Scale-up of Hydrogenation of Nitrobenzene, Data-Rich Experimentation approach

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Identification of optimal operating conditions of a chemical process by combining knowledge of kinetic and thermodynamic parameters is shown in this case study through the catalytic hydrogenation of aromatic nitro compounds. This reduction is an industrially important process for the introduction of amino functionality into pharmaceutical and agrochemical intermediates and in polyurethane chemistry. Aromatic nitro compounds are hydrogenated easily, and hydrogenations have been carried out under a wide range of conditions including the vapor phase.
They are known to be potentially hazardous reactions, especially because the hydroxylamine intermediates formed are often thermally unstable and can decompose with a significant temperature increase, causing large explosions.
Hydrogenation of nitro-compounds was studied at lab scale with EasyMax and RC1mx reactor systems from METTLER TOLEDO to understand the process and to access the role of mass transfer limitation. The goal was to define the necessary rules to run the hydrogenation experiments in the chemical reaction regime and characterize the influence of gas-liquid mass transfer to support kinetic modelling for scale-up purposes.

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