A STUDY ON MATHEMATICAL MODELLING OF DISTILLATION COLUMN IN A PETROLEUM PROCESS

Er. Ravi Baliyan[1], Akram Taher Ahmed Ali Al Zubidai[2]

[1]*Assistant Professor, HOD, Dept. of Petroleum Technology, Bhagwant University, Ajmer*
[2]*M.Tech Scholar, Petrochemical Engineering, Bhagwant University, Ajmer*

ABSTRACT

The aim of this paper a study on Mathematical Modelling of Distillation Column. This paper introduces a calculation procedure for modeling and control simulation of condensate distillation column based on petroleum process. Most distillation control systems, either conventional or advanced, assume that the column operates under a constant pressure. Pressure fluctuations make control more difficult and reduce performance. The petroleum process behavior of distillation columns can be described strictly by a set of algebraic equations. The distillation column is said to contain a known number of trays. The mass balance and overall mass and energy balance on each component on each tray give rise to a set of algebraic equations that can be solved simultaneously to obtain the dynamical behavior. In this paper, modeling and simulation are completed in three stages: the basic nonlinear model of the plant, the full-order linear model, and the low-order linear model. In this paper, calculations and simulations are implemented using the MATLAB (version 7.0) software package.

Keyword: - *PP, Industry, Control, Strategies, Distillation Column etc.*

1. INTRODUCTION

Petroleum Refining Processes Chemical engineering processes and conversion of crude oil into petroleum refineries (also known as oil refineries) into useful products such as liquefied petroleum gas (LPG), gasoline or petrol, kerosene, jet fuel, diesel oil Is used for. And fuel oil. [1] [2] [3] Petroleum refineries are very large industrial complexes consisting of many different processing units and ancillary facilities such as utility units and storage tanks. Each refinery has its own unique arrangement and the combination of refining processes is largely determined by the refinery location, desired products and economic considerations. Some modern petroleum refineries process between 800,000 and 900,000 barrels (127,000 to 143,000 cubic meters) of crude oil per day. In recent years, the interest of process engineers in the control of industrial processes has increased. Due to the widespread application of distillation in the process industry, effective control of distillation columns has gained immense importance. Several advanced control strategies are available to improve the control of distillation columns, but to properly implement these control schemes, it is important to understand the dynamic behavior of the columns. A lot of work has been done in this area using digital computers and several models have been developed to describe the unstable state behavior of distilled columns. The trend is towards better predictability of mobility. This study attempts to continue that trend. The first mathematical model of dynamic behavior of distillation columns was proposed in 1947 by Marshall and Pigford (17). He considered the inclusion of columns by interconnecting equilibrium means by currents. Material balance was made on each tray for each component. The drawback of the model was that for a simple column with a low number of trays, there were many differential equations to solve simultaneously. Further work using the tray-by-tray model was done by Peiser and Grover, who simulated the dynamics of a multiplexing. Distillation columns with flooding trays near the bottom of the tower. Wagner and Holland had developed a column model using a similar approach but assuming that the potential of the plate was known. A generalized model that takes into account the effect of hydraulics and mixing on the tray was presented by Tetlo. Morris and Svrcek, in response to the inability of traditional equilibrium means to handle absorbing and discrete problems, developed a distillation tray model based on a mass transfer approach. The model was tested with data obtained from a 75-stage industrial distillation unit, but the general application of this model to other columns still requires prior knowledge of the mass transfer characteristics of the components. In a distillation process, the liquid and vapor flowing counter-

current come into continuous contact on a series of trays. The complexity of the process can range from a simple column with a single feed and two product streams to multiple feed streams, multiple side and product streams, and non-ideal reactive chemical species on all trays. Rigorous modeling of such a process requires simultaneous treatment of material balance equations and energy balance equations. In North America, the first oil well was drilled in 1858 in Ontario, Canada by James Miller Williams. In the United States, the petroleum industry began in 1859 when Edwin Drake found oil near Titsville, Pennsylvania. [4] The industry developed slowly in the 1800s, mainly producing kerosene for oil lamps. In the early twentieth century, the introduction of internal combustion engines and its use in automobiles created a market for gasoline that was the inspiration for the fairly rapid development of the petroleum industry. Early discoveries of petroleum such as those in Ontario and Pennsylvania were soon ruled out by large oil "booms" in Oklahoma, Texas and California. [10] (Source: Jaspal Singh Sabharwal, 1991)

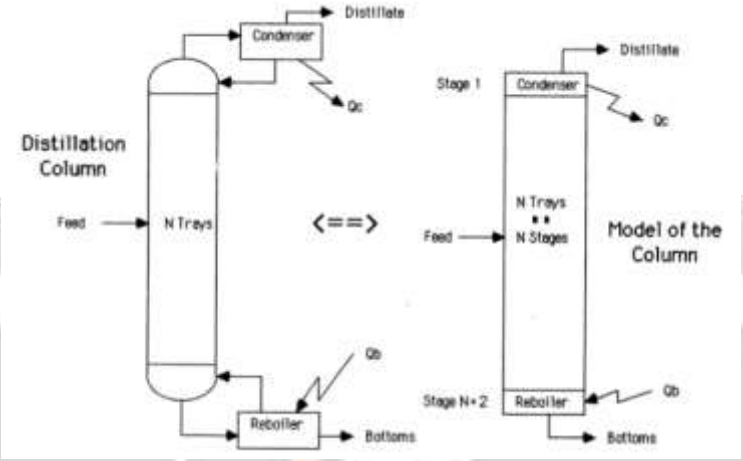


Figure 1.1: A Distillation Column and 1ts Equivalent Model (**Source:** Jaspal Singh Sabharwal, 1991)

2. PROCESSING UNITS USED IN REFINERIES

- Crude Oil Distillation Unit: Distributes crude oil to other units in different degrees for further processing.
- Vacuum distillation unit: Separates the residue oil from the bottom of the crude oil distillation unit. Vacuum distillation is performed at a pressure below atmospheric pressure.
- Naphtha Hydrotreatment Unit: Uses hydrogen to remove naphtha fraction from crude oil distillation or other units within the refinery.
- Catalytic Reforming Unit: Converts reflexed naphthal molecules into high-octane molecules to produce an improvement, a component of the end-product gasoline or petrol.
- Alkylation unit: Converts isobutane and butenase to alkylate, a very high-octane component of end-product gasoline or petrol.
- Isomerization Unit: Converts linear molecules into high-octane branched molecules such as common pentane for blending into end-product gasoline. In addition linear normal butane is converted to isobutane for use in an alkaline unit.
- Distillate Hydrotreaty Unit: Uses hydrogen to extract some other distilled fractions from a crude oil distillation unit (eg diesel oil).
- Merox (mercaptan oxidizer) or similar units: LPG, kerosene or jet fuel by oxidizing undesired mercaptans into organic disulfides.
- Amine gas turet, claus unit and tail gas treatment to convert hydrogen sulfide gas from hydrocreators to end-product element sulfur. The majority of the 64,000,000 metric tons of sulfur produced worldwide in 2005 was the production of sulfur from petroleum refining and natural gas processing plants. [11] [12]
- Fluid Catalytic Cracking (FCC) unit: Upgrades crude oil distillation by converting heavier, higher-boiling fractions into lighter and lower-boiling, more valuable products.

- Hydrocracker Unit: Uses hydrogen to upgrade heavier fractions from crude oil distillation and heavy distillation units to lighter, more valuable products.
- The Viscoer unit upgrades heavy residual oils from the vacuum distillation unit into a thermometer by cracking into lighter, more valuable low-viscosity products.
- Delayed coking and liquid coking units: convert very heavy residual oils into end-product petroleum coke as well as naphtha and petrol oil by-products.

3. SOLUTION METHOD FOR THE SYSTEM OF LINEAR AND NONLINEAR ALGEBRAIC EQUATIONS

Large sets of algebraic equations must be solved at each time step of the simulation when implementing the integration algorithm. For a distillation column with no PumaRide, the coefficient matrix structure of these algebraic equations is triangular in structure, and the system of equations can be solved very efficiently with the Thomas algorithm. Suppose the system of equations is

$A_{nxn} \cdot X_{nx1} = d_{nx1}$

Where A is the coefficient of triad is matrix

lower diagonal elements a_k k = 1,2, ... ,n-1

diagonal elements b_k k = 1,2, ... ,n

upper diagonal elements c_k k = 2,3, ... ,n

and x and d are nx1 vectors.

According to the Thomas algorithm, the equations can be directly solved as follows

$A_1 = b_1$

$B_1 = d_1 / A_1$

$C_k = b_k - (a_k c_k\text{-}1)/C_{k-1}$ k= 2, .. ,n

$D_k = (d_k - a_k C_{k-1})/ak$ k = 2, .. ,n

and finally,

$x_n = Bn$

$x_k = Bk - (c_k x_{k-1})/C_k$ k=n-1, .. ,1

4. SOLUTION METHOD FOR SYSTEM OF ALGEBRAIC EQUATIONS

The calculation of liquid and vapor fluxes for the case of continuous molar holdup involves the solution of two sets of algebraic equations, namely mass balance and energy balance on each tray. Since the coefficient matrix is not trinomial, the Thomas algorithm described in the previous section does not apply. For this case, the Gauss Sedale iteration method is used. This method requires reasonable initial estimates of the variables being calculated. However, this is not a problem because the values from the last time step can be used as an initial estimate. Consider a set of equations

$f_l(x_2,x_3, ... ,x_n)=0$

This set of equations can be transformed to

$x_l = F_l(x_2,x_3, ... ,x_n)$

$x_2 = F_2 (x_1 ,x_3 , ... ,x_n)$

$x_3 = F_3(x_l,x_2,x4, ... ,x_n)$

.....

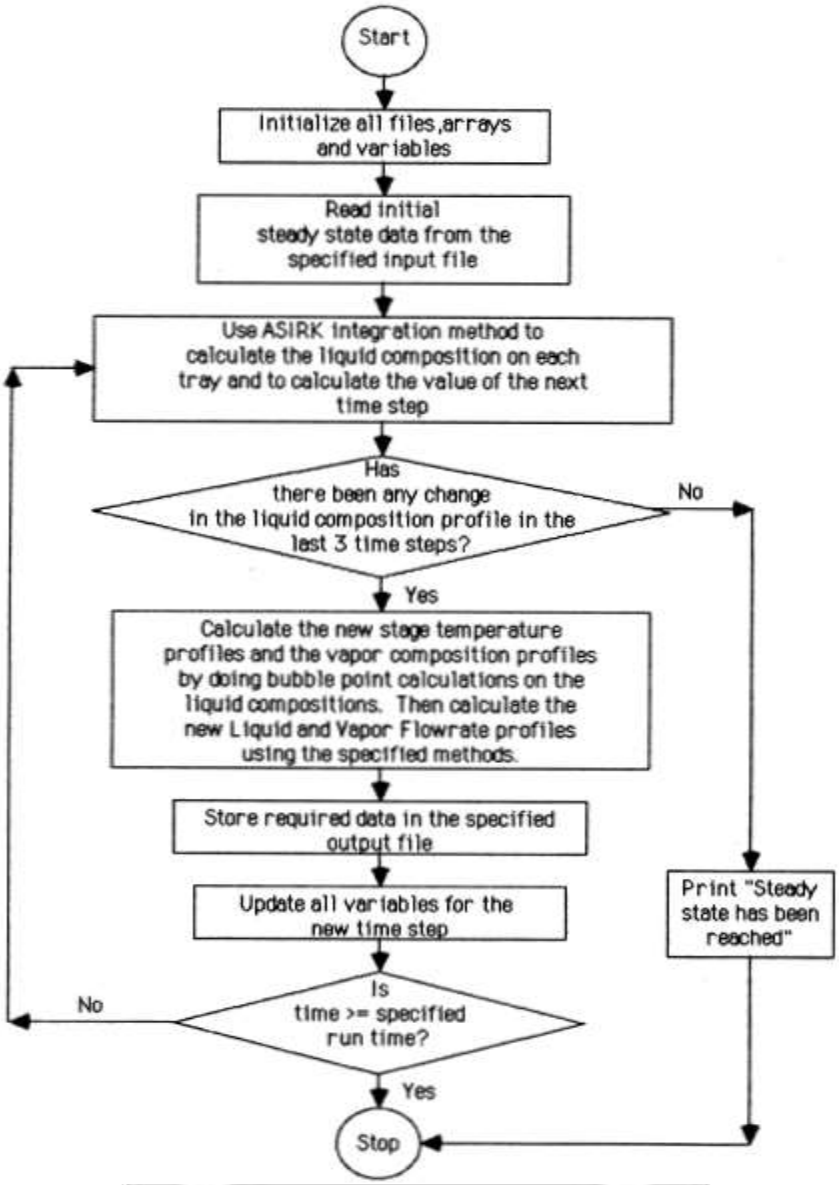
.....

.....

$x_n = F_n(x_l,x_2,x4, ... ,x_{n-1})$

The new value of x_1 is calculated from the equation, using initial estimates of x_2, x_3, .., x_n. This value of x_1 and the initial estimates of x_3, x_4 .., x_n are used to calculate the new value of x_2 from the equation. This process continues with all the equations, Recursively, until the values of x_l, x_2, · · ·, x_n are stabilized within a specified tolerance. It is worth noting here that the latest estimate of the variable is always used.

Flowchart of the simulation algorithm(Source: Jaspal Singh Sabharwal, 1991)



(Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

5. PROCESS MODEL AND SIMULATION RESULTS

The feed can be considered as a pseudo-mixture of ligas iso-butane, n-butane and propane and naphthas iso-pentane, n-pentane and higher components. The column is designed with N = 16 trays. The model is simplified by combining some components with pseudo components and modeling the dynamics of the column is based only on these pseudo components (3). (Source: Vu Trieu Minh and Ahmad Majdi Abdul R

(Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

$$y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n},$$

Where x_n is the liquid concentration at nth stage; y_n nth is the vapor concentration at the stage; α is relative volatility.

Table 1.1: The main streams (Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

Stream	Condensate	LPG	Raw gasoline
Temperature (^{0}C)	120	48	154
Pressure (atm)	5.8	5	5.8
Density (kg/m^3)	680	590	730
Volume flow rate (m^3/h)	24.68	9.67	22.90
Mass flow rate (kg/h)	16580	5162	11406
Plant capacity (ton/year)	140000	44000	88000

Table 1.2: The steady state values of concentration s x_n and y_n on each tray. (Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

Stage	Bottom	Tray 1	Tray 2	Tray 3	Tray 4	Tray 5	Tray 6	Tray 7
x_n	0.0375	0.0924	0.1561	0.2121	0.2475	0.2630	0.2712	0.2742
y_n	0.1824	0.3666	0.5142	0.6142	0.6458	0.6685	0.6777	0.6821
Stage	Tray 8	Tray 9	Tray 10	Tray 11	Tray 12	Tray 13	Tray 14	Distillate
x_n	0.2842	0.3166	0.3944	0.5338	0.7141	0.8453	0.9372	**0.9764**
y_n	0.6895	0.7285	0.7876	0.8670	0.9341	0.9689	0.9891	0.9985

Table 1.3: Product quality based on changes in feed rates(Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

	Purity of the distillate product x_D (%)	Impurity of the bottoms product x_B (%)
Normal feed rate	97.56	4.85
Reduced feed rate 10%	91.25	0.88
Increased feed rate 10%	98.35	12.88

6. LINEARIZATION OF THE DISTILLATION PROCESS

To derive a linear control model for this nonlinear algebraic system, we assume that the variables diverge only slightly from certain operating conditions (10). The non-linear algebraic equation can then be extended into Taylor's series. (Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

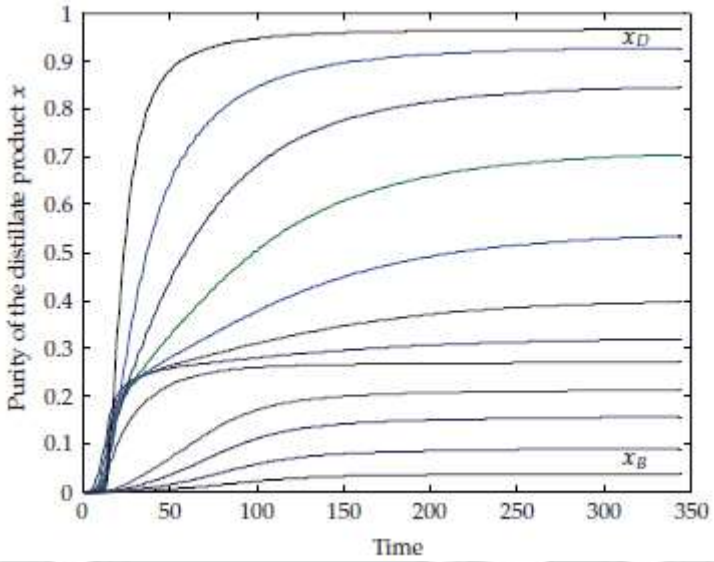


Figure 1.1: The steady-state values of concentrations *xn* on each tray. (Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

We assume that the low-order linear model can also maintain stable output, similar to the basic stationary model.

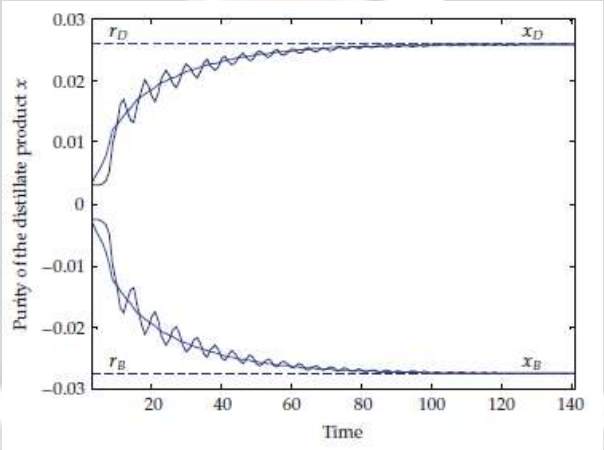


Figure 1.2: Correlation of plant outputs, model outputs, and reference setpoints. (Source: Vu Trieu Minh and Ahmad Majdi Abdul Rani, 2009)

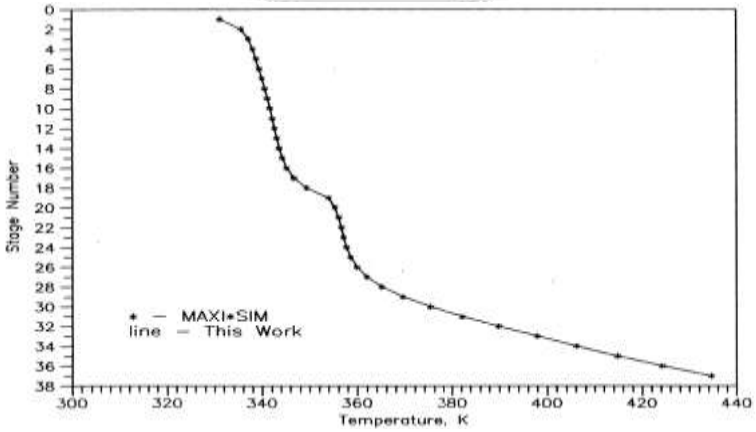


Figure 1.3: Depropanizer Tray Temperature Profile Comparison(Source: Jaspal Singh Sabharwal, 1991)

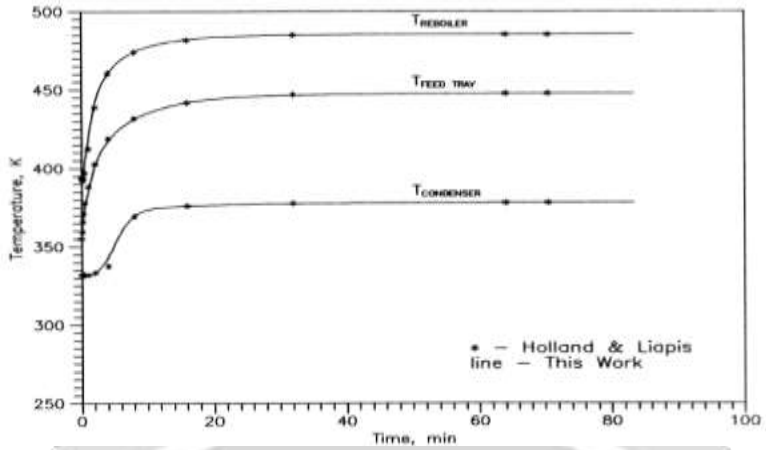


Figure 1.4: Temperature Profile Comparison(Source: Jaspal Singh Sabharwal, 1991)

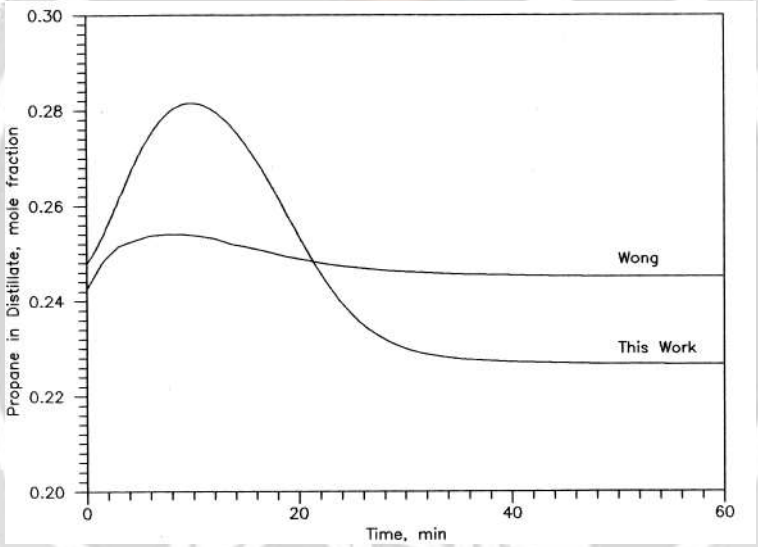


Figure 1.5: Response of Distillate Propane Composition to a 10 Percent Increase in Reboiler Duty(Source: Jaspal Singh Sabharwal, 1991)

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