38c Mixing Effects on Homogeneous Catalytic Hydroformylation of 1-Octene in Co_2 - Expanded Solvent

Debangshu Guha, M. P. Dudukovic, P. A. Ramachandran, and Bala Subramaniam

Hydroformylation reaction converts olefinic petrochemicals into oxygenated hydrocarbon compounds, i.e. aldehydes, which are important for the production of fine chemicals and pharmaceuticals. CO2 – expanded liquids (CXLs) combine the reaction benefits of organic solvents and the environmental benefits of compressed CO2, and this makes CXLs very suitable as environmentally benign reaction media. Much higher turnover numbers (TON) for aldehyde formation can be obtained with CXL as the reaction media compared to neat solvent. The higher TON in CXLs is attributed to enhanced syngas solubility in CXL. The purpose of this work is to model the mass transfer and mixing effect of syngas on hydroformylation of 1-octene in CXL and compare with some data obtained in a small laboratory scale reactor. The experimental data shows the presence of a significantly large induction period (~2 hours). The model can capture the trends that are observed in the experimental results. A simplified kinetic scheme as well as a detailed kinetic scheme is used in the model and the predictions are compared. Due to the inhibitory effect of CO, the increase in mass transfer rate may not be always beneficial. Sensitivity of the predictions to different model parameters is also studied. This insight will lead to optimization of the process condition for the reaction. The experimental data can also be fitted to estimate the kinetic parameters of the reaction.