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Liquid Phase Ethylene Production by Hydrogenation of Acetylene: Kinetics and Multiscale Modeling

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Highlights
- Kinetics of the commercial catalyst for liquid phase hydrogenation was studied
- The kinetic parameters were included in the multiscale model
- The reactor performance for the hydrogenation reaction varied for different models

1. Introduction

Ethylene is a primary building block in petrochemical industries produced mainly by steam cracking of naphtha. Acetylene is the byproduct of the cracker effluent, and selective hydrogenation of acetylene to ethylene has been conducted in industries to increase the yield. Moreover, using acetylene as a primary source for manufacture of ethylene, considering ethylene's demand, is beneficial. Catalytic conversion of ethylene to higher hydrocarbons will be an alternate process for fuel production. Hydrogenation of acetylene in the gas phase has been commonly practiced in industries with the risks of runaway conditions as well as early catalyst deactivation due to green oil formation.[1] Liquid phase hydrogenation has been a recent focus of research to overcome these issues along with increasing the conversion and selectivity. [2, 3] The liquid phase which selectively absorbs acetylene from the effluent gas mixture also acts as an efficient heat transfer medium. The formation of green oil on the catalyst due to oligomerization can be reduced in the liquid phase which increases the stability and life of the catalyst. This work aims at understanding the kinetics of a commercial Pd/Al_2O_3 catalyst for the liquid phase acetylene hydrogenation. Also, the obtained kinetics will be used in a mathematical multi-scale model to predict and validate the reactor performance. Most of the models in literature were reported with various assumptions making them less reliable as they do not forecast the exact operating conditions. Also, the models rely on assuming single effectiveness factor for the catalytic reaction for whole the reactor while this parameter varies with the variation of the reactants concentration which varies spatially. A robust model should integrate the kinetics and the reactor hydrodynamics to capture the physical phenomena in the catalytic reactor at both particle and reactor scale levels. This model must be able to simulate the catalytic reactions thereby predicting the performance of a fixed bed reactor for both trickle and two-phase upflow.

2. Methods

The kinetics studies will involve the hydrogenation of acetylene in the presence of a solvent acting as the liquid phase over a commonly used gas phase hydrogenation catalyst. A 300mL three phase stirred tank reactor will be used, and experiments will be conducted in both slurry and basket modes. The high-pressure autoclave can operate in a batch, semi-batch or continuous mode at pressure up to 2000psi and temperature up to 500C. The effluent samples were analyzed using a gas chromatograph with FID. A kinetic model was developed and fitted on simple power law equations and Langmuir-Hinshelwood-Hougen-Watson approach. The predictions of these approaches on the acetylene conversion were compared. The parameters studied to understand the liquid phase kinetics were temperature, $H_2:C_2H_2$ feed ratio, catalyst loading, and operating pressure. The obtained reaction kinetics will be included in the multi-scale model, a one-dimensional mathematical axial dispersion

flow model integrated with a particle scale model. The kinetics and the related parameters involved in the processes were accounted in the model along with different particle to liquid wetting conditions. The multi-scale model accounts for the variation of the local catalyst effectiveness factor along the height of the reactor due to the change in reactants concentrations, bed hydrodynamics, and transports. The reactor scale model identified the local concentration of the reactant species while the local effectiveness factor was accounted by the particle scale model for the corresponding local concentration and local hydrodynamics in terms of liquid holdup and catalyst wetting efficiency. The modeling strategy solved the mass balance equations for convergence numerically to evaluate the local reactant concentration, and conversion in the flow direction.

3. Results and discussion

The multiscale model was operated at different operating conditions integrating the kinetics from the experiments. The comparison helped in understanding the conversion at different LHSV. Figure 1 is a representation of the predictive reactor performance from the model results to understand the variation in the conversion while using the multiscale model with axial dispersion model and plug flow model. Further results of kinetic studies will be integrated and simulated by the model.
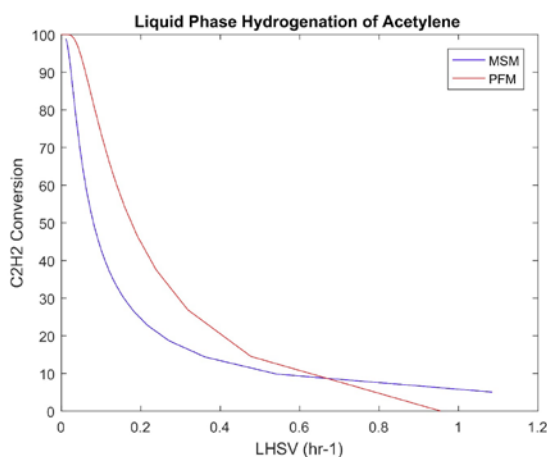
Figure 1. Reactor performance prediction for liquid phase hydrogenation of acetylene by comparing the multi-scale model (MSM) and plug flow model (PFM) at T= 80C, P= 1.5MPa, Superficial gas velocity = 3.8cm/s, Superficial Liquid velocity = 0.236 cm/s

4. Conclusions

This work integrates the kinetics studies in the reactor scale modeling for liquid phase hydrogenation of acetylene for ethylene production. The prediction of the reactor performance guides the fixed bed experiments which in turn can optimize operating parameters, time and number of trials.

References

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