

عنوان مقاله:

Hybrid model formulation for the unsteady state simulation of a packed bed reactor for CO₂ hydrogenation to methanol

محل انتشار:

دهمین کنگره ملی مهندسی شیمی ایران (سال: 1384)

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خلاصه مقاله:

Carbon dioxide emission is well known as the main source of global warming and reduction of carbon dioxide by hydrogen is the interesting topic for prevention of this side effect. For studying the CO₂ removal a hybrid Neural Network Model (NNM) was developed to estimate outlet of a differential methanol reactor as a function of time, temperature, pressure CO, CO₂, H₂O and H₂ mole fractions. The hybrid model consists of two parts; a mechanistic model and a neural model. The mechanistic model consist of heat transfer, mass transfer and pressure drop equations which calculate the effluent temperature of a differential reactor by taking outlet mole fraction from neural model. Neural model provides estimation of outlet mole fraction of a differential reactor. This estimation is fed to mechanistic model. The prepared hybrid model is used to simulate and identify an industrial methanol reactor. The bed of reactor was assimilated to pile of layers, each corresponding to a Neural Network (NN) so the associate NN could predict outlet composition of each layer as a function of time. The model was successfully tested with plant experimental data. The insights of this research indicate a very fast responding model in comparison to traditional models to demonstrate CO₂ reduction as a function of time and reactor length. Variation of temperature and other compositions with time and bed height are investigated in this article.

کلمات کلیدی:

CO₂ reduction; Methanol synthesis; Neural Network; Packed Bed Reactor

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