445c Finding Exact Separation Boundaries in Synthesis and Design

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Separation has always been an important task in the production of petrochemicals, pharmaceuticals, food, and other commodities and products. Azeotropic, extractive, reactive distillation, and crystallization are among the most widely used techniques for product purification, the separation of chemical or biochemical intermediates, and solvent recovery. Even with the recent shift in emphasis and efforts toward unifying the physical and biological sciences, separation will remain an important workhorse in production and product/process design. The theory of residue curve maps has a long history (roughly one hundred years), has made a significant impact in the way many new separation processes are synthesized and designed, and will continue to impact the synthesis and design of new separations as industries shift their focus from process to product design. The key synthesis/design concept in this approach centers on understanding the ways in which constant boiling or constant melting mixtures (i.e., azeotropic and eutectic points) define separation boundaries. It is now well established that these azeotropes and eutectics often define curved separation boundaries for mixtures of three or more components that place strict limitations on the degree of separation that can be achieved using open evaporation or condensation. Despite this, there remains no clear and exact understanding of separation boundaries and no straightforward way of accurately computing them in practice.

The main contributions of this talk are two-fold and have widespread application in separation synthesis and design. First, a new geometric methodology is presented that shows that exact separation boundaries can be defined through the use of differential geometry and dynamical systems theory and formulated as a constrained global optimization problem. This new geometric approach to separation boundaries is rigorous and general. Second, the underlying theory is constructive and therefore leads to several practical algorithms for computing exact separation boundaries in a reliable and efficient manner. Our novel approach is based on the observation that, for ternary liquids, separation boundaries correspond to local maxima in the line integral within a given separation region. These local maxima have interesting algebraic structure and correspond to one-sided cusps. Thus, special numerical tools for the global optimization of one-sided differentiable functions are absolutely necessary since several local maxima can exist within any separation region. It is also shown that this new methodology readily extends to mixtures with four or more components by finding local maxima in surface areas, volumes, etc. and applies to reactive separations, non-equilibrium models, and other processes like crystallization and vapor degreasing. Therefore the proposed approach has widespread application in chemicals and plastics, petroleum products, pharmaceuticals, protein and other bio-separations, the cleaning of medical equipment, metallurgy, and advanced materials. Several examples of pharmaceutical separations, bio-separations, and medical cleaning will be presented, including some involving crystallization, along with results that clearly show that this new geometric approach can reliably and efficiently find exact separation boundaries. Many geometric illustrations will be used to elucidate key ideas.