Selective oxidation of benzyl alcohol in dense CO2: Insight by phase behavior modeling

Catalytic reactions in pressurized CO2 are often strongly affected by the phase behavior. Knowledge on phase behavior is therefore desirable for optimizing the reaction conditions but often requires considerable experimental effort. Here, a previously established thermodynamic model for complex systems, based on the Cubic Plus Association (CPA) equation of state, is utilized in order to gain insight into the phase behavior during the palladium-catalyzed selective oxidation of benzyl alcohol to benzoic acid. The catalytic reaction was studied in a tubular continuous reactor both under biphasic and single phase conditions at different flow rates, compositions and oxygen concentrations. In general, biphasic conditions resulted in the highest reaction rate which was also found when running the reaction in a batch reactor. On transition to a single phase a gradual deactivation of the catalyst was observed. Hence, the model predictions can be beneficially applied in order to find optimal reaction conditions. In the continuous reactor under biphasic conditions, the substrate was found to accumulate in the reactor due to segregation. The study indicates that a direct comparison between the catalytic performance observed in the continuous flow system and batch reactor under biphasic conditions requires knowledge on the influence of the segregation on flow conditions and mass transfer, which is often ignored in the literature.

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