Modeling of a dynamic adiabatic trickle-bed reactor

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Modern refinery operations cover a wide and complex variety of processes. Consider, for example catalytic hydrotreatment, it is crucial to obtain fuels with improved quality and low polluting compounds content (sulfur, nitrogen, aromatics) but also, vital for further refining stages. In these cases, it is not always possible to directly measure the important state variables online which are needed by the operator to judge if the reactor is behaving as planned or not. If these variables cannot be determined by direct measurements, then the information can be constructed by means of a state estimator using a process model.

Currently, catalytic hydrotreating takes place in trickle-bed reactors. Trickle-bed reactors are tubular reactors with a bed of packed catalyst and usually comprise a gas and a liquid phase that make them difficult to operate. The coupling between transfer phenomena, non-linear kinetics and the distributed nature can lead to temperature hot spots in the catalytic bed or formation of an undesired compound.

Now, consider that operation conditions of trickle-bed reactors are too hostile or fouling for sensors to work. In most cases, the information acquired from the reactors is restricted to temperatures and pressures along the catalytic beds in the reactor. Concentration measurements are made whether by sampling and lab analysis, which results are issued with significant delay, or using state estimators that may also incorporate information of known disturbances from feed mixture analysis or upstream data. Therefore, achieving high quality online information of the process is a challenge, moreover, it is important for the operator, or any model based control algorithm for process optimization, to ensure product quality as well as a safe and reliable process operation.

It is clear that mathematical models of the systems play a crucial role. Previous researches have approached the problem of trickle-bed reactor modeling [1] [2] [3] [4]. It is interesting that these models consider whether two-phase systems, isothermic, or steady-state behavior. This can be explained by the fact that steady-state isothermic models are used to study the reactions kinetics, nonetheless for literature is limited regarding large-scale industrial trickle-bed reactor models able to describe dynamic behavior with adiabatic characteristics.

This work will show the development of a dynamic model of an adiabatic trickle-bed reactor. Using the traditional framework describing reactive flows from a differential control volume and is able to describe the dynamic concentration and temperature profiles from two different modelling approaches, plug-flow reactor, and a series of continuous stirred-tank reactors. The accuracy of the model is validated with experimental data acquired from an industrial trickle-bed reactor at steady-state operation.

References

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