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Coated wall reactor modelling - Criteria for neglecting radial concentration gradients. 2. Reactor tubes filled with inert particles

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Abstract

The influence of radial mass transport limitation on the conversion in a coated wall reactor filled with inert particles was investigated in a modeling study. Criteria are developed to allow neglecting the radial concentration gradients, and to use the simple plug-flow model for performance testing and kinetic studies using the measured conversion. The simulations were carried out using Athena Visual Studio 10.0 for several reaction orders in a tubular reactor filled with inert particles of different size. It was verified that the entrance effects, that enhance the radial mass transfer, can be neglected in most typical situations.

The criterion for the conversion is a function of the modified Péclet number (*Pe*'), the reaction order (*n*), and a constant *a* that depends on the reactor geometry and the internal tube radius/particle size ratio.

$$X_{CWR} < \frac{1.42a}{a + nPe'}$$

The criterion is valid for both gases and liquids as long as the viscous contribution to the pressure drop is much larger than the turbulent contribution. This applies for most gas-phase applications and some liquid-phase applications. At conditions where the turbulent contribution becomes comparable or larger than the viscous contribution, the criterion for the modified Péclet number becomes stricter. In that case the criterion with assuming $d_p = 0$ can be used as a conservative estimate. The most relaxed criterion is obtained for relatively large particles, up to $d_p/d_t = 0.4$.

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