242c Stability of Equilibrium Staged Reactive Systems

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Equilibrium staged processes for separation are among the most important and energy intensive processes in use in the chemical and petro-chemical industry. Of them, reactive distillation is especially important because of its potential advantages of enhanced conversion, improved product selectivity and reduced equipment cost. Despite its economic attractions, the control and stability analysis of these systems have so far been limited to (local) linear analysis, simulation and experimental studies. The only general nonlinear stability result for distillation is due to Rosenbrock (1960) and this result is limited to binary systems. We are not aware of any results applicable to reactive columns.

In an excellent paper on distillation, Doherty and Perkins (1982) claimed that the multi-component flash (single stage distillation) is stable. The method of analysis is based on Lyapunov's second method and is only valid for systems with independent k-values. Rouchon and Cref (1996) extended the result to multi-component, single stage, non-reactive systems and they showed that stability under restrictive flow conditions by showing that the flash dynamics can be represented as a gradient flow using results from no-equilibrium thermodynamics. The methods of analysis used by Doherty and Rouchon cannot easily be extended to multi-stage systems. Many papers report that instability and multiplicity of steady states are possible in equilibrium multi-stage distillation (Bekiaris et al, 1993; Jacobsen and Skogestad, 1991; Jacobsen and Skogestad, 1994; Magnussen et al, 1979). These results are supported by experiments (Kienle, Groebel and Gilles, 1995; Guttinger, Dorn and Morari, 1997).

This objective of this paper is to describe advances in the stability analysis of staged equilibrium systems. The systems we are interested in comprise systems with two or more phases and chemical reaction under equilibrium conditions. The approach for stability analysis is derived from thermodynamics principles and passivity theory. The method of analysis can be related to the Lyapunov direct method when we use a storage function based on the concavity of entropy function. We first study the multi-component reactive flash problem. We then extend the results to the multi-stage problem. The results do not at all contradict the examples reviewed above since the boundary conditions (feedback controls) we impose are different. The favored boundary conditions for instability simulation appear to be closely related to the Dirichlet conditions. Our boundary conditions are more closely related to the Neumann conditions.

The application of the theoretical results will be illustrated by simulating an unsteady state multi-stage model of a moving bed packed column. The column is used for reacting Aluminum and Aluminum Oxide off-gases from a Carbothermic Aluminum reactor with Carbon in order to generate Aluminum Carbide in a Carbothermic Aluminum reactor. The PDE model of the column will be approximated as a multi-stage (20 stages) equilibrium system. The thermodynamics are modeled using the FACTsage system with equilibrium calculated by ChemApp's Gibbs free energy minimization procedures. This system has been interfaced with Matlab for solving the material and energy balances.