Modeling and Simulation of Low Temperature Water Gas Shift Reactor

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ABSTRACT

The Water Gas Shift Reaction (WGSR) is a reaction traditionally used for the Production of Hydrogen from synthesis gas which is further used for ammonia Production in the fertilizer industry, petroleum refineries for a variety of Operations and recently as fuel for power generation and transportation. This reaction depends mainly on the catalyst used and it's properties, so study of different metal based catalyst including Cu, Fe, Ni, Pd, Rh and Ru is in Centre of interest.

Generally all gas phase reaction is carried out in catalytic bed and all the reaction kinetics is based on some mechanisms and also depends on catalyst property. Some of mechanism and kinetics of catalytic reaction is illustrated from researcher's literature and also from catalyst manufacturer.

Mathematical model for such water gas shift reaction is beneficial for study of the weight of the catalyst needed to achieve a higher CO conversion %.

The aim of the present work is to develop a mathematical model that describes the low temperature water gas shift reaction in a fixed bed reactor using Copper-Zinc catalyst.

The mathematical model was used to calculate the amount of catalyst needed to achieve a certain conversion percentage.The effects of different parameters on the weight of the catalyst used inside the reactor to achieve certain conversion were studied. These parameters are: the operating pressure, temperature and initial molar flow rate of carbon monoxide and water. The model was validated against a real plant data from "AlexFert Company " and also by using published data and the results show good agreements with both the real plant data and the published data with a deviation (6.22%,4.24%) respectively.

A sensitivity analysis was carried out to study the effect of the parameters on the model and it was found that the feed temperature and the initial molar flow rate of H_2O was the most effective parameter where the operating pressure initial molar flow rate of CO was the least effective parameter.