A Hybrid Approach to Reconstruct a Complete TBP Curve from Blended Gas Condensates

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Successful operations of a natural gas condensate fractionation unit requires the feed's True Boiling Point (TBP) curve to be reconstructed and its' bulk properties to be predicted. In this work, a hybrid approach combining the Generalized Distribution Model (GDM) and Pseudo-component Linear Equation (PcLE) methods are proposed. The proposed method is simple and requires limited information from readily available laboratory analysis data. The method was demonstrated using a refinery case study and found that the hybrid approach were able to reconstruct a pure component TBP curve from the blended feed data with error of less than 5%. Consequently the approach is very useful during preliminary stage for refinery engineers to explore and exploit the operational flexibility in a current distillation column to maximize the desired product yields.

KEYWORDS: crude blend; pseudo-component; condensates; refinery; distillation.

INTRODUCTION

Condensate Fractionation Unit (CFU) is the front-end unit operations in a refinery to process the incoming natural gas condensates feed (C5+) into a range of petroleum products. Condensates are separated into several fractions according to boiling point ranges. The typical petroleum products include LPG, naphtha and kerosene. Raw materials cost makes up the largest proportion or about 90% of the overall refinery input cost (Li et al., 2005). Therefore, the selection of which condensate to process is of primary importance to the refiners. Different feed yields different products palate. In addition, competitive markets, stringent environmental laws and regulations, high crude prices, and advancement in process design technology, have all driven refiners to deploy

process optimization on their unit operations. The main input to process optimization is feed distillation data (Li et al., 2005). Mathematical methods such as linear programming (LP) are used to optimize the current unit operating parameters to maximize profitability while achieving the desired product yields and the required properties (Prakash, 2003). Towards this end, analysis and characterizations of refinery feedstock become crucial for refineries because deviation in bulk properties would affect the qualities and specifications of the petroleum products.

Condensate Characterization

Condensates, like crude oil and other petroleum fractions, are complex hydrocarbon mixtures. Determining the exact composition of crude oils and heavy condensates is not possible. Instead it is sufficient to characterize them in bulk properties such as Reid vapor pressure (RVP), flash point and pour point. The characteristics can also be defined graphically using true boiling point (TBP) curve. Other properties, such as molecular weight (MW), specific gravity (SG) and viscosity may also be determined as specific cumulative volume or mass percentage. All these properties are defined as the condensate distillation curves. SG and MW are commonly supplied as "bulk properties" which are measured for the overall petroleum sample. These boiling curve measurement and bulk properties are then related to the physical properties of the condensates using correlations. For example, the two-parameter empirical equation by Riazi and Daubert (1980) uses TBP and SG to predict other properties of the petroleum fraction such RVP for volatile products and kinematic viscosity (Kvis) for heavy distillates. Other options for properties prediction may include the use of MW, refractive index and carbon to hydrogen weight ratio (Riazi, 2005).

current Methods to Reconstruct TBP Curves

TBP curves and other distillation data are naturally non-linear. Accurate reconstruction of a TBP curve is difficult due to lack of knowledge about the functional form of the underlying equations (Eckert and Van ek, 2005). A conventional method to predict properties of the distilled fraction is the Narrow Cut Method (NCM). NCM uses the concept of pseudo components and involves iterations until the property of the desired component is reached (Prakash, 2003). With the advancement of mathematical modeling, linear regression and linear recursion modeling have been widely used. Riazi (1997) developed characterization of C7+ fractions from crude oil to reconstruct the complete TBP curve. Generalized distribution model (GDM) is the most versatile model that can be applied to all major characterization parameters as given below.

$$P = \left[\frac{A}{B}\ln\left(\frac{1}{x_c}\right)\right]^{\frac{1}{B}}$$

In Eq. (1), *P* is a desired property, such as TBP, molecular weight (M), or specific gravity (SG). Moreover, x_c is the cumulative fraction of interest such as weight, mole, or volume fraction, while A and B are correlation coefficients. Other works that have been developed are the Molecularly Explicit Property Prediction (MEPP) model (Albahri, 2006), and the utilization of a substitute mixture of real components in the simulation of crude oil processing (Eckert and Van^{*}ek, 2005). Other rigorous modeling tools are also available on commercial software such as Petro-SIM from KBC Advanced Technology and Aspen HYSIS[®] From AspenTech Inc.

The commonly used technique to reconstruct feed TBP curve is by using distillate products data followed by data reconciliation on a commercial process simulator. Moreover, high end analytical equipment, like gas chromatograph, infrared spectroscopy, and nuclear magnetic resonance spectroscopy, have also been used to performed direct analysis of feed TBP curve and the properties of petroleum products.

Problem Statements

The deviation in condensate feed properties would affect the qualities and specifications of the distilled fractions leading to final products give away. Reconstruction of feed TBP curve and bulk properties is important to ensure optimum operations of the refinery. There is a trade-off between accuracy and complexity of methods used. However, the lack of a simple, low cost yet accurate method has led many refiners to operate their CDUs and CFUs based on experience or based on operating parameter recommended by consultants during detailed design stage.

PROPOSED METHOD

A new method employing Pseudocomponent Linear Equation (PcLE) is proposed to

(1)

reconstruct the TBP curves and predict selected bulk properties of pure components in blended feed. A non-linear TBP curve and bulk properties distribution in condensate or other petroleum fractionates are considered as a build-up up from a series of pseudo-components, which are linear within specified boiling range of temperature cuts. For example, Figure 1 shows a typical TBP curve of pure condensate. If this non-linear TBP-curve is divided into smaller boiling ranges, it becomes possible to develop simple linear equation of each pseudo component. The linear relation or PcLE is found by calculating the gradient, m, and constant, c, as given in eq. (2) below.

$$y_i = m_i x + c_i \tag{2}$$

In the above equation, y_i is the TBP of ith pseudo-component at *x* mass fraction. When all the PcLEs are combined and arranged into a composite curve of cumulative mass fraction, then a complete non-linear TBP curve for a particular condensate or petroleum fraction can be reconstructed as illustrated in Figure 2. Any overshooting of PcLE beyond the specified boiling range is removed from the composite curve.

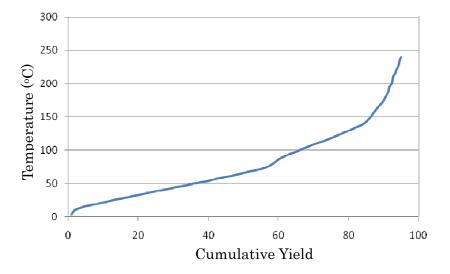


Figure 1. True Boiling Point (TBP) Distillation Curve

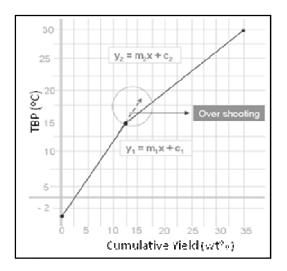


Figure 2. TBP reconstruction through PcLE composite curve

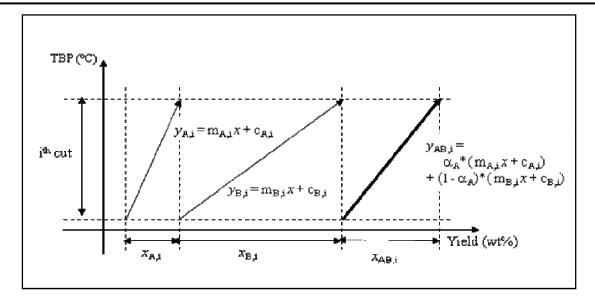


Figure 3. A composite curve of blended PcLE at specified cut points

When two or more condensates or petroleum fractions are blended as a crude feed to a separation unit, the resulting feed TBP curve and bulk properties are weighted against the blending ratio of the mixtures. This is given as follows:

$$\mathcal{Y}_{i,j\dots n=\sum_{j=n}^{j=1}\alpha\times(mx+c)_{ij}} \tag{3}$$

Where $i = i^{th}$ pseudo-component, j is condensate type {j=1, 2, 3, ...,n,} and \boxtimes is the blending ratio. It is worth to note that the specific gravity (SG) is linear additive and assumed constant within the boiling ranges is constant. Figure 3 shows the reconstruction of blended PcLE at a specified cut point.

The proposed method can also be used to predict pure condensate TBP from the blended feed. The TBP and bulk properties distribution of pure condensate can be determined if the blending ratio of each pure condensates of the blended feeds are known. For example when two PcLEs are combined, the individual equation can be determined if two sets of mixed ratios are known. Consider the following illustrations:

Let $y'_{12} = m'_{12}*x + c'_{12}$ at α blending ratio and $y''_{12} = m''_{12}*x + c''_{12}$ at β blending ratio. As a result, m_1 and m_2 can be calculated by,

 $m_1 = m'_{12} + (m''_{12} - m'_{12}) * (1-\alpha)/(\beta - \alpha)$ and

$$\begin{split} m_2 &= m'_{12} + (m''_{12} - m'_{12}) * (-\alpha)/(\beta - \alpha) \\ \text{Similarly for constant } c, \\ c_1 &= c'_{12} + (c''_{12} - c'_{12}) * (1 - \alpha)/(\beta - \alpha) \quad \text{and} \\ c_2 &= c'_{12} + (c''_{12} - c'_{12}) * (-\alpha)/(\beta - \alpha) \end{split}$$

Furthermore, for the known blended condensates TBP curve at two different feed blending ratios, the model is capable to reconstruct an accurate TBP curve of pure condensates and predict the properties of the pure condensates as well. The algorithms of PcLE method to predict pure condensates TBP curve and bulk property distribution from blended feed is given in the Appendix.

Case Study – Feed TBP Curve for CFU

A case study was carried out on Condensate Fractionating Units (CFU) at a local refinery complex. A schematic diagram of CFU is shown in Figure 4. Two condensates, Bintulu Condensate (BNC) and Terengganu Condensate (TNC), are blended prior to entering the condensate tower. The top product is sent to the condensate stabilizer while the bottom product is sent to the crude distillation unit (CDU). A side-stream heavy naphtha product from the condensate tower is sent to the product blending unit. Typical blend fractions comprising 100% BNC (α =1.0) and 50% BNC (α =0.5) were used in this case study.

The lab result for all distillate products are

reported in ASTM distillation. A conversion of ASTM to TBP was carried out using the method by Daubert (1994). The whole range feed TBP curves at α =1.0 and α =0.5 were reconstructed using GDM (Riazi, 1997). The whole range Feed TBP curve was divided into pseudo-components each with a step of 10°C boiling range. The slope and constant of linear equation for each pseudo-component at α =0.5 and α =1.0 were further calculated. Finally, the series of linear equations at the unknown pure TNC feed (i.e. α =0) was further solved using Gaussian Elimination method (Kreyszig, 1999).

The reconstructed and laboratory analysis of TBP curves for BNC and TNC are compared in Figure 5. The discrepancies between the analytical and the modeled values were measured using standard deviation (%D) and absolute average deviation (%AAD) as shown in Table 1.

The results showed that %AAD for BNC and TNC are 5.22% and 6.07%, respectively. The desired product in this case is side-stream heavy naphtha from condensate tower. From historical runs, the average product boiling range is between 70°C and 170°C. Based on the laboratory TBP curve, the product yield is lying between 35% and 85% and between 50% and 90% of the cumulative volume fraction for BNC and TNC, respectively. Therefore, by discounting the data for cumulative volume <30% and >90%, as illustrated in Figure 5, the %AAD for both BNC and TNC is 2.7% and 4.55% respectively. The results demonstrate that the method proposed in this study is simple, low cost and capable to reconstruct TBP curves with sufficient accuracy within practical operation range.

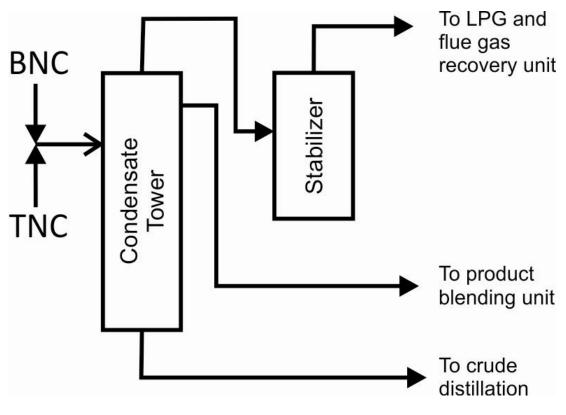


Figure 4. Condensate Fractionating Unit (CFU)

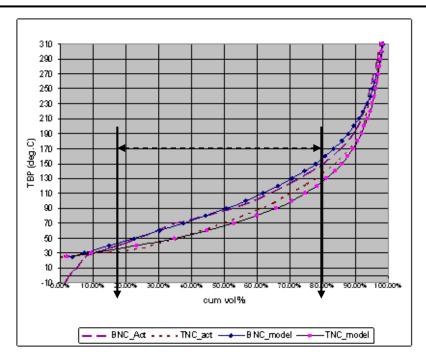


Figure 5. Reconstructed Pure TBP curves

Table 1. Error Analysis of the Reconstructed TBP C	Lurves
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	BNC			TNC		
cum						
yield (%)	TBP_{Assays}	TBP_{model}	[% D]	TBP_{Assays}	TBP_{model}	[% D]
10	29.83	33.81	13.34	29.06	29.91	2.92
30	60.96	59.81	1.88	43.44	45.37	4.44
50	86.67	89.04	2.73	71.02	66.69	6.10
70	123.00	128.35	4.35	108.94	99.75	8.44
90	194.31	203.11	4.53	179.07	172.36	3.75
95	257.85	246.34	4.46	244.79	218.86	10.59
		%AAD	5.22		%AAD	6.07
		Practical	2.70		Practical	٨٢٢
		%AAD*			%AAD*	4.55

*excluded data from 10% and 95% cumulative yield fractions

CONCLUSIONS

A hybrid approach combining Pseudocomponent Linear Equation (PcLE) and the Generalized Distribution Model (GDM) methods have been proposed to reconstruct TBP curves for condensates. A case study on CFU feeds showed that the hybrid approach were able to reconstruct a pure component TBP curve from the blended feed data with error of less than 5%. The discrepancy can be reduced further with increasing accuracy of feed and distillate products flow rates measurements. The proposed hybrid approach would be useful to refinery planners and engineers to screen opportunities for profit improvement. The inputs can be extracted from readily available databank. Despite its simplicity and low-cost, the accuracy of the results from the hybrid approach is sufficient enough to match other results obtained from commercial software or expensive on-line analyzers.

REFERENCES

- Albahri, T.A. (2006), Enhanced Method for Predicting the Properties of Light Petroleum Fractions, *Fuel*, 85, 748–754.
- Daubert, T.E (1994), Petroleum Fraction Distillation Inter Conversion, Hydrocarbon Processing, 73(9) 75 - 78.
- Eckert, E. and T. Van ek (2005), New Approach to the Characterisation of Petroleum Mixtures used in the Modelling of Separation Processes, *Comp. Chem. Eng.*, 30, 343–356.
- Kreyszig, E. (1999), Advance Engineering Mathematics, Singapore, *John Wiley*.
- Li et al., (2005), Integrating CDU, FCC and product blending models into refinery planning, *Comp. Chem. Eng.*, 29, 2010–2028.
- Prakash, S. (2003), Refining Processing Handbook, Amsterdam, *Elsevier*.
- Riazi, M.R. (2005), Characterisation and properties of Petroleum Fraction, *ASTM annual series*.
- Riazi, M.R. (1997), A Distribution Model for C7+ Fractions Characterisation of Petroleum, Ind. Eng. *Chem. Res.*, 36, 4299-4307.
- Riazi, M.R. and T.E. Daubert (1980), Improved Characterization of Wide Boiling Range Undefined Petroleum Fractions, *Industrial and Engineering Chemistry Research*, 26(3), 629-632