A NEW APPROACH TO DISTILLATION OF CONTINUOUS MIXTURES: MODELLING AND SIMULATION

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Abstract— Continuous Mixtures are mixtures of so many components that is no longer useful to distinguish among chemical species. Instead, an index is chosen to characterize each molecule, such as carbon atoms in each substructure, chromatographic retention time or normal boiling point and the continuity of this index is admitted. The present work aims the mathematical formulation and the simulation of a distillation column in which a continuous mixture is fed. This is performed with the assumption of a mixture of linear paraffins, in which ideal mixture hypothesis in both liquid and gas phases are reasonable. A quadrature method is employed to calculate the integrals which turns the functional-algebraic problem into a numerical one.

Keywords— Continuous Mixtures, Distillation, Quadrature Method

I. INTRODUCTION

The concept of continuity of a given mixture is applied whenever that mixture is so complex that it is no longer worthwhile to distinguish among individual chemical species; instead, an index (such as number of carbon atoms, boiling point or chromatographic retention time) is chosen to characterize each component and the continuity of the index is assumed. Mole fraction $x_i$ of species $A_i$ is replaced by $f(x)dx$, the molar fraction of material with an index in the $(x, x + dx)$ interval. Function $f(x)$ is known as the mixture distribution function (DF), where $x$ is the continuous index of the mixture. In some cases, more than one index must be used to completely characterize the continuum of species, which increases the mathematical complexity of any phenomena described with a continuous approach.

Distribution functions exhibit an obvious normalization condition given by:

$$\int_{0}^{\infty} f(x)dx = 1.$$  \hspace{1cm} (1)

Vapor-liquid equilibria (VLE) calculations for complex mixtures has been traditionally accessed through a Pseudo-Component Method, that is basically a "lumping" approach in which key components are chosen to fully characterize the whole mixture. In this way, a simple modelling procedure can be adopted, but results are highly dependent on the choice of the set of pseudo-components (Chachamovitz, 1993).

The development of the continuous thermodynamics had shown great advantages in many aspects (Peixoto et al., 2000). When applying continuous thermodynamics, a critical point is the choice of the continuous index. Some authors chose a natural identification variable, such as molecular weight or boiling point (Du and Mansoori, 1986; Cotterman and Prausnitz, 1985). However, it is sometimes difficult to relate such indices with other thermodynamic properties, especially equations of state (EOS) parameters, and fitted polynomials have been employed (Cotterman et al., 1985).

The simulation of distillation columns using a continuous approach was previously addressed by Kehlen and Rätzsch (1987) and Rätzsch et al. (1989). However, these authors employ boiling-point temperature as the continuous index, differing essentially of this work.

This work aims the modelling of distillation columns in which a continuous mixture is fed, the most important examples being paraffinic fractions of petroleum. The well-established Quadrature Method (Cotterman and Prausnitz, 1985; Peixoto et al., 2000) is employed for solving the problem. This method was considered the most suitable, once it does not show the error in material balance of the Method of Moments (Cotterman et al., 1985). The VLE is accessed through its most simple form, once paraffinic mixtures are one of the most common examples of mixture with ideal be-