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Characterization of crude feed and products from operating conditions by using continuous probability functions and inferential models

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Abstract−The purpose of this paper is to provide information for the characterization of the products and feed of a crude fractionator, hard to get from a hardware system, by using probability function and inferential model of real-time operating conditions. TBP is a major characteristic of CDU products and feed. It has become possible to consider that the TBP of component can be predicted by using an inferential modeling technique such as partial least square (PLS) or artificial neural network. On the other hand, knowing that the characteristic of each product of a crude distillation unit follows a continuous probability distribution function, variables of the probability distribution function can be calculated from operating conditions in the same way. In general, the proposed model can provide a tool for doing more efficient operations to maximize profit.

Key words: TBP, Crude Characterization, Petroleum Crude, Probability Distribution Functions, Inferential Model

INTRODUCTION

Characteristics of feed can be utilized for the production and control strategy that all products meet their quality target so as to maximize the profit. Many approaches have been proposed to control the crude product qualities. Friedman [1994] proposed model-based control of crude product qualities by using simplified heat-balance equations for estimating the crude TBP curve. But the model under-predicted crude TBP by about 5%. Model predictive control (MPC) technology and neural network models were commonly used by a number of researchers for the optimum product control [Zhu et al., 1997; Friedman, 1994]. Other related researches were done by Dhaval et al., 2002; Kumar et al., 2001; Chatterjee and Saraf, 2003; El-Hadi et al., 2005 and Hwang et al., 1995. On-line analyzers can be strategically placed along the process vessels to supply the required product quality information to multivariable controllers [Chen et al., 1998; Kresta et al., 1991]. However, on-line analyzers are very costly and are limited to maintain the product specification.

In this paper, a method to identify the feed and product is proposed that is able to provide the information for down-stream scheduling, production, and control. Two key ideas are used to identify the feed characteristic as a real time basis. The first is that the characteristic, TBP of component of feed and products, follows a specific probability function. The other is that the variables of the function can be correlated with operating conditions by using an inferential modeling technique such as partial least squares regression analysis.

PRODUCT CHARACTERIZATION AND PROBABILITY DISTRIBUTION FUNCTION

Generally, there are several products coming out of the CDU (Crude Distillation Unit) such as LPG, Naphtha, Light Kerosene (LK), Heavy Kerosene (HK), Light Gas Oil (LGO), Heavy Gas Oil (HGO), Residue Crude (RC). Each product has its own specification such as boiling point range, and the specifications are controlled by the operating conditions. TBP is a major characteristic of CDU products and feed. Product TBP range of a particular crude feed is shown in Fig. 1 and TBP curves for each of its product are shown in Fig. 2.

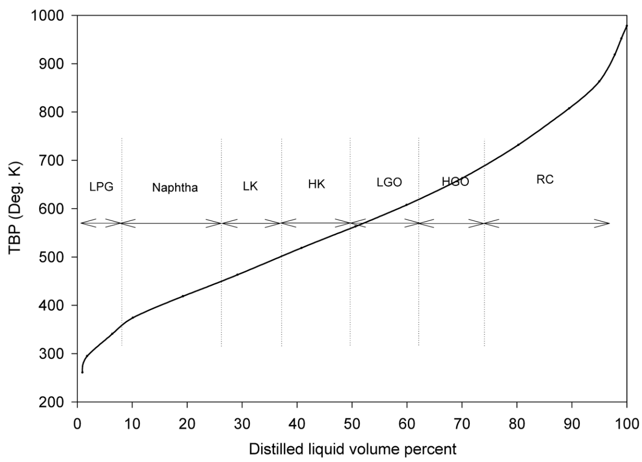

Fig. 1. TBP range of a crude oil for each product.

Probability distribution functions of TBP of products in the specific CDU are shown in Figs. 3 and 4. The laboratory TBP data and crude assay used in Figs. 3 and 4 were supplied by one of the major oil companies in Korea, and the simulation data from crude assay for CDU products are generated by our research team; these data are also used in these Figs. 3 and 4. Crude unit always possesses a high degree of inherent flexibility for the operation of the unit. Nevertheless, there has been always motivation to improve the accuracy of calculation methods not only to further reduce the possibility of a serious performance problem, but also to give a greater degree of

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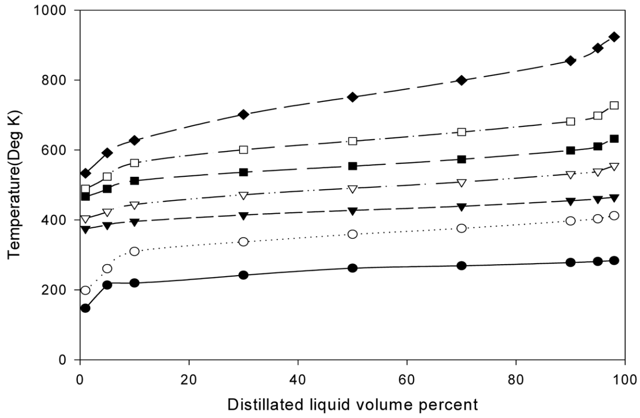

Fig. 2. TBP curve for CDU products of a crude oil.

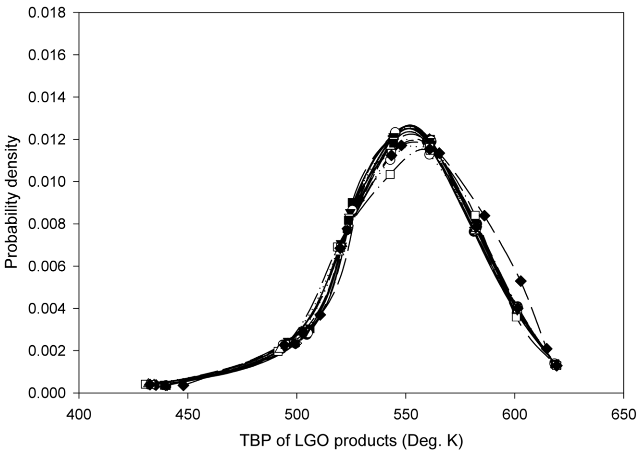

Fig. 3. Probability density of LGO products.

confidence in developing process designs, equipment specifications and performance guarantees. As shown in Figs. 3 and 4, CDU products can be represented well with a continuous probability distribution function in terms of TBP. Therefore, utilization of a general probability function to TBP vs. distilled liquid volume percent (LV %) of products is able to improve the predictive capabilities of the CDU process.

In this paper, two probability functions are used to represent the TBP data of products. One is Hill's probability equation and the other is developed in the course of our research and proposed here. These functions can be expressed by the integrated form of probability distribution function. Hill's probability equation can be written as the following.

$$D(\text{Distillate},\%)=100/((T_H/T)^{B_H}+1) \tag{1}$$

where T_H stands for average and B_H stands for variance of the function for each product. T is true boiling temperature. The other equation can be introduced to a following case. Knowing the end boiling point for each product and variance for each product cut, the production and control strategy for all products can be efficiently utilized. In doing so, the following probability function is developed by trial and error.

$$D(\text{Distillate},\%)=100/\exp((T_L-T)/B_L)^2, (T_L>T) \tag{2}$$

where T_L stands for end boiling temperature of each product and B_L stands for variance of each product cut. T is true boiling temperature. Distribution function for each product has two parameters: T_L and B_L. So T_H and B_H, at Eq. (1) or T_L and B_L at Eq. (2) parameters can be used for TBP identification of each distribution of products also feed. In the petroleum industry, the desired product specifications of TBP of products can also be used such as TBP_{50}, temperature at 50% distillate, and TBP_{90}, temperature at 90% distillate. In Eqs. (1) and (2), it is clear that D=50 when T equals to TBP_{50}, a temperature at 50% distillate, and D=90 when T equals to TBP_{90}, a temperature at 90% distillate. As a result, parameters of Eq. (1) and (2) can be converted into those in Eqs. (3) and (4), respectively.

$$T_H=TBP_{50} \tag{3}$$

$$B_H=\frac{-2.197}{\ln(TBP_{50}/TBP_{90})}$$

$$T_L=\frac{0.833*TBP_{90}-0.325*TBP_{50}}{0.508}$$

$$B_L=\frac{T_L-TBP_{50}}{0.833} \tag{4}$$

It should be also noted that for the desired product specification, the two points of TBP (TBP_{50}, TBP_{90}) can be used to obtain parameters of the probability function of TBP.

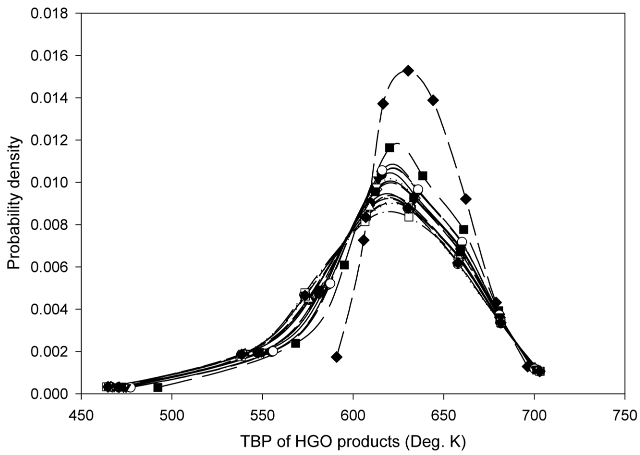

Fig. 4. Probability density of HGO products.

The multiple correlation coefficient is a measure of how well the regression model describes the data. By using least square regres-

Table 1. Optimized parameters in Eq. (1) (Dimensionless Unit)

Parameter	LPG	Naphtha	LK	HK	LGO	HGO	RC
B_H	5.3016	17.4541	36.4592	32.4062	27.3499	23.6067	12.2731
T_H	262.8636	373.3009	441.9055	494.6851	550.5835	619.354	749.7262

Table 2. Optimized parameters in Eq. (2) (Dimensionless Unit)

Parameter	LPG	Naphtha	LK	HK	LGO	HGO	RC
B_L	148.198	79.269	46.9499	58.367	76.866	100.985	194.103
T_L	391.268	442.278	481.8223	544.615	616.630	705.908	914.873

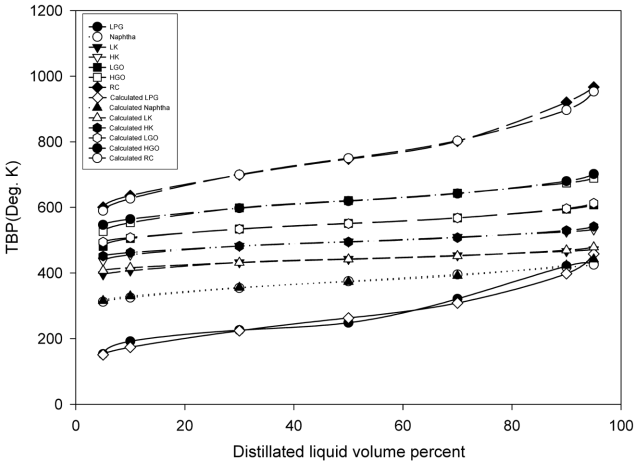

Fig. 5. Experimental vs calculated TBP's by using Eq. (1).

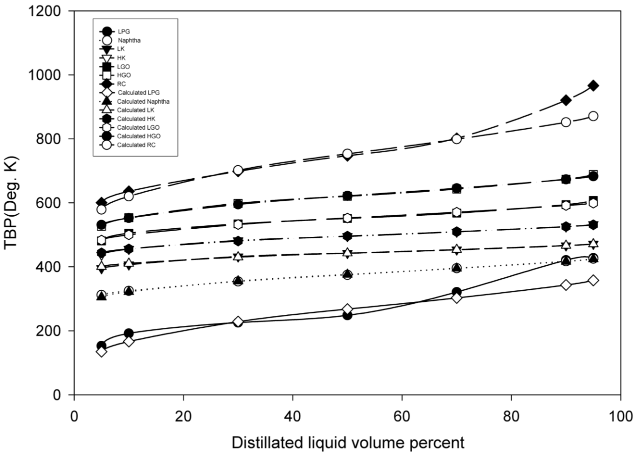

Fig. 6. Experimental vs calculated TBP's by using Eq. (2).

sion method, parameters of probability functions can be obtained as shown in Tables 1 and 2 in which the laboratory TBP data and the simulation data from crude assay of CDU products are used; from now on we call them as experimental data. Tables 1 and 2 show optimum parameters of Eqs. (1) and (2) for seven different products of CDU. Figs. 5 and 6 show the comparisons between experimental TBP and predicted TBP by probability function. Table 3 shows standard prediction error from Eq. (1) and Eq. (2). Eq. (1), in general, fits well with experimental TBP. However, Eq. (2) fits more precisely in the range of specific TBP of Naphtha, LK, HK, LGO, HGO products with experimental data. Because Eq. (2) has limits in itself, it gives good prediction to all side products having special ranges. It should also be noted that there exists distinctive measuring error especially for light and heavy fractions. So the combination of Eq. (1) and Eq. (2) will produce a good fit to predict crude TBP.

Table 3. Standard prediction error from Eq. (1) and Eq. (2)

	Standard error of estimated TBP (K), R-square	
	Eq. (1)	Eq. (2)
LPG	4.8784	7.6849
Naphtha	3.0299	1.2799
LK	3.5634	1.7239
HK	3.0393	1.3010
LGO	2.6599	1.5658
HGO	2.5888	1.7313
RC	1.6068	4.9685

For different feed systems, similar results will be obtained. In the next sections, parameters of probability function are used by correlating with operating variables. In this report, Partial Least Squares Projections to Latent Structures (PLS) technique [Bjorn et al., 1992; Kresta et al., 1991] is used for correlating the parameters of probability function with the variables of operating conditions.

RELATIONS BETWEEN THE PARAMETERS OF PROBABILITY FUNCTION AND OPERATING CONDITIONS BY PLS METHOD

Characteristics and quantities of product for CDU can be changed by adjusting the following operating conditions. The variables are as follows:

1. Supplied steam quantity
2. Pressure compensated tray temperatures
3. Product flow rate
4. Over flash ratio
5. Outlet temperature of furnace
6. Reflux ratio
7. Heat duty of condenser,
8. Pump-around duties
9. Etc.

Parameters of probability function or products qualities can be optimized by the above variables. In this paper, PLS technique was used for predicting the parameters of probability function in terms of the variables of operating conditions. PLS technique is commonly used in multivariate calibration, i.e., the predictor block consists of variables that are less expensive, less time consuming, or more easily calculated than the responses of control variables. The two points of TBP (TBP_{50}, TBP_{90}) can be correlated with operating variables as shown in the following.

$$TBP_{50}=\sum_{i=1}^{n}C_{50,i}*X_i,\quad TBP_{90}=\sum_{i=1}^{n}C_{90,i}*X_i \qquad (5)$$

where $C_{50,i}$ and $C_{90,i}$ are constants and X_i is the functional value of

Table 4. Operating variables for prediction of TBPs of HGO product in Eq. (5)

i	Variable X	$C_{50,i}$	$C_{90,i}$
1	Constant	210.06	657.24
2	HK draw temp. (Deg·K)	0.16656	0.018195
3	LGO draw temp. (Deg·K)	−0.42937	−0.030752
4	HGO draw temp. (Deg·K)	−0.65854	−0.041505
5	RC draw temp. (Deg·K)	1.6048	0.080707
6	HK flowrate/feed flow rate	0.24134	0.020104
7	LGO flowrate/feed flow rate	−0.54573	−0.064349
8	HGO flowrate/feed flow rate	0.65828	0.24049
9	RC flowrate/feed flow rate	−0.24681	−0.031697
10	Overflash ratio	0.41874	−0.027407

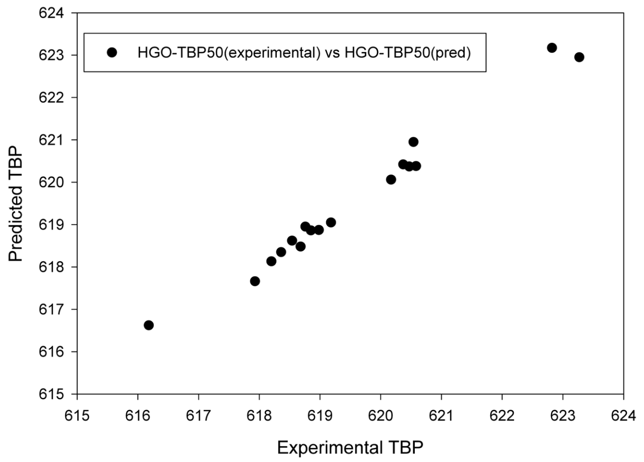

Fig. 7. Experimental vs predicted TBP's by using operating variables.

operating variables. For example, the two points of TBP for HGO product can be correlated with independent variables which are shown in Table 4. Fig. 7 shows predicted TBP from operating variables shown in Table 4. To find these correlations, commercial software, Simca-P was used.

Parameters of TBP probability functions can be correlated with TBPs by using operating variables of CDU system with Eq. (3) or Eq. (4) for each probability function. This correlation model can be applied for other products. The models made by PLS technique predict each parameter of probability function by operating variables and the TBP of each product can be calculated by these parameters. Finally, the TBP of feed from operating conditions can be obtained by summing all predicted products as written in Eq. (6).

$$D(T, L_1, L_2, L_3, L_4, L_5, L_6, L_7, \Lambda) = \frac{\sum_{i=1}^{7} L_i * D_i(T)}{\sum_{i=1}^{7} L_i} \qquad (6)$$

where D is the liquid volume distillate percent at temperature T, Di(T) is the liquid volume distillate percent of each product at temperature T, and Li is the liquid volume of each product. Finally, the TBP of feed can be obtained with all predicted product TBP shown in Fig. 8. Fig. 8 shows that predicted TBP from Eq. (1) is more close

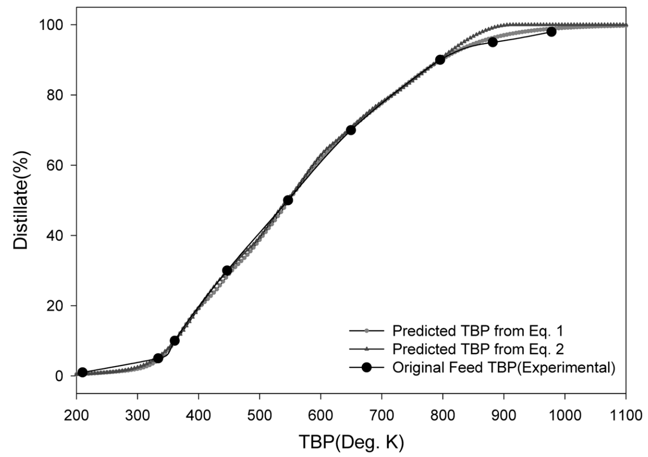

Fig. 8. Comparison of predicted TBP's of feed for using different probability equation.

to provided TBP. The reason is Eq. (1) fits more precisely in the region of RC, which is about 50% of crude feed. So the final results show that the Eq. (1) is better than Eq. (2). The combination of Eq. (1) and (2) will give better results.

It should be noted that the selection of the continuous probability functions and operating variables is rather arbitrary; a better choice of these selections could result in better predictions.

CONCLUSIONS

Utilizations of the proposed probability equation and PLS technique has enabled us to correlate the parameters of probability functions with operating conditions for TBP's of each product and resulting feed. The choice of probability function is rather arbitrary and other equally versatile distribution functions or combined functions can also be used. It should be also noted that for desired product specification, the two points of TBP can be used to get feed and product TBP's by applying the continuous probability distribution function.

Overall, the proposed method can be effectively used for controlling process optimization, downstream operation, and scheduling for better profit.

NOMENCLATURE

D : distillated liquid volume percent
T_H : parameter of probability function (dimensionless unit)
B_H : parameter of probability function (dimensionless unit)
T_L : parameter of probability function (dimensionless unit)
B_L : parameter of probability function (dimensionless unit)
TBP_{50} : TBP at D is 50 [Deg·K]
TBP_{90} : TBP at D is 90 [Deg·K]
L : liquid volume [liter]

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