \frac{b}{a + nPe'}$$

The criterion is valid for both gases and liquids.

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