ABSTRACT

Dynamic Modeling of Industrial Fixed Bed Catalytic Reactors: A Comparative Study

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Steady-state and dynamic modeling of packed bed reactors have attracted considerable attention. Interest in dynamic modeling can be explained by the necessity to understand important practical problems such as reactor start-up and shutdown and process stability, i.e. response of the reactor to disturbances in operating conditions. In this thesis, dynamic models for three reactors in an industrial ammonia production facility were developed. These are a Primary Reformer, a Secondary Reformer and an Ammonia Converter.

The modeling was done comparatively using the software packages HYSYS.Plant and MATLAB/Simulink. For step disturbances in the feed conditions to the primary steam reformer, the HYSYS.Plant model predicted considerably larger gains and longer settling times than the MATLAB/Simulink model. It was determined that these differences were as a result of the fact that, for the HYSYS.Plant model, a fixed heat duty was employed to represent energy transferred from the furnace section of the reformer, while the MATLAB/Simulink model assumed a fixed tubeskin temperature. For the secondary steam reformer, the gains and settling times predicted by both models were quite similar. No limit cycle behaviour was observed for the ammonia

converter, from either model. However, there was a greater degree of nonlinearity in the responses from the MATLAB/Simulink model.

The modeling was done using a computer equipped with a Pentium 4, 2.4 GHz processor and 512 MB of memory. The computational speed for the MATLAB/Simulink models was, on average, 5 times faster than for the HYSYS.Plant models. Based on the superior numerical methods available in MATLAB/Simulink, and the extent to which it can be customized, it is recommended that MATLAB/Simulink be the package of choice for future modeling projects.

Keywords: Omar Davis; Primary Steam Reformer; Secondary Steam Reformer; Ammonia Converter; MATLAB/Simulink; HYSYS.Plant.