Kinetic modeling of the catalytic hydrogenation of nitrile esters to amino esters

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In this research, the catalytic hydrogenation of nitrile esters to amino esters was studied. The application of amino acids as monomers for production of polyamides is well-known for use in a broad scope of products in automotive, oil and gas, and electronic cables industries due to the high resistance to hydrocarbons. Amino-esters are alternative monomers to produce these polymers.

The hydrogenation of nitrile ester was performed in a stirred tank reactor. The mixing of the fluids was carried out using a gas induction stirrer with a hollow shaft. An appropriate amount of ammonia has to be dissolved into the reaction mixture in order to avoid side or consecutive reactions, whereas the starting material nitrile ester was diluted by applying methyl-cyclohexane as solvent.

The reaction study was carried out at temperatures varying from 90 - 120 °C, pressures ranging from 70 - 90 barg and stirring speeds from 1000 - 1200 rpm. The influence of the amount of dissolved ammonia and the hydrogen solubility in the reactants and in the chosen solvent were considered in this study.

A reaction mechanism is proposed from the gas chromatographic and mass spectrometric analysis of the experimental data.

A mathematical model, which describes the proposed reaction mechanism of intermediate species and products was proposed for this hydrogenation reaction. The data were fitted using the least square method and the relevant kinetic rate constants were determined.

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