469d A Thermodynamic Approach to the Stability of Equilibrium Mass Transfer Units and Multi-Stage Distillation Columns

Luis T. Antelo, B. Erik Ydstie, and Antonio A. Alonso

Multi-component separation systems have been widely studied by the process control community as distillation is one of the basic units of a real chemical plant. The aim of this paper is to go into depth in the study of stability of separation units because it is a fact that some of them (e.g. azeotropic distillation columns) can exhibit multiple steady states (Bekiaris *et al.*, 1993 and 1996) or even limit cycles (Lee *et al.*, 1999). Multiplicities may cause operation and control problems in the plant as some perturbations may change the column profile from the desired state to an undesired one which, for instance, does not satisfy the quality condition for the product. Even if these changes do not occur, the appearance of multiplicities can make the column to exhibit unexpected behaviors like sustained oscillations that cause periodic movements of the profiles inside it. To overcome these issues, we propose an alternative approach for stability analysis of mass transfer units (MTU) based on the tools that irreversible thermodynamics, process networks and system theory provide us. In relatively recent papers, Ydstie and Alonso (1997) and Alonso and Ydstie (2001) proposed a formal approach for stability analysis of open process systems using a generalization of the available work as a Lyapunov function candidate. The approach settles its roots on the properties of the entropy (S) function (homogeneity and concavity). However, there are two drawbacks related to availability when it is used for stability analysis of systems far from stationary steady states. The first is that the reference state chosen has to be time invariant. This can lead to poor estimates of stability regions for nonlinear systems too far from the steady state. The second problem is that it is difficult to use the availability for systems exhibiting flow instability. To avoid these issues, we define a new well stated concave storage function(R) based also on the entropy and its properties, to perform the stability analysis. We also introduce the concept of process network to systematize the process representation. For the mass transfer unit network case, the network is composed by nodes representing the liquid and vapor phases interconnected through dissipative mass transfer fluxes. Nodes are related with the environment by convective input/output flows. This formal representation allows us to define the network dynamics by a DAE system based on a time scale decomposition: a) *Network fast dynamics* are associated to dissipative transfer terms due to thermodynamic driving forces. Such fast transient phenomena (compared to the convective one) result in a MTU representation as a closed network where dissipative mass flux are only present between nodes. Once the equilibrium is reached, the thermodynamic potentials become equal and the transient dynamics disappears. b) *Network slow dynamics* are related to the convective phenomena between nodes and between nodes and the environment. In this case, the MTU network can be represented by independent nodes connected with the surroundings through convective mass and energy fluxes. With such decomposition it is possible to explore the dynamic behavior of the network and understand how these two phenomena affect to its stability. Applying Lyapunov direct method -making use of function R defined previously- it can be proved that both fast and slow dynamics are stable. The thermodynamic approach presented for the general mass transfer unit is applied to establish the stability conditions of a multi-component flash distillation under the consideration of a constant molar overflow (CMO) model. The method also extends in a straight forward manner to the analysis of multiple interconnected MTU to represent a distillation column showing that, under suitable conditions, multi-component homogeneous distillation columns also have a unique, asymptotically stable singular point.

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