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Oral contribution

# Styrene Synthesis: High Yield over Unpromoted Iron Oxide Model Catalysts

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Dehydrogenation of ethylbenzene to styrene is usually run over potassium promoted iron oxide based catalysts at 870 K in presence of steam. Here we present conversion yield measurements on unpromoted single crystalline α-$Fe_2O_3$ (0001) model catalysts by combining surface science techniques with an in-situ micro flow reactor (Fig.1). The influence of $H_2O$ and $O_2$ on the reaction was investigated by varying the composition of the feed. The initial conversion over $Fe_2O_3$ is always high (5-8%, Fig. 2), independent of the type of the feed composition. Only the length of this period depends on the feed composition. In presence of $O_2$ ($EB:H_2O:O_2$ = 2:20:1), the high yield period can be maintained, in absence of $O_2$ (EB: $H_2O$ = 1:10) it decreases in two steps of about a factor of 2-3 each. The reaction was interrupted in the different yield regimes, and the sample structure and composition was analyzed. The high yield is related to $Fe_2O_3$ with almost no carbon deposits. $O_2$ in the feed maintains this phase. Without $O_2$, $Fe_2O_3$ is reduced to $Fe_3O_4$ and the yield drops to the intermediate region. The same yield is observed on clean $Fe_3O_4$. Carbon deposits increase but do not yet limit conversion. This happens at the transition to the low yield regime where a thick layer of carbon deposits is observed. With $H_2O$ in the feed, the oxide below the carbon deposits remains $Fe_3O_4$, without $H_2O$, it is reduced to metallic Fe. We ascribe the low yield to catalysis by carbonaceous species. The study shows that the high yield is typical for $Fe_2O_3$ and can be maintained by proper admixture of $O_2$ to the feed.

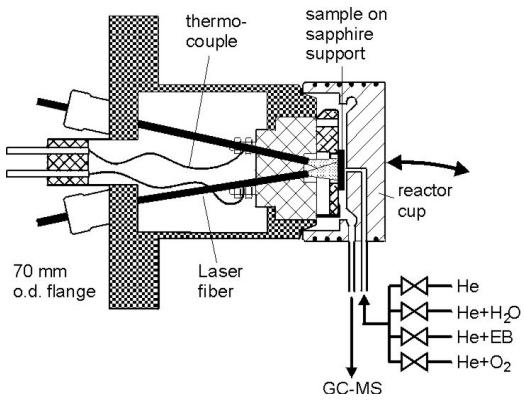


Fig. 1: Micro flow reactor

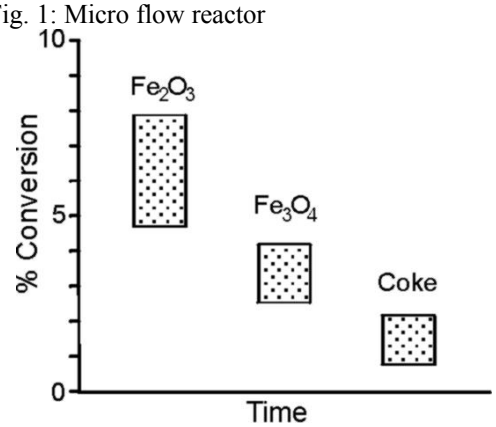


Fig. 2: Styrene yield over $Fe_2O_3$ and its decrease by reduction to $Fe_3O_4$ and by coking, schematically.