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Hybrid Model for Optimization of Crude Distillation Units

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Abstract

Planning, scheduling and real time optimization (RTO) are currently implemented by using different types of models, which causes discrepancies between their results. This work presents a single model of a crude distillation unit (preflash, atmospheric, and vacuum towers) suitable for all of these applications, thereby eliminating discrepancies between models used in these decision processes. Product TBP curves are predicted via partial least squares model from the feed TBP curve and operating conditions (flows, pumparound heat duties, furnace coil outlet temperatures). Combined with volumetric and energy balances, this enables prediction of crude distillation on par with a rigorous distillation model, with 0.5% RMSE over a wide range of conditions. Associated properties (e.g. gravity, sulfur) are computed for each product based on its distillation curve and corresponding property distribution in the feed. Model structure makes it particularly amenable for development from plant data.

1. Introduction

Crude distillation units (CDUs) separate feed to a refinery into intermediate products which are further process by the downstream units or blended into the final products. CDUs are complex distillation towers, producing several products and having many degrees of freedom which can be used to fine-tune the operation. Fig. 1 shows an example of a CDU in Aspen Plus[1] consisting of a preflash tower (which remove light components from the feed), atmospheric distillation (which operates at atmospheric pressure and separates bulk of the crude into several products), and vacuum distillation (which operates under vacuum to separate heavy end of the crude into several products).

Since crude oil typically consist of large number of compounds, and its chemical compositions is not known, petroleum refining community has adopted crude characterization in a form of

crude assays. An assay describes a crude oil in terms of increasing boiling point temperatures at which specific parts of the crude will evaporate; this is so called true boiling point (TBP) curve, as shown in Fig.2. The entire TBP curve is divided into non-overlapping sections ("cuts"). Other crude properties, e.g. % sulfur or gravity or viscosity, also vary from one temperature range to another temperature range (from one cut to another), as shown in Fig. 2.

If CDU is capable of perfectly sharp separation, each product stream from CDU will have the yield corresponding to the width of the cut and its TBP curve will overlap its section of the crude TBP curve. In reality, product distillation curves differ significantly from their respective section of the crude TBP curve. Fig.2 shows crude TBP and product distillation curve for a typical atmospheric distillation tower. Back end a product TBP curve is above the crude TBP curve and the front end of the product TBP is lower than the crude TBP curve. One should note that the back end of the lighter cut and the front end of the adjacent heavier cut are not equidistant from the crude TBP curve. Similarly, midpoint of a TBP distillation curve for a cut does not lie on the crude TBP distillation curve. Such pattern as a rule appears in practically all industrial CDUs. Unfortunately, vast majority of the published works on simplified crude distillation modelling assume that (i) the back end/front end points of adjacent products are equidistant from the crude distillation curve and (ii) the midpoint of a product distillation curve lies on the crude distillation curve.

Accurate and robust models capable of predicting CDU product yields and properties took several decades of rigorous distillation tower model developments. The first commercial flowsheet simulation software capable of solving reliably complex distillation tower models was SSI/100 by Simulation Sciences, which was released in mid 1970s. In 1974 Boston and Sullivan published "inside-out" algorithm for rigorous tray to tray simulation of distillation towers, which has become the basis for all present day algorithms for distillation of wide boiling mixtures. In mid-1980's HYSIM introduced the use of property curves, such as % of sulfur, and their mixing via pseudo components to predict product properties other than distillation curves (Svrcek, 1989)[2]. This was soon followed by similar development in AspenPlus and Pro/II. Since early 1990s process simulation, design, and real-time optimization applications have relied on these large scale (10,000 equations or more) nonlinear model capabilities to predict accurately the outcome of processing crude feedstocks under specified set of operating conditions.

In addition to rigorous distillation tower models, commercial simulators usually offer a simplified, fractionation index based models of complex distillation towers (e.g. Aspen Plus 11.1 Unit Operation Models.[3]). These have been provided to fill the need for easy to configure and easy to tune models of complex distillation towers.

Rigorous distillation models available in simulation software have many equations, are highly nonlinear and are not suitable for use in production planning and scheduling. In order to

accomplish reasonable solution times for planning and for scheduling models, crude units have traditionally been represented by various forms of linear and recently simplified nonlinear models of CDU behavior, as described in the next section. RTO on the other hand uses tray to tray rigorous distillation models, which makes them too large for use in planning and scheduling.

Production planning and production scheduling models require multiple representations of the same crude unit, either because there are many periods and each period has at least one crude unit, or because the crude unit is represented by several modes of operation. Two simplifying assumption which as a rule are used in these simplified models are: (i) equidistance between the back end of the lighter cut and the front end of the heavier cut, and (ii) the midpoint of a product TBP curve lies on the crude TBP curve. However, if one examines product distillation curves from actual crude distillation towers (or from rigorous tray to tray simulations), I becomes apparent that both of these assumptions are incorrect and that they introduce significant errors in predictions by the models which rely on them.

This work introduces a high accuracy hybrid model of a crude unit. The model does not rely of the assumptions (i) and (ii). Hence, the model computes correctly product TBP curves that are observed in actual CDUs. In addition, we illustrate how product and crude TBP curves and property distribution curves can be used to compute bulk properties (e.g. % sulfur) of the product streams. Results computed by the hybrid model are compared with those from a rigorous tray to tray model. Differences between the predictions by the two models are within the error of the analytical instruments used to measure product distillation curves.

In section 2 of this paper we present a brief review of the prior work on the simplified models of crude distillation towers. Section 3 we present a sample crude unit and summarize computation of overall mass and energy balances based on approximate thermodynamic data and examines their accuracy vs. balances based on rigorous thermodynamic properties. Prediction of product distillation curves is described in Section 4, while Section 5 describes computation of other stream properties (e.g. specific gravity and sulphur). Comparison of hybrid model predictions with a rigorous tray to tray model predictions is given in Section 6 via several case studies and an example of optimizing the operation of the sample CDU. Conclusions are given in Section 7.

2. Prior work on simplified crude distillation models

Simplest approach to modelling crude units in a mathematical programming planning model is to represent each cut by its yield and approximate its distillation curve by

(i) adding some "delta differences" ΔTB_i (where *i* can be e.g. 90%, 95%, 99%, 100%) to the crude distillation points at the back end of the product, and

(ii) subtracting some delta differences ΔTF_i (where *i* can be e.g. 10%, 5%, 1%, 0%) from the crude distillation points at the front end of the product.

Such approximation is not realistic, since CDU unit can operate under variety of conditions, which leads to different sharpness of separation between adjacent products. In other words, deviations from the crude TBP curves are not constant. In addition, this model assumes that the middle section of the product distillation curve (including 50% midpoint) correspond to the crude distillation curve, which is practically never correct.

Frequently used improvement is to define distinct operating states (modes) that will be employed for the crude unit by Brooks et al.[4]. Each operating state is then characterized by different set of "delta differences" for each product. This approach improves somewhat prediction of the product front end and back end distillation points, but still suffers from the fact that these predefined operating modes cannot represent changes in separation which may be required to optimize product blending for a particular demand pattern. Similarly, middle section of the product TBP curve leads to erroneous computation of other properties.

An improved method is to define a swing cut, i.e. amount of the front end of the heavier cut which is transferred to the back end of the adjacent light cut (or the amount of the back end of the lighter cut which is transferred to the front end of the heavier cut). Purpose of the swing cuts is to approximate product distillation curves. Swing cut is an assumed cut between the two adjacent products, most often with constant properties. The size of the cut is assumed as a fixed ratio (volume or weight based) to the total feed to the distillation tower, or as a TBP interval of specific size. If there are more than one crude present in the feed, then the swing cuts from all crudes are mixed and the resulting "mixed swing cut" is distributed among the adjacent products. Since the assumption is that the properties of each swing cut are constant for the entire TBP range of the swing cut, this methodology can not represent accurately the fact that the properties are distributed nonlinearly across TBP intervals.

Once product TBP curve is known, its bulk properties can be computed by the methodology which is used by rigorous simulation models (pseudo components "carry" with them other properties and are blended to compute product bulk properties), as illustrated by Menezes et al.[5]. Menezes et al divided each swing cut into "light part" and "heavy part". Their approach still leaves open the question of how to determine the size of the cut in relationship to the separation capabilities of the distillation tower.

In order to apply the swing cut methodology one must decide on the amount of the transferred components and on their distillation properties. Zhang et al.[6] applied swing-cut model by taking into account how fractions of the same distillation points swing between adjacent cuts. Li et al.[7] employed weighted average of the yield changes by using the weight transfer ratio of each product cut. Guerra et al.[8,9]also employed swing cut model. Recognizing the limitations of swing cut methodology, Pinto et al.[10] and Neiro and Pinto[11]proposed use of nonlinear models to derive delta models and swing cuts.

Alattas and Grossman[12] derived an approximate nonlinear crude distillation model which uses fractionation indices and proposed that the fractionation indices be tuned for different sets of operating conditions. This is similar to the simplified models used in the process simulators (e.g. AspenPlus) and also is similar to models used by some refining companies in their planning models. They also assumed equidistance between the back end of the lighter cut and the front end of the adjacent heavier cut. Alatas and Grossman did not publish a comparison of their model with rigorous tray to tray results.

All of the above research efforts have relied on the equidistance assumption and on the assumption that the midpoint of the product TBP curve lies on the crude TP curve. Mahalec and Sanchez[13] presented a model of an atmospheric pipestill which does not assume equidistance between adjacent (back, front end) pairs and also does not assume that the midpoint of the product TBP curve lies on the crude TBP curve. The model was designed with real time applications in mind. Hence, they assumed that the temperature profile in the towers could be estimated from several available tray temperature measurements. This enabled accurate computation of the internal vapor and liquid flows in the tower in mass units (not mole units) and the internal reflux. Product TBP curves were then computed based on the crude TBP data, product yields, stripping steam flows, and pumparound duties. The model was demonstrated to predict product TBP pints typically with less than 1% error (for 5% to 95% points on the distillation curve). An example application of the model led to an optimum which was verified as feasible via AspenPlus simulation and it was better that the result computed by optimization of the corresponding rigorous tray to tray model in AspenPlus.

Ochoa-Estopier et al.[14] presented a review of various efforts to create reduced order crude distillation models. They developed a very accurate neural network based model of a crude distillation unit and compared its results to a rigorous simulation.

3. Material and energy balances

Sample crude distillation unit (see AspenTech "Getting Started with Petroleum Distillation Modelling") used in this work is shown in Fig. 1. It consists of a preflash tower, an atmospheric distillation tower, and of a vacuum distillation tower. Rigorous model of this unit is used in this work as a substitute for an actual crude distillation unit. "Plant data" used in this study have been generated from this rigorous model. All volumetric flows are expressed as liquids at the standard conditions; all measurements will be expressed in imperial units, as it is customary in North American refineries.

If each tower in the CDU was carrying out perfect, sharp separation, then the entire feed would be separated into cuts as shown by dashed vertical lines in Fig. 2 and each product would have TBP curve identical to the corresponding section of the crude feed. Note that Fig. 2 represents all products from the CDU. Since separation is not perfect, the actual product distillation curves are represented by S shaped curves as shown in Fig. 2.

CDU distillation towers have a significant amount of stripping steam as their feeds. Since water does not mix with hydrocarbons, volumetric or mass balances for hydrocarbons in each tower will be considered separately from the water balances. Volumetric balances (on a dry basis) for the three distillation towers are:

Preflash tower:

$$F_{crude}(dry) = F_{lgh}(dry) + F_{nph}(dry) + F_{ap-feed}(dry) \quad (1)$$

Atmospheric pipestill:

$$F_{ap-feed}(dry) = \\ F_{hnph}(dry) + F_{kero}(dry) + F_{dsl}(dry) + F_{ago}(dry) + F_{vp-feed}(dry) \quad (2)$$

Vacuum pipestill:

$$F_{vp-feed}(dry) = F_{lvgo}(dry) + F_{hvgo}(dry) + F_{resid}(dry) \quad (3)$$

Water mass balances are:

Preflash tower:

$$MF_{pf-stm} = MF_{pf-water} \quad (4)$$

Atmospheric pipestill:

$$MF_{ap-stm} + MF_{ap-stm,kero} + MF_{ap-stm,dsl} + MF_{ap-stm,ago} = MF_{ap-water} \quad (5)$$

Vacuum pipestill:

$$MF_{vp-stm} = MF_{top-vapor} \quad (6)$$

Energy balances will also be written separately for hydrocarbons and for water.

Preflash tower:

$$F_{crude}(dry) * \rho_{crude} * h_{crude} + Qduty_{pf-f} = F_{lgt}(dry) * \rho_{lgt} * H_{lgt} + \\ F_{nph}(dry) * \rho_{nph} * h_{nph} + F_{ap-feed}(dry) * \rho_{ap-feed} * h_{ap-feed} + Q_{cond}(dry) \quad (7)$$

$$MF_{pf-stm} * H_{pf-stm} = MF_{pf-water} * h_{pf-water} + Q_{cond}(water) \quad (8)$$

$$Q_{cond}(wet) = Q_{cond}(dry) + Q_{cond}(water) \quad (9)$$

Atmospheric pipestill:

$$\begin{aligned} &F_{ap-feed}(dry) * \rho_{ap-feed} * h_{ap-feed} + Qduty_{ap-f} = \\ &F_{hnph}(dry) * \rho_{hnph} * h_{hnph} + F_{kero}(dry) * \rho_{kero} * h_{kero} + F_{dsl}(dry) * \rho_{dsl} * h_{dsl} \\ &+ F_{ago}(dry) * \rho_{ago} * h_{ago} + F_{vp-feed}(dry) * \rho_{vp-feed} * h_{vp-feed} + \sum_{i=1}^{2} Qduty_{QPA_i} + +Q_{cond}(dry) \end{aligned} \quad (10)$$

$$\begin{aligned} &MF_{ap-stm} * H_{ap-stm} + \sum_{i=1}^{3} (MF_{ap-ss,i} * H_{ap-ss,i}) = \\ &MF_{cu-water} * h_{cu-water} + Q_{cond}(water) \quad i = 1, 2, 3(kero, dsl, ago) \end{aligned} \quad (11)$$

$$Q_{cond}(wet) = Q_{cond}(dry) + Q_{cond}(water) \quad (12)$$

Vacuum pipestill:

$$\begin{aligned} &F_{vp-feed}(dry) * \rho_{vp-feed} * h_{vp-feed} + Qduty_{vp-f} = F_{LVGO}(dry) * \rho_{LVGO} * h_{LVGO} \\ &+ F_{HVGO}(dry) * \rho_{HVGO} * h_{HVGO} + F_{resid}(dry) * \rho_{resid} * h_{resid} + \sum_{i=1}^{2} Qduty_{QPA_i} \end{aligned} \quad (13)$$

$$MF_{vp-stm} * H_{vp-stm} = MF_{top-vapor} * H_{top-vapor} \quad (14)$$

Steam balance for VP tower (Eq. 14) assumes that the entire vapor stream from the top of the VP tower is steam.

We need to compute unit enthalpies *[energy/mass]* of hydrocarbon streams, energy supplied by the furnace, energy removed by the condenser, and the pumparound duties. We assume that at some base operating conditions we have available bulk thermodynamic properties (stream enthalpy, specific heat capacity, density, and heat of vaporization). Thermodynamic properties at conditions different from the base case are then computed as incremental changes from the base case. We will also assume that the pressure in each distillation tower does not vary significantly from the pressure at the base operating state, as is the case in refinery operations. Computation of energy balances is carried on a dry basis, disregarding steam balances. This does not have an impact on the accuracy of calculation, since the stripping steam flows through the tower without a large change in the steam enthalpy and it is condensed at the top of the tower.

Since the model will be used to predict operation under a variety of conditions, temperatures of the liquid streams leaving e.g. atmospheric distillation tower will vary. If we employ *[energy/mass]* instead of *[energy/mole]*, we will notice that the specific heat capacities of hydrocarbons of similar molecular weights are approximately the same. Therefore, if the composition of a stream varies around some base composition, the specific heat capacity of the

material remains practically constant. For instance, if kerosene 95% point changes by 10 or 20 deg F, there are some changes to its composition but its specific heat capacity remains practically constant. Since rage of changes in operating conditions is relatively small with respect to the base case, we can also assume that the specific heat capacities of individual streams do not vary with temperature when the distillation tower moves from one operating state to another. Therefore, unit enthalpy of a stream can be calculated by Eqs. (15) and (16) for liquid and vapor streams, respectively.

$$h_p = h_p^0 + C_{p,L}(T_p - T_p^0) \tag{15}$$

$$H_p = H_p^0 + C_{p,V(T_p - T_p^0)} \tag{16}$$

Temperature of a stream leaving a side-stripping tower differs from the temperature of the main tower draw-off tray by some difference. This difference changes somewhat from one set of operating conditions to another, but for purposes of energy balance calculations it can be assumed to be constant. Hence, if we can estimate the temperature at the draw-off tray, then we can calculate the temperature of the stream leaving the side-stripping tower. Temperature at the draw-off tray varies with the boiling point of the material on that tray, which is also the same material as the one leaving the main tower and it is closely related to the product stream from the side-stripper. Front end of the distillation curve of the product stream is heavier than the front end of the material on the draw-off tray, due to additional separation and the steam used in the side-striper. These considerations lead us to a relationship between the draw-off tray temperature, the product cut point temperature, and (stripping steam/product flow) ratio S_p, Eq. (17) for each of the side products p.

$$T_{drawoff\ tray,p} = a_0 + a_1 * T_{cut,p} + a2 * S_p \tag{17}$$

and the product p stream temperature is then:

$$T_p = T_{drawoff\ tray,p} + a_3 \tag{18}$$

Heat duty of the condenser for the atmospheric tower can be computed from the heat of vaporization of the distillate and the total liquid leaving the condenser. Maxwell[15]presented heats of vaporization for hydrocarbons at various pressures, showing that at the pressure of 1 atmosphere the heats of vaporizations of C7 to C10 hydrocarbons are within 5% of each other. Since naphtha composition can vary significantly from one operating state to another, and since the condenser is a very large contributor in the energy balance, heat of vaporization of naphtha needs to be estimated as accurately as possible. Mid-point at the distillate TBP distillation curve T50,d is a good surrogate for naphtha composition. We can use linear approximation around the base operating conditions, as shown by Eq. (19), to compute the heat of vaporization of the distillate. Fig. 3 shows the relation between naphtha TBP 50% point and the latent heat for naphtha. Fig. 4 shows the comparison of the predicted value of latent heat and the latent heat

value from AspenPlus. Approximated heat of vaporization has at most 2.5% error compared to the rigorous calculation from a comprehensive thermodynamic package.

$$\lambda_d = \lambda_d^0 + a_4 * (T_{50,d} - T_{50,d}^0) \tag{19}$$

More accurate computation of the latent heat of naphtha can be accomplished by an iterative procedure by estimating naphtha TBP curve from the model, recalculating the heat of vaporization, estimating again naphtha heat of vaporization, etc. until the desired accuracy is achieved. Since the model predictions are already very accurate, such iterations are not necessary and we have verified such conclusion by experiments.

4. Predicting product distillation curves

Distillation curves shown in Fig. 5 illustrate that the product distillation curves as a rule do not overlap with the feed distillation curve. This is the case in general, not just for the example model used in this work. Hence, we can not assume that the middle section of the product TBP curve coincides with the feed TBP and then add corrections to the front end and the back end. Such procedure leads to an erroneous product TBP curve which then leads to inaccurate prediction of other properties, since they are computed via their association with the product pseudo component distribution.

Instead of assuming that the middle section of the product TBP curve lies on the feed TBP curve, we need to estimate it from tower operating data, as introduced by Mahalec and Sanchez[13](Fig. 5). After that, deviations from the front and the back ends of the line are estimated, as shown in Fig. 5.

The middle section of the curve is predicted as by partial least squares (PLS) model using feed TBP curve and the yield of individual products. This section represents how a given distillation tower separates the bulk of the crude among the products, based on the tower structure. It is not directly impacted by changes in other operating conditions, other than through their impact on the yield of individual products. The vertical deviations between the middle section straight line and the front and back sections are predicted by a different PLS model using cut information and operating conditions.

Cumulative cut width of each product ($CCWP_i$) is defined as:

$$CCWP_i = \sum_{l=1}^{i}, p_l/F \quad i = 0, 1, 2, 3 \tag{20}$$

Then the cut point temperature (cutti) of each product can be calculated from the feed TBP curve as shown in Fig. 6.
Separation in the tower is governed by the number of trays and by the internal reflux. Since in production planning and scheduling we do not know the temperature profile in the tower, the model uses external reflux to determine the separation in the tower. In order to account for the internal vapor flows in the tower, the model uses fraction of the feed that vaporizes at the furnace coil outlet temperature (COT).

Preflash Tower

Purpose of the preflash tower is to separate the light components from the crude. From planning or scheduling viewpoint, specifying the overhead distillate flowrate is the most important decision. In order to increase accuracy of the predictions, the model requires the condenser temperature (which can be to be assumed constant for planning and scheduling applications), stripping steam flow and overflash. In addition to product properties, the models calculates furnace COT (see Table 1). Alternatively, for use in plant operation, one can specify COT and the model calculates the overflash, as shown in Table 2.

Preflash tower model was developed from simulation data for very light crude and for very heavy crude (total of 54 cases). The model was then tested against a crude feed consisting of mixtures of medium crude (total of 27 cases). Range of changes in operating variables is shown in Table 3.

Equations to predict product TBP curve of the liquid distillate are as follows:

The straight line through the middle section:

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * \sum TBP_{crude,k} + a_{i,j,2} * ccwp_i + a_{i,j,3} * cutt_i + a_{i,j,4} * pf_{stm}$$
$$i = 0(nph)\ j = 30, 50, 70\ where\ k\ are\ points\ on\ the\ distillation\ curve \quad (21)$$

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * \sum TBP_{crude,k} + a_{i,j,2} * ccwp_{i-1} + a_{i,j,3} * cutt_{i-1}$$
$$i = 1(ap - feed)\ j = 30, 50, 70\ where\ k\ are\ points\ on\ the\ distillation\ curve \quad (22)$$

The deviations from the straight line are defined as:

$$TBP^d_{i,j} = TBP^{'}_{i,j} - TBPi, j \quad i = 1(ap - feed) \quad k = 1, 5, 10 \quad (23)$$

$$TBP^d_{i,j} = TBPi, j - TBP^{'}_{i,j} \quad i = 0(nph) \quad k = 90, 95, 99 \quad (24)$$

The deviations for the front and the back sections are given by:

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,1} * COT + a_{i,j,2} * CCWP_i + a_{i,j,3} * cutt_i + a_{i,j,4} * pf_{stm} \quad i = 0(nph) \quad j = 90, 95, 99 \tag{25}$$

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,1} * COT + a_{i,j,2} * CCWP_{i-1} + a_{i,j,3} * cutt_{i-1} + a_{i,j,4} * pf_{stm} + a_{i,j,5} * \sum TBP_{crude,k} \quad i = 1(ap - feed)\ j = 01, 05, 10\ where\ k\ are\ points\ on\ the\ distillation\ curve \tag{26}$$

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,l} * \sum TBP_{crude,k} + a_{i,j,4} * CCWP_{i-1} \quad i = 1(ap - feed) \quad j = 90, 95, 99\ l = 1, 2, 3\ where\ k\ are\ points\ on\ the\ distillation\ curve \tag{27}$$

TBP curve of the feed to the atmospheric distillation tower is computed by estimating its front end; the remainder is copied from the TBP curve of the preflash tower feed. Results from the model testing are presented in Table 4. Maximum error is for 99 vol% TBP point and this is still less than 1% error.

Atmospheric pipestill

Input and output variables for the atmospheric distillation tower are shown in Table 5. Note that we use ratio [reflux/(reflux + distillate), i.e. R/(R+D)] instead of [reflux/distillate], since it represents more closely the internal reflux in the tower. Energy balance requires that we either specify one of the pumparounds and compute R/(R+D) or specify R/(R+D) and compute the second pumparound. Various options for specifying the model are given in Table 6.

Data for development of the atmospheric pipestill model have been generated by simulating operation with a light crude feed and with the heavy crude feed for a range of operating variables (192 cases), as shown in Table 7. The feed was calculated by the rigorous simulation of the preflash tower, since this represented the feed as it would be produced in a real plant. The model was then tested (96 cases) against predictions from rigorous simulations for a mixed crude feed (between the light and the heavy crude). Results of the model testing are shown in Table 8. In these tests, all TBP points computed by the hybrid model in these test were less than 1% from the TBP points computed by the rigorous simulation.

Product distillation curves are computed from the following equations:

The straight line through the middle section:

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * \rho_{ap-feed} + a_{i,j,2} * ccwp_i + a_{i,j,3} * cutt_i$$
$$i = 0(hnph) \quad j = 50, 70 \tag{28}$$

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * \rho_{ap-feed} + a_{i,j,2} * ccwp_i + a_{i,j,3} * cutt_{i-1}$$
$$+ a_{i,j,4} * cutt_i \quad i = 1, 2, 3(kero, dsl, ago) \quad j = 30, 50, 70 \tag{29}$$

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * \rho_{ap-feed} + a_{i,j,2} * ccwp_{i-1} + a_{i,j,3} * cutt_{i-1}$$
$$+ a_{i,j,4} * \sum TBP_{ap-feed,k} \quad i = 4(vp - feed) \quad j = 30, 50, 70$$
$$where\ k\ are\ points\ on\ the\ distillation\ curve \tag{30}$$

The deviations from the straight line are defined as:

$$TBP^d_{i,j} = TBP'_{i,j} - TBPi, j \quad i = 1, 2, 3, 4(kero, dsl, ago, vp - feed) \quad j = 1, 5, 10 \tag{31}$$

$$TBP^d_{i,j} = TBPi, j - TBP'_{i,j} \quad i = 0, 1, 2, 3(hnph, kero, dsl, ago) \quad j = 90, 95, 99 \tag{32}$$

The deviations for the front and the back sections are given by:

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,1} * y_{ap,0} + a_{i,j,2} * y_{ap,1} + a_{i,j,3} * ap_{SS_1}/y_{ap,1}$$
$$+ a_{i,j,4} * \sum \Delta TBP_{l,m} + a_{i,j,5} * RefluxRatio$$
$$i = 0(hnph) \quad j = 90, 95, 99 \quad or \quad i = 1(kero) \quad j = 01, 05, 10$$
$$where\ l, m\ are\ adjeacent\ product\ steams \tag{33}$$

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,1} * y_{ap,i} + a_{i,j,2} * y_{ap,i+1} + a_{i,j,3} * ap_{SS_{i+1}}/y_{ap,i+1}$$
$$+ a_{i,j,4} * \sum \Delta TBP_{l,m} + a_{i,j,5} * CCWP_i + a_{i,j,6} * \varphi$$
$$i = 1, 2, 3(kero, dsl, ago) \quad j = 90, 95, 99$$
$$where\ l, m\ are\ adjeacent\ product\ steams \tag{34}$$

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,1} * y_{ap,i-1} + a_{i,j,2} * y_{ap,i} + a_{i,j,3} * ap_{SS_i}/y_{ap,i}$$
$$+ a_{i,j,4} * \sum \Delta TBP_{l,m} + a_{i,j,5} * CCWP_{i-1} + a_{i,j,6} * \varphi$$
$$i = 2, 3, 4(dsl, ago, vp - feed) \quad j = 01, 05, 10$$
$$where\ l, m\ are\ adjeacent\ product\ steams \tag{35}$$

$$TBP^d_{i,j} = a_{i,j,0} + a_{i,j,1} * CCWP_3 + a_{i,j,2} * cutt_3 + a_{i,j,3} * \varphi$$
$$i = 4(vp - feed) \quad j = 90, 95, 99 \tag{36}$$

Vacuum pipestill

Vacuum pipestill is much simpler that the atmospheric tower. Hence it has a much smaller number of input and output variables, as shown in Table 9. There are two possible sets of specifications as presented in Table 10. Data for model development have been developed by 276 simulations (light crude, heavy crude, various operating conditions in the atmospheric tower, and the vacuum tower). Table 11 summarizes the range of operating conditions used for data generation. The model was tested with 147 additional sets of data for medium mix of crudes in the feed and various operating conditions. Shown in Table 12 are the test results for the models. Similarly to the atmospheric and preflash tower models, the vacuum tower model predicts TBP points within 1% of the rigorous simulation.

TBP curves for the products from the vacuum pipestill are described by Eqs. (38) to (40), which have been obtained by PLS.

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * y_{vp,0} + a_{i,j,l} * \sum TBP_{vp-feed,k}$$
$$i = 0(lvgo) \quad j = 1, 5, 10, 30, 50, 70, 90, 95, 99 \quad l = 2, 3, 4, 5$$
$$where\ k\ are\ points\ on\ the\ distillation\ curve \tag{37}$$

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * y_{vp,0} + +a_{i,j,2} * y_{vp,1} + a_{i,j,l} * \sum TBP_{vp-feed,k}$$
$$i = 1(hvgo) \quad j = 1, 5, 10, 30, 50, 70, 90, 95, 99 \quad l = 3, 4$$
$$where\ k\ are\ points\ on\ the\ distillation\ curve \tag{38}$$

$$TBP_{i,j} = a_{i,j,0} + a_{i,j,1} * CCWP1 + a_{i,j,l} * \sum TBP_{vp-feed,k}$$
$$i = 2(resid) \quad j = 1, 5, 10, 30, 50, 70, 90, 95, 99 \quad l = 2, 3, 4, 5, 6$$
$$where\ k\ are\ points\ on\ the\ distillation\ curve \tag{39}$$

5. Predicting other properties

Product distillation curves determine properties related to volatility, e.g. flash point. It is also important to calculate additional properties, such a specific gravity, sulphur, pour point, etc. These properties are either quality constraints or are very important for downstream processing units. There are two categories of these properties, volumetric based (e.g. specific gravity) and weight based (e.g. sulfur). In this article we employ TBP based properties prediction method to Predict specific gravity and sulfur of crude and fractions as illustration.

The specific gravity and sulfur curves for the base case with the light crude feed are shown in Fig. 7 and Fig. 8. As you can see, the curves are 'S' shaped and are similar to the TBP curves of products. Hence, linear interpolation based on the fractions of the TBP curve can be used to predict the properties of the product streams. Details of the computational will be presented in a separate paper. There are main 3 steps to predict specific gravity and sulfur properties of the products:

1. For each crude oil that is part of the feed to the CDU unit, calculate properties curves from the crude assay data (e.g. specific gravity and sulfur).
2. Calculate TBP curve for the mixture of the crudes that is the feed to CDU; then calculate specific gravity and sulfur curves for this mixed crude. Computation is based on the linear combination of the specific gravity and of sulfur data for same TBP point on the constituent crudes
3. From the hybrid model of the CDU unit compute product TBP curves. Then calculate the product specific gravity and sulfur curves by linear interpolation by using properties of the mixed crude for a given TBP point in the product curve. After getting specific gravity and sulfur curve of one product, then accumulate to get bulk properties for that fraction.

Properties computed from the hybrid model have been compared with the results from AspenPlus (Table 13).

6. Model Testing

Test results presented in Section 4 were for individual distillation towers, e.g. atmospheric pipestill was tested by using the crude feed computed by AspenPlus. In this section we present results of testing the hybrid model of the entire CDU unit, i.e. atmospheric tower feed is computed by the hybrid model of the preflash tower, and the bottoms product of the hybrid model of the atmospheric tower is the feed to the vacuum tower.

There are totally 4 tests in this section. The detail of each test is as following:

- Test #1: The purpose of this test is to evaluate the TBP properties prediction for different crudes (Heavy, medium and light crude, see Table 14). The operating conditions for each crude are getting from Aspen plus under same specifications. (see Table 15). Then enter these operating conditions into this hybrid CDU unit to generate results for comparison. The compared results are shown in Table 16.
- Test #2a: The purpose of this test is to evaluate the TBP properties prediction for different product strategies for the light crude. Different specifications based on different production strategies were set up in Aspen plus (see Table 17). After that the flows computed by rigorous tray to tray model in Aspen Plus were used in the hybrid model and the product TBP curves were computed from the hybrid model. The comparison of the results is shown

in Table 18. Most of the products TBP are less that 1% away from the rigorous model prediction. An exception if 95% point for Heavy Naphtha, which has an error of 1.3%.

- Test #2b. The purpose of this test is to evaluate how accurately the hybrid model predicts the product flows. Product specifications from Table 17 were used in both hybrid model and rigorous tray to tray model in Aspen Plus. Then the flows from the hybrid model were compared to the flows from AspenPlus model as presented in Table 19. Flow of heavy naphtha is up to 3% different from AspenPlus. Flow of kerosene is has 2.4% error for the max diesel operation. All other flows have errors less than 1%

- Test #3: The purpose of this test is to examine AP tower hybrid model performance in an optimization application. The objective function is described by Eq.40. Constraints are presented in Table 20. We used specification set 4 described in section 4. The optimization problem was solved by using GRG nonlinear solver in excel and AspenPlus model was solve in equation oriented mode by DMO. In order to verify hybrid model for TBP prediction, the hybrid model product flows were entered into AspenPlus. The results are shown in Table 21. It can be seen that the optimum computed by the hybrid model leads to the operating point which is within the specified constrains The main difference between the two models is that the hybrid model recognizes that maximization of pumparound heat duties is advantageous and increases them to the maximum allowed. AspenPlus model stopped at a significantly lower pumparound duty which results in the objective function being approx. $ 3.8k per day lower.

$$Z = max(24 * y_{ap,0} + 23.42 * y_{ap,1} + 23.1 * y_{ap,2} + 22.5 * y_{ap,3} - 0.84 * ap_{stm} - 0.60 * ap_{ss1} - 0.60 * ap_{ss2} - 0.60 * ap_{ss3} - 53.95 * Q_{ap-f)} \quad (40)$$

7. Conclusions

This paper addresses the issue of inconsistency of predictions between the models which are used for planning, for scheduling, and for real time optimization of refinery operations. Over the last decade there have been many proposed versions of simplified crude distillation models. Most of these models rely on the assumption that at be boundary of the product cut the distance from the crude distillation curve to the front end of the heavier product is equal to the distance to the back end of the lighter product. In addition, many models assume that the mid-point of the product distillation curve lies on the crude distillation curve. Both of these assumptions are not correct as it can be seen from rigorous crude unit simulation or from plant data.

Hybrid model presented in this paper removes both of these assumptions. It is a small size model of the crude unit (preflash, atmospheric, and vacuum towers) which predicts the unit behaviour with very small discrepancies (vast majority of them less than 1%) with respect to the

rigorous tray to tray model. The model is linear, with exception of the reflux/(reflux+distillate) variable for the atmospheric tower. Volumetric and energy balance equations are complemented by PLS models which relate the operating variables to product distillation curves. Other product properties, (e.g. sulfur, specific gravity) are computed by an approach analogous to the pseudo-component based calculation in the rigorous simulation models. In this work we used simulated plant data, generated from rigorous tray to tray simulations. Structure of the model makes it also very amenable for development from the plant data.

Extensive model testing has been carried out by comparing the model predictions with rigorous tray to tray model of the crude unit in AspenPlus. An optimization example demonstrates that the optimum computed from the hybrid model is feasible and at least as good as the optimum computed by AspenPlus equation oriented mode.

Small size of the model and excellent convergence properties make it suitable for applications in production planning, scheduling, and real-time optimization refinery applications. Therefore, this type of the hybrid models can be used to eliminate discrepancies (caused by different models) in the decisions between these business processes.

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