OPTIMAL PROGRAMMING OF BATCH DISTILLATION: VESSEL NETWORK OPERATIONS

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***Abstract*-- This work presents an alternative structure for multivessel batch distillation and focuses on the determination of an optimal programming for it. The system is composed by a set of heated or cooled vessels connected by total reflux distillation cascades. This structure is able for separating multicomponent mixtures achieving simultaneously desirable specifications for all components, without loss of material and avoiding complex control strategies. An optimization problem is formulated in order to maximize a profit function assigned to a separation task. Transformed decision variables together with a smooth price function, are used to pose the problem according to an unconstrained form. The decision variables are the vapor molar flow rate and the operating time of each column. Batch separations of ideal quaternary mixtures are optimally programmed regarding purity specifications under fixed number of stages in each cascade and with an upper bound on the total rate of heat consumption.**

***Keywords*: Batch Distillation, Optimal Programming and Vessel Network.**

I. Introduction

The recent expansion of specialty chemical industries has led to a renewed interest in batch distillation. This may be attributed to the inherent simplicity of batch distillation and its flexibility to process small volumes. Batch distillation may be divided into single vessel and multivessel. Single vessel batch distillation includes the Batch Rectifier (BR), the Batch Stripper (BS) and the Middle Vessel Column (MVC). Hasebe et al. (1995) extended the MVC concept to a Multivessel Batch Distillation (MVBD). The MVBD uses a single reboiler and a single condenser, operating at total reflux with intermediate vessels (one per product) connected to the liquid downflow circuit of the column. The MVBD separates *Nc* components with *Nc* constant hold-up vessels, calculated from the feed composition. Wittgens *et al*. (1996) pointed that MVBDs have comparative advantages to BRs because there is no need of optimal times for slop cuts. However they mentioned that the constant hold-up policy may hinder the achievement of specifications. To overcome this, Hasebe *et al.* (1995, 1997) controlled composition by manipulating vessel hold-ups, while Skogestad *et al*. (1997) did the same by controlling column temperatures.

The object of this work is an alternative batch distillation scheme, the Vessel Network (VN). VN exhibits comparative advantages to the MVBD. The idea is to by-pass the drawbacks of the MVBD due to the fact that vessels access only *the liquid circuit*. If, for instance, a light impurity goes to a vessel rich in heavy species, it can only be removed by (slow) elution, i.e. the impurity would be protected against a (fast) expulsion by stripping. So, it is no surprise that MVBDs require maneuvers on the vessel streams to meet stringent specifications.

VNs resemble MVBD configurations, but they work differently. For ideal or non-ideal moderate systems, VN separates multicomponent mixtures achieving specifications for all components without flow rate maneuvers, loss of material or slop cuts. It operates with constant mass where heat is continuously supplied to some vessels and removed from others.

An important aspect is that VN vessels are contacted with both vapor and liquid streams, so that stripping and rectifying effects occur inside and around them. A VN is composed by a set of vessels operating with constant hold-up, arranged in a vertical planar frame (Fig. 1) interconnected by total reflux distillation cascades. Total reflux cascades establish true constant hold-up in all vessels, so each vessel must be charged with a hold-up equal to the amount of product designed to be recovered there. The network connectivity is determined by cascades, defining oriented connections according to the flow of vapor phase (arcs) between vessels (vertices). VNs can be represented as digraphs (Mah, 1990) if we choose the orientation of arcs according to the vapor flow. For global separation of a mixture there must exist at least one oriented path for vapor and liquid between any two vessels.

In general, a VN with higher degree of connectivity will accomplish a separation task in a shorter time at expenses of higher capital costs. Assuming, as a basis of reasoning, a certain level of available heating utility, an optimization problem then arises as a compromise between operational time (i.e., productivity) and capital costs. Optimal batch distillation campaigns dealing with cheap products, will probably distort the above compromise to favor the choice for simpler equipment. On the other hand, with gradual increase of the unitary separation reward (i.e. the monetary value difference