Estimation of variation in Vapour Liquid Equilibrium constants for modeling a multicomponent crude distillation column

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Abstract: In this paper, the mathematical model of a multicomponent crude distillation column is investigated which aimed at predicting the concentration (mole fraction) of any component on each tray of the column. In literature, it is observed that there is a drastic up and down variations in the steady state composition profile of various multicomponent at each tray of the column. These variations are due to the assumption that Vapor Liquid Equilibrium (VLE) ratios are kept constant throughout the tray for any component and are not true in real time petroleum industries. The proposed method shows a proper procedure for choosing equilibrium constants by using an estimation technique by reverse calculation of Thomas algorithm. Hence, a reverse calculation is performed using a Tridiagonal matrix method for estimating the VLE values from the steady state composition profile for each component mixture. Further, the composition profile for various components, mainly Whole Naphtha, Straight Run Kerosene (SRK), Light Diesel Oil (LDO), Heavy Diesel Oil (HDO) and Atmospheric Residue (AR) are estimated and compared. This modified algorithm is a simple technique for ideal and non-ideal systems with ease of implementing a composition profile for a multicomponent mixture and reduction in computational complexities.

Keywords: Multicomponent, Vapor liquid **e**quilibrium, modeling, crude distillation column**.**

1. INTRODUCTION

Distillation is the process of separation of various hydrocarbons into its component parts or fractions based on the differences in their relative volatilities or boiling points. The separation is done in a large column that contains a number of trays where hydrocarbon gases and liquids interact. The liquid flow down the column and the vapor goes up (Charles, 1997). Crude oil is mainly a complex mixture of hundreds of hydrocarbons, which are fractionated in a petroleum refinery, into useful crude oil products, mainly whole Naphtha, Kerosene, diesel and different gas oil by means of fractionation. Light distillate products are the most profitable, hence the design of the atmospheric column is targeted towards maximizing the production of these lighter components. Major products extracted from the column are Whole Naphtha (130-150 $^\circ$C), SRK (140-270/250 $^\circ$C), LDO (250/270-320 $^\circ$C), HDO (320-380 $^\circ$C) and AR/Reduced crude oil (Abdullah et al., 2007 and Rosendo, 2003).

VLE parameters are important in the optimization of thermodynamic cycle. In a gas-liquid system, the main parameters include pure vapour pressure data and VLE data for mixtures. Modeling a crude distillation column with side stripper is difficult process, since the parameters are based on VLE constants as the composition profile of each component changes with variation in the VLE. Due to the strongly interacting nonlinear algebraic equations, the solution procedures are difficult and tedious. In literature the Bubble-Point (BP) and Sum-Rates (SR) methods are relatively

simple, but are limited to ideal mixtures and allowable specifications.

The Thomas algorithm uses forward elimination procedure for solving the linearized set of equations starting from stage1 to stageN. In the proposed method, same popular Thomas algorithm using the reverse calculation procedure is implemented to estimate the values of VLE from the steady state composition on each tray of the column. The models applied to the distillation column reported in Jackson et al. was calculated based on constant VLE for individual component in the column. The simulated results obtained from the composition profile of mole fractions on each tray have a drastic variation (up and downs) due to constant VLE, which is not seen in any chemical process industries (Bandyopadhyay, 2002 and Bennett et al., 2010). A smooth variation in composition profile variation of any component mixture is noticed in various industries. This is achieved by different VLE values on an individual tray of the column for any mixture. This method estimates the variability in VLE values on each tray from the steady state composition profile of each component of crude and is capable of estimating the concentration of any component of interest of the mixture on the trays of the column. The developed model predicts the composition of five components at each tray of the column.

2. MODEL DESCRIPTION

A mathematical model of a distillation column is useful in all phases of research and in development to plant operations, and also in economic studies. The design of multi component separation requires the determination of pressures,

temperatures, stream compositions, stream flow rates, and heat-transfer rates at each stage by solving energy-balance, material-balance, and equilibrium for each stage. Unfortunately, these equations are strongly interacting non-linear algebraic equations. So, solution procedure becomes difficult.

A proper model is necessary in sizing and arrangement of processing equipment for performance analysis. Although various methods are available for solving multi component separation problems, approximate methods are generally used for design to establish optimal design conditions. Also, process synthesis is studied to determine optimal separation sequences with initial approximations for rigorous, iterative methods. The mathematical model describing the separation process like distillation consists of four sets of basic equations, called mesh equations which are Mass balance equation, Equilibrium relations, Sum (or conservation) equation and Enthalpy balance relations.
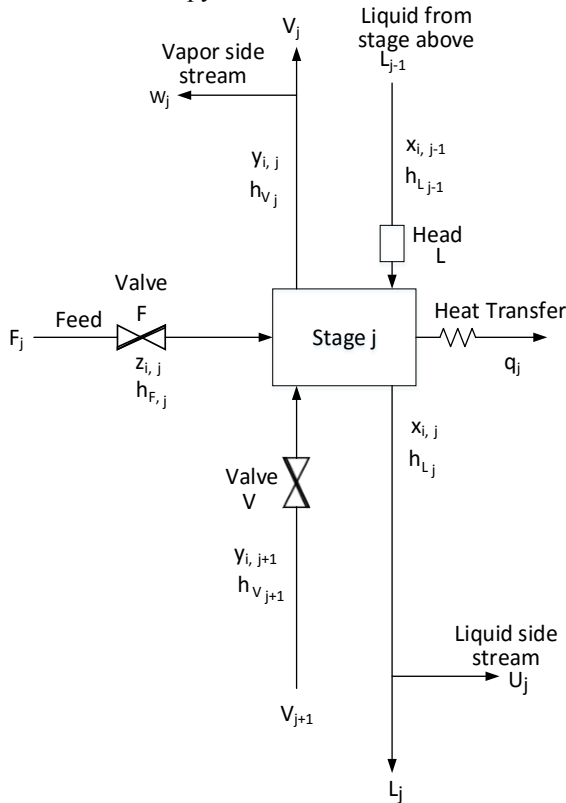

Fig. 1. General Equilibrium stage

where,

F is Feed flow rate.
$Z_{i,}$ is Composition of feed
L_j is Liquid flow throughout the column
V_j is Vapor flow throughout the column
x_j is Mole fraction of Liquid in the column
y_j is Mole fraction of vapor in the column
h_{vj} is Enthalpy of vapor in the column
h_{Lj} is Enthalpy of Liquid in the column
W_j is Side stream flow rates of the vapor
U_j is Side stream flow rates of the liquid
q_j is heat transfer

The mathematical model proposed in this paper has 48 trays numbered from top to bottom, including the condenser numbered 1 and a re-boiler numbered as 48. The liquid molar

flow L and vapor molar flow V are coming from the stage j from a VLE. The feed stream F is in the 43rd tray and vapor (SV) side stream are planned at the top tray for Whole Naphtha, 12th tray for SRK, 25th tray for LDO, 35th tray for HDO and 48th tray for AR. Normally, for obtaining the model till now the value of vapor liquid equilibrium ratio is considered to be constant.

Fig. 1, represents vapor liquid equilibrium case where the trays are numbered from top to bottom. Feed of molar component is entering stage j with a flow rate F_j, with composition $z_{i,j}$ in mole fractions of component i and molar enthalpy h_{Fj}.

2.1 Assumptions

- To obtain the model reported in Jackson et al., a 48 tray column model is chosen.
- The residence time on each plate is such that equilibrium is attained between the liquid and the vapour. Hence $Yn = Kn * Xn$
- The flow rate of the side streams is equal to the flow rate of the reflux which is assumed from Seader, J.,(2011)
- From the example 10.1, sighted in Seader, J.,(2011) the reflex ratio is considered to be 2.
- The flow rate of the vapour throughout the column is considered to be the summation of the three side streams and reflux of the three side streams. i.e.,
  $V_j = W_{12} + W_{25} + W_{35} + $ reflex ratio$*(W_{12} + W_{25} + W_{35})$.
- The liquid flow rate is also considered to be constant throughout the column.
- The mass balance doesn't match for the inflow rates and out flow rates reported in Jackson et al,. Hence by considering only the feed flow rate and the feed compositions new values of side streams are calculated and liquid flow rate are calculated.
- With reference to Jackson et al., only vapour side streams are present. The liquid side stream flow rate is zero.

2.2 Process variables

Generally, for obtaining the model reported in Jackson et al., the values of VLE ratios are assumed to be constant for each component of the tray column. But, the values of VLE will change tray by tray for every component mixtures in the column. Hence, in this work, an algorithm is implemented to determine/estimate the VLE ratios at each tray using reverse calculation in Tridiagonal method developed by Thomas algorithm. Using this new proposed algorithm the sudden rise and fall in composition profile is minimized.

Similarly, in stage j the liquid from the above stage L_{j-1} is also entering from the top tray with the composition $x_{i,j-1}$, in mole fractions and similarly from stage j+1, the vapor V_{j+1} is also entering from the bottom of the tray with the composition $y_{i,j+1}$, in mole fractions. Leaving stage j is the vapor V_j and liquid L_j with mole fraction compositions $y_{i,j}$ and $x_{i,j}$ respectively. This stream can be divided into a vapor side stream of molar flow rate W_j and an interstage stream of