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Modeling of CO₂-assisted liquid phase oxidation of para-xylene catalyzed by transition metals/bromide

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Abstract: The promoting effect of CO₂ on liquid phase oxidation of para-xylene (PX) catalyzed by transition metals/bromide was investigated in batch experiments under conditions of industrial interests such as temperature, pressure, and catalyst. On the basis of free radical chain reaction mechanism of alkyl aromatics oxidation, the kinetic model of CO₂-assisted PX oxidation involving six parameters was developed. The model fits the PX oxidation kinetics well with narrow confidence intervals of rate constants under conditions of various CO₂ addition, temperatures, and catalysts. It was found that the presence of CO₂ could obviously promote the chain initiation reactions that are the rate-limiting steps, while it has no impact on the propagation reaction kinetics. Only the rate constant concerning chain initiation was dependent of different experimental conditions while other model parameters kept constant. The promoting function of CO₂ can be ascribed to the formation of active peroxocarbonate that results from a synergistic interaction of CO₂ and O₂. This postulated specie may participate in the generation of free radicals by oxidizing Co^{II} to Co^{III}. Hopefully, the kinetic model proposed in this work can be used to optimize the CO₂ assisted PX oxidation process and bring insights into PX oxidation mechanism with the presence of CO₂.

Keywords: Liquid phase oxidation; Alkyl aromatics; Kinetic model; Carbon dioxide; para-Xylene.

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