

CFD Simulation and Optimization of the Oxidative Dehydrogenation of Butene to Butadiene using Artificial Neural Network

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In this work, the CFD analysis and synthesis of butadiene via the Oxidative Dehydrogenation of butene in a multi-tubular and water-cooled reactor was executed. The impact of operating parameters such as temperature, flow rate, and inlet concentrations on performance of the reactor (e.g., selectivity and yield of butadiene) was investigated. Validation of the CFD model showed that simulation results agreed well with the experimental data. Data generation for the ANN model was performed by the CFD model using a varying range of process conditions along with domain expert knowledge. The developed surrogate model proved beneficial for predicting future outputs. Lastly, the optimization of the key operating parameters was carried out to maximize the yield of butadiene.

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