

Simulation of a reactor for the partial oxidation of o-xylene to phthalic anhydride packed with ceramic foam monoliths

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In this study, the potential of ceramic foams as catalyst carriers in the oxidation of o-xylene to phthalic anhydride (PA) is evaluated theoretically. The main objective is to show the effect of ceramic foams on reactor operation, PA selectivity and space-time-yield in comparison to conventional fixed catalyst beds consisting of particles.

The heterogeneously catalysed gas phase oxidation of o-xylene is the most important industrial process for the production of phthalic anhydride (PA). In the cooled multi-tubular reactors employed in this process, high reaction and heat production rates cause pronounced radial and axial temperature gradients across the catalyst bed. If the operating conditions slightly change, the risk of a thermal reactor runaway is given. In addition, temperatures above 500°C accelerate an irreversible deactivation of the catalyst. As a consequence, industrial PA-reactors are forced to operate at low o-xylene inlet concentrations and low temperatures, resulting in lower PA space-time-yields than theoretically possible. One opportunity to improve the performance of industrial PA reactors could be the application of ceramic foams as structured carriers for the V_2O_5/TiO_2 catalysts. First literature data indicate that these open cell materials with high surface areas generally enable improved heat and mass transfer as compared to conventional catalyst bodies like spheres or hollow cylinders. In addition, the high porosities of ceramic foams lead to a considerably reduced pressure drop over the catalyst bed.

We developed one- and two-dimensional, pseudo-homogeneous models to simulate the behaviour of industrial PSA reactors filled with catalytic spheres, hollow cylinders or ceramic foams. Kinetic models as well as correlations for heat and mass transfer were taken from the literature. The results achieved with fixed beds of catalyst particles were used as a reference for different case studies which we performed with reactors packed with ceramics foams.

Our simulations show that axial and radial temperature gradients are much less pronounced when ceramic foams are applied as catalyst carriers. Thus, the risks of both, reactor runaway and catalyst deactivation are reduced. Furthermore, the lower temperature gradients allow for operation at higher inlet and salt bath temperature which, according to the kinetic models, enhances the PA yield. The inlet concentration of o-xylene can also be increased such that up to three times higher PA space-time-yield are achievable at constant PA selectivity and yield. A further boost of the PA space-time-yield is possible with foams because their high surface area per volume in combination with the low pressure drop makes it possible to increase the space velocity at constant modified residence time. Besides improved operating conditions, the simulations show that larger diameters of the single tubes can be installed when foam packings are used instead of particle beds. This could result in a considerable reduction of the costs for construction and operation of the multi-tube reactor.