Proceedings of the Canadian Society for Mechanical Engineering International Congress 2022
CSME Congress 2022
June 5-8, 2022, Edmonton, AB, Canada

Experimental investigation and modeling of nickel carbonyl formation in a fluidized bed reactor

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ABSTRACT

Nickel tetracarbonyl, known primarily as nickel carbonyl gas, is formed through the reaction between nickel powder and carbon monoxide at moderate temperatures and pressures. This process is known as the Mond process and has been used in the industry for nickel purification over a century. Most of the studies published on this process are few and primarily based on empirical models or purely have exploratory nature. In this presentation, experimental investigation, theoretical modeling, and computational fluid dynamic (CFD) simulation of nickel tetracarbonyl formation through the Mond process under different conditions in a fluidized bed reactor is presented. The fluidization process is simulated through CFD case studies for a range of conditions and compared to experimental observations of fluidized beds of nickel powder. In theoretical models, nickel carbonyl formation progress is modeled as a function of reaction temperature, inlet gas pressure, and carbon monoxide flow rate. Experimental results were obtained using a fluidized bed reactor. A diffusion-kinetics and a two-phase bubbling bed model were developed to compare with experimental results. The reactor is considered as a differential flow reactor for the theoretical modeling. The reaction rate is strongly dependent on carbon monoxide gas pressure. The models developed are rather simple yet provide significant improvement in predictions of the reaction rate compared to the existing models in the literature. Rate of reaction is measured in a fluidized bed and used for the verification of the studied models. The best performing model is a kinetic-diffusion model with a rate of reaction that obeys $r_{em} = K_{em}([CO])^n$, in which K_{em} is a function of mass transfer as well as kinetic variables, but is primarily temperature dependent. Also, n for low-pressure and high-pressures regions is −1 and −3, respectively.