Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Catalysis Science & Technology

Electronic Supplementary Information

Enhancing internal mass transport in Fischer-Tropsch catalyst layers utilizing transport pores

Henning Becker, Robert Güttel and Thomas Turek

Evaluation of the productivity of micro channel reactors requires careful choice of the reference volume as the overall absolute production rate, R_{C5+}, is not independent of reactor size and overall catalyst inventory, which is influenced by transport pore fraction and layer thickness (Fig. (1), left).

$$R_{C5+} = (1 - \varepsilon_{TP}) \cdot A \cdot \int_0^t r_{CO}(x) \cdot S_{C5+}(x) dx$$

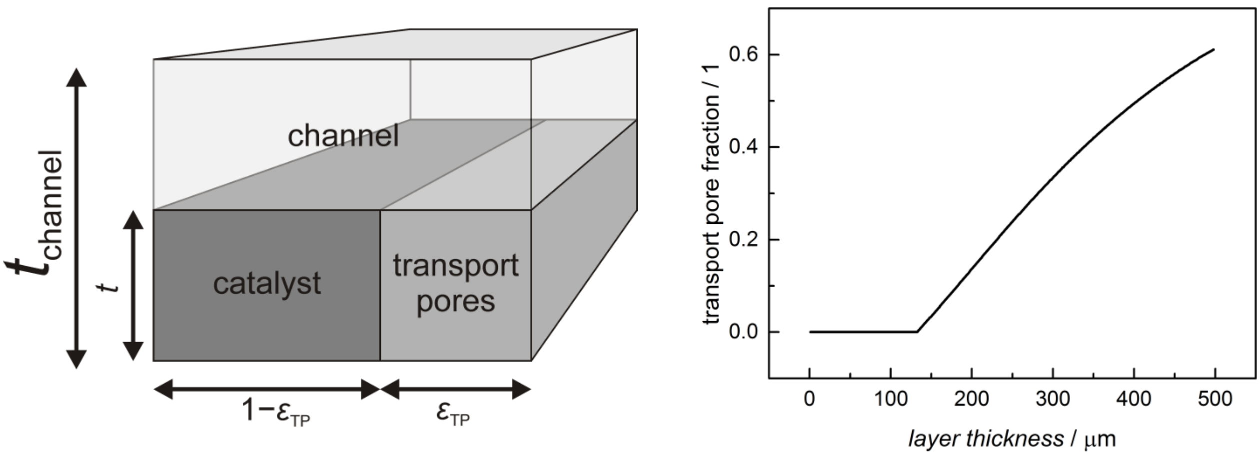
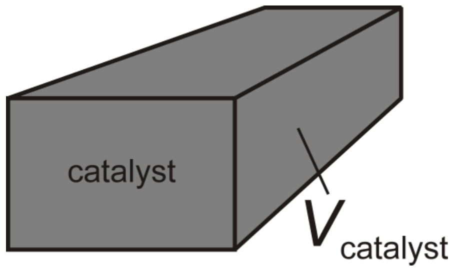


Figure 1: Schematic of wall coated micro-reactor with catalyst, transport pore and micro channel volumes (left); transport pore fraction as function of layer thickness; T = 493.15 K, p = 21 bar, H_2/CO = 2, ε_{Cat} = 0.4, τ_{cat} = 3, τ_{TP} = 1 (right).

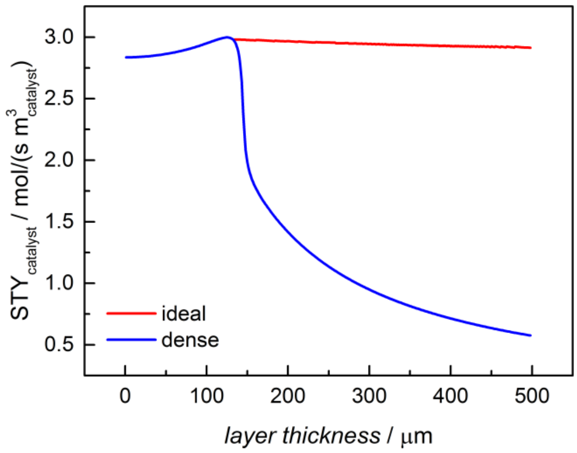
Optimization of productivity for a certain layer thickness requires an ideal transport pore fraction that maximizes C_{5+} production rate. Repeating this for several layer thicknesses lead to the ideal transport pore fraction as function of layer thickness (Fig.1, right). These conditions are also used for subsequent evaluation of productivity measures.

Catalyst volume



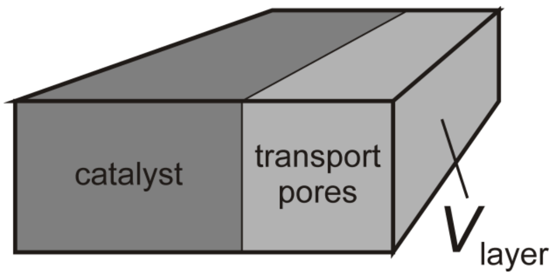
$$STY_{catalyst} = \frac{R_{C5+}}{V_{catalyst}}$$

$$= \frac{1}{t} \cdot \int_0^t r_{CO}(x) \cdot S_{C5+}(x)dx$$



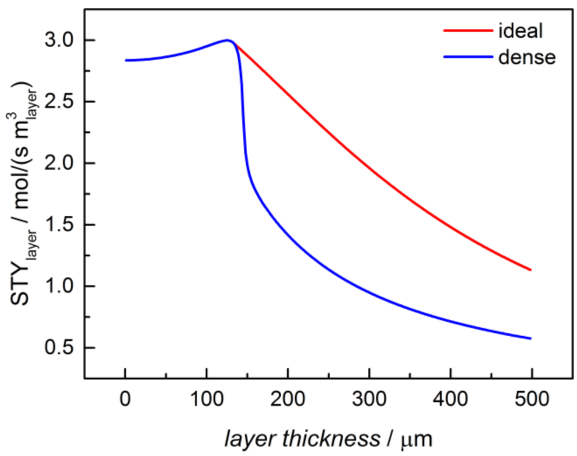
The typically used space time yield with the catalyst volume as basis, STY_{catalyst}, does neither take into account that the amount of catalyst is reduced by transport pores nor the ambiguous effect of layer thickness, the increase of which leads to higher diffusion limitations, but also to higher catalyst inventory. Thus, results highly overestimate the improvement for a certain layer but do not show a positive effect of transport pores.

Layer volume



$$STY_{layer} = \frac{R_{C5+}}{V_{layer}}$$

$$= \frac{(1-\varepsilon_{TP})}{t} \cdot \int_0^t r_{CO}(x) \cdot S_{C5+}(x)dx$$

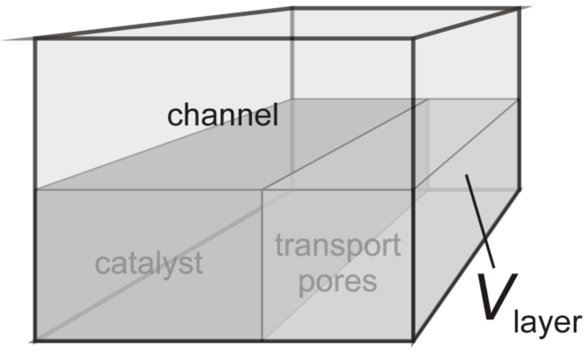


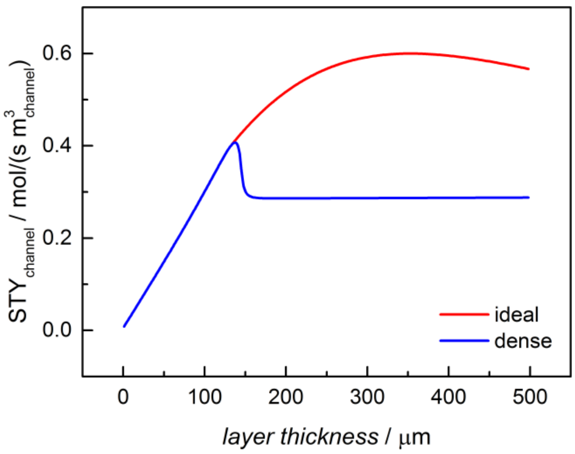
If one uses the layer volume as basis, the resulting STY_{layer} properly accounts for the effect of transport pores, but the impact of layer thickness is still neglected. Therefore, this property is not useful for comparison of layers with different thickness.

Catalysis Science & Technology

Electronic Supplementary Information

Channel volume



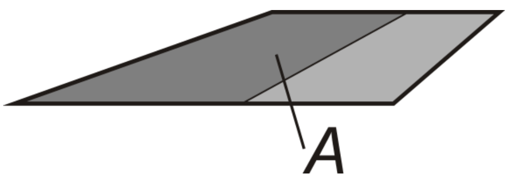


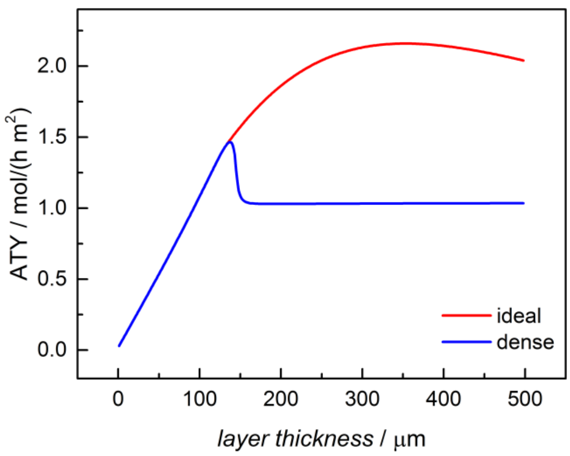
$$STY_{channel} = \frac{R_{C5+}}{V_{channel}}$$

$$= \frac{(1-\varepsilon_{TP})}{t_{channel}} \cdot \int_0^t r_{CO}(x) \cdot S_{C5+}(x)dx$$

The use of the complete channel volume, including the catalyst layer, would be the best for evaluation of reactor productivity. But channel thickness can only be realistically evaluated by using an integral reactor model, considering gas and liquid flow and pressure drop. Since this was not the objective of this work, an arbitrarily fixed value of 1 mm was used.

Layer surface area





$$ATY = \frac{R_{C5+}}{A}$$

$$= (1-\varepsilon_{TP}) \int_0^t r_{CO}(x) \cdot S_{C5+}(x)dx$$

The area specific yield, ATY, considers effects of thickness and transport pore fraction properly, but avoids problems related to the channel thickness. Hence ATY is the ideal measure for assessment of productivity.