

An Alternative Approach for the Oxidation of o-Xylene to Phthalic Anhydride: New complex Molybdates as Active Compounds in an Advanced Process Scenario

Stephan Andreas Schunk, Nadine Brem,

hte Aktiengesellschaft, Heidelberg, Deutschland

Andrey Karpov, Christine Deissler, C. Dobner, Hartmut Hibst, Frank Rosowski,

BASF SE, Ludwigshafen, Deutschland

Within the framework of the BMBF project “NanoSelOx” (promotional reference 03X2007A) BASF SE, hte AG, the TU Munich, the TU Karlsruhe and the RWTH Aachen tried to elaborate the options of an alternative process for the production of phthalic anhydride. The main process routes that were followed as potential leverages were: i) the oxidation of o-xylene in alternative reaction media, especially supercritical CO₂, ii) the oxidation of o-xylene in liquid phase using heterogeneous catalyst candidate systems iii) a two stage gas phase oxidation approach. Within this presentation we will focus on the results the two stage gas phase oxidation approach.

General Considerations regarding Process Improvements in o-Xylene

Oxidation

The general idea for a substantial improvement of the existing oxidation process went back to the finding at SASOL in the 1990's, that the established catalyst within the system for o-xylene to phthalic anhydride, namely vanadia on TiO₂ in the modification of anatase, can oxidize partial oxygenates like tolyl alcohol, tolyl aldehyde or the like with much higher selectivity to phthalic anhydride than the standard educt of the reaction, o-xylene. This was the fundament for the new potential process schemes that were envisaged and brought to test. In this process scheme that was developed as alternative for gas phase operation the development goal was to establish a pre-oxidation process which would allow generating a pre-oxidized feed gas mixture which could then be passed over the standard catalyst system at conditions similar to the current process.

New Catalyst Families for the Alternative Gas Phase Oxidation Process

Scheme

The new gas phase oxidation process faced a number of challenges concerning catalyst and process development. Apart from the fact that new catalyst systems had to be identified which would only oxidise a feed of o-xylene partially, the resulting feed-stream had to be suitable in terms of composition for further conversion by the established catalyst system. In order to accelerate the development process in search of a new catalyst family, high throughput experimentation was employed as leveraging toolbox. Three distinct new catalyst types were developed: one catalyst family of complex Copper Molybdates which allows conversion of o-xylene to tolyl aldehyde with high selectivity within the conversion-window between 10 and 20%, a family of Molybdates with Copper combined with either Silver or Iron which render a mixture of oxygenates at conversion levels between 30 and 50% also at high levels of selectivity. And finally a family of Silver Molybdo-Vanadates which could be tuned to deliver useful properties for the high conversion corridor. In our presentation we discuss the structural motives relating the different catalyst families and the resulting structure property relationships.

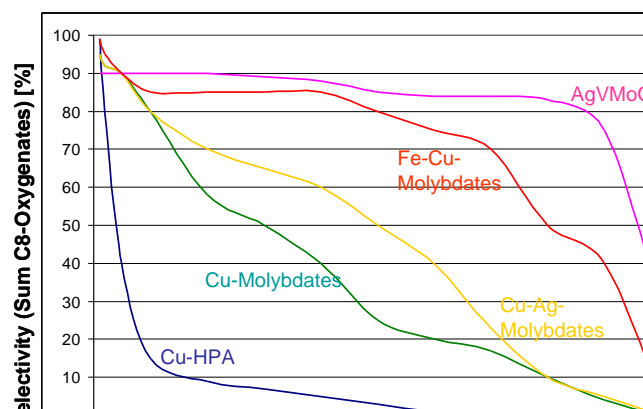


Figure 1: Comparative conversion selectivity plot for the catalyst families discussed.

Conclusions for an Alternative Process Scheme

A range of new and useful catalyst families could be identified for the alternative process scheme. We will discuss drawbacks and advantages for different process scenarios highlighting materials properties.