

### **397b Dynamic Analysis and Controllability Issues in Reactive Distillation Columns**

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Methyl tert-butyl ether (MTBE) production and hydrodesulfurization of diesel (HDS) are two important processes in the refinery, whose traditional process flowsheets consist of a reactor followed by a sequence of distillation columns. The alternative configuration to these processes is the reactive distillation (RD) involving reaction and separation in a single unit operation, with several advantages such as: capital and operation costs are reduced, energy integration is improved, reactant conversion is increased and product selectivity is improved.

In general, RD has a complex behavior, such as high non-linearity due to complex kinetics and thermodynamic models, strong input-output interactions, steady state multiplicity, high potential to instability, sensitivity to disturbances, etc. However, the complexity of the RD process is known to create unusual responses to changes in operating variables. Many of these effects are related to the phenomenon of multiplicity of steady states (which occurs as either input or output multiplicity) and have significant implications on the effectiveness of operability and control schemes. On the other hand, from a thermodynamic point of view, as the driving force is increased, the separation becomes easier, the energy consumption is reduced and the control requirement becomes easier. Moreover from a control point of view, it is reported that passive systems are easy to control and a passive state, in chemical processes, is related to state of minimum entropy production [1]. Thus, analyses of both steady state and dynamic behavior, together with thermodynamics concepts, facilitate the studies related to process operation, control, monitoring and optimization of existing plants.

In this research project, the main objective is the study of the (steady state and dynamic) behavior and controllability aspects based on the equilibrium (element-based) approach [2] and thermodynamic analysis for reactive distillation columns, with emphasis in the MTBE and HDS process. The element-based approach has the advantage of obtaining reduced order models (i.e. smaller number of states, since the number of elements are always less than the number of compounds), making easier the selection of the control structure. While from the thermodynamic analysis, controllability insights can be obtained by using the driving force and the Gibbs energy concepts: a state related to the largest driving force and to the minimum Gibbs energy will provide a passive system, and therefore a system easier to control. These conclusions are corroborated through steady state and dynamics simulations on ICAS and ASPEN. The results show the implications of both input and output multiplicities on the column operation, design and control; and a passive control configuration is proposed.

#### References

- [1] Coffey, D.P., Ydstie, B. E., and Farschman, C.A. (2000) *Comp. Chem. Eng.* 24, 317.
- [2] Pérez-Cisneros, E.S., Gani, R., and Michelsen, M.L. (1997) *Chem. Eng. Sci.* 52, 527.