Front. Eng. Manag. 2018, 5(2): 195–201
https://doi.org/10.15302/J-FEM-2017052

RESEARCH ARTICLE

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Impact of crude distillation unit model accuracy on refinery production planning

Abstract In this work, we examine the impact of crude distillation unit (CDU) model errors on the results of refinery-wide optimization for production planning or feedstock selection. We compare the swing cut + bias CDU model with a recently developed hybrid CDU model (Fu et al., 2016). The hybrid CDU model computes material and energy balances, as well as product true boiling point (TBP) curves and bulk properties (e.g., sulfur % and cetane index, and other properties). Product TBP curves are predicted with an average error of 0.5% against rigorous simulation curves. Case studies of optimal operation computed using a planning model that is based on the swing cut + bias CDU model and using a planning model that incorporates the hybrid CDU model are presented. Our results show that significant economic benefits can be obtained using accurate CDU models in refinery production planning.

Keywords impact of model accuracy on production planning, swing cut + bias CDU model, hybrid CDU model, refinery feedstock selection optimization, optimization of refinery operation

1 Introduction

Refinery planning models employ linear or successive linear programming (LP or SLP) to compute the best production plans. A crude distillation unit (CDU) separates a crude oil feed into intermediate streams, which are used to either blend the final products or become feeds to downstream conversion units. The accurate representation of the CDU in a planning model is important because the CDU model dominates the outcome of planning model optimization. The CDU is commonly represented by a linear model to facilitate convergence, thereby often compromising accuracy. Various forms of simplified CDU models have been devised over the past several decades. The delta model adjusts the front and back ends of the product true boiling point (TBP) curve by adding the differences to the deviations from the crude TBP. Brooks et al. (1999) described the use of multimode delta models, in which the CDU is represented by several models of operation in each period having different deltas for each mode. A variation of the delta model is the swing cut model, which requires the estimation of the product boiling point range and the corresponding yield. Zhang et al. (2001) assumed a fixed-size swing cut. Li et al. (2005) introduced the weight transfer method for adjusting product yields on the basis of different operating modes. Alattas et al. (2011) introduced a fractionation index-based CDU model and integrated it into a simple refinery model; this model requires that the fractionation indices be fine-tuned for different operating modes. Menezes et al. (2013) divided swing cuts into light and heavy parts to improve the prediction of product properties.

All of these methods assume that the crude TBP curve lies in the middle between the end point of the light cut and the initial boiling point of the heavy cut. Figure 1 shows that the yield based on the equidistance assumption is incorrect. Guerra and LeRoux (2011) used biases, sometimes as much as 4% of the feed volume (which can be more than 20% to 30% of the product amount), to correct the product yields.

The use of biases has been a common practice in the industry since the early days of LP-based planning models. Research over the past couple of decades has focused on searching for the best methods, which will reduce the size of the biases and/or increase their accuracy. In this study, we determine how to eliminate the biases by using the hybrid CDU model (Fu and Mahalec, 2015). This model employs mass and energy balances combined with

Received June 16, 2017; accepted August 21, 2017

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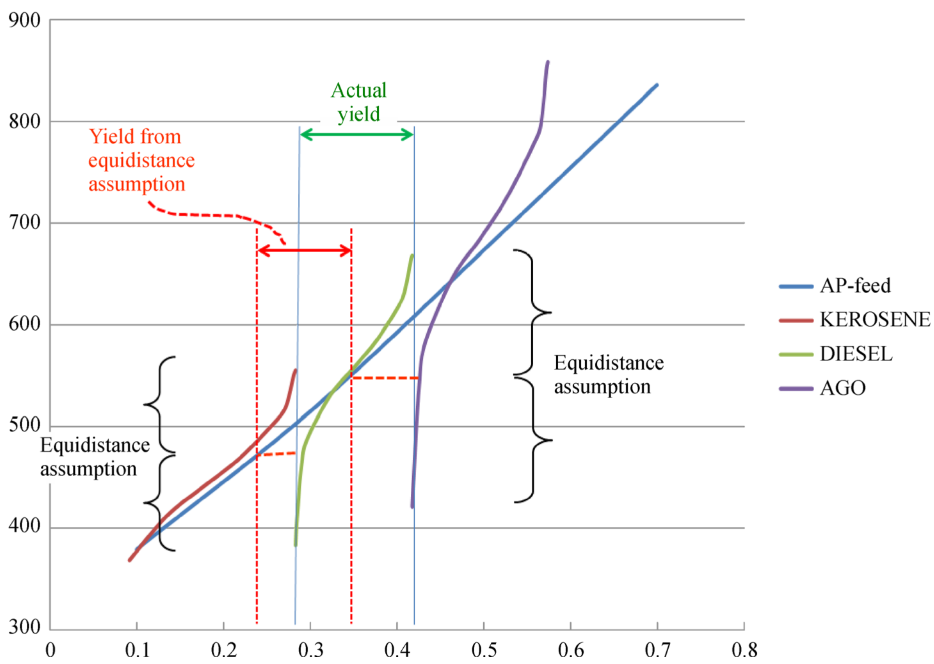

Fig. 1 Actual yield vs. yield from equidistance assumption

projection on latent space models, which predict product distillation curves and other stream properties. The hybrid CDU model uses feed TBP and property curves (e.g., sulfur, cetane, octane, etc.), as well as operational degrees of freedom (i.e., product flows, stripping stream flows, pumparound heat duties, reflux-to-distillate ratio, and furnace coil outlet temperature), to predict product stream properties. The model has approximately 200 equations and predicts the product TBP curves with less than 1% error (expressed in °F). The model does not have to be used in a specific operating mode because it employs operational degrees of freedom corresponding to an actual distillation tower. The optimization algorithm determines the actual operating conditions that correspond to the optimum value of the objective function. The model is suitable for use in refinery-wide models for planning or scheduling because of its small size and small number of nonlinear terms. This work shows that using such a high-accuracy CDU model leads to production planning outcomes that substantially differ from those of the swing cut + bias CDU model, which is the most accurate model currently employed in industrial practice.

2 Hybrid model of a CDU

A sample CDU is shown in Fig. 2. The unit is described in detail in AspenTech's manual on the modeling of petroleum processes. The CDU model must be able to predict the TBP distillation curves of each product, as well as the bulk properties (e.g., specific gravity % sulfur, etc.) of each of the product streams. Our approach is to compute the product TBP curve from the known feed TBP curve and the operating variables associated with a distillation tower. This means that the bottom product (AP feed) from the preflash tower is predicted from the feed TBP curve and the preflash tower operating conditions. Similarly, the products from the atmospheric distillation tower (AP tower) are predicted from the properties of the AP feed and tower operating conditions.

The main idea is to predict the straight line through the middle section of the product distillation curve and then predict the deviations from that straight line. For instance, the kerosene TBP can be represented as shown in Fig. 3. Fu et al. (2016) showed that the straight line through the middle section of the TBP curve depends only on how the tower feed is cut into different products (i.e., cumulative volumetric percentage corresponding to the front and back of each product) and the corresponding temperatures on the feed TBP curve. In other words, for a given tower configuration, the middle section is determined by the properties of the feed and by the amounts of the feed allocated to each product. The deviations of the product TBP curve from the straight line through the middle section are due to imperfect separation in the tower. These deviations depend on the operating conditions in the tower (e.g., reflux ratio, heat supply in the furnace, heat removal via pumparounds, and stripping steam supplied to each of the side strippers). Although the CDU operation is nonlinear, equations for the straight line through the middle sections and for the deviations from these lines are linear in the operating variables. Nonlinearities occur via certain ratios (e.g., reflux/distillate, stripping steam/product flow, and pumparound heat duty/feed flow). In

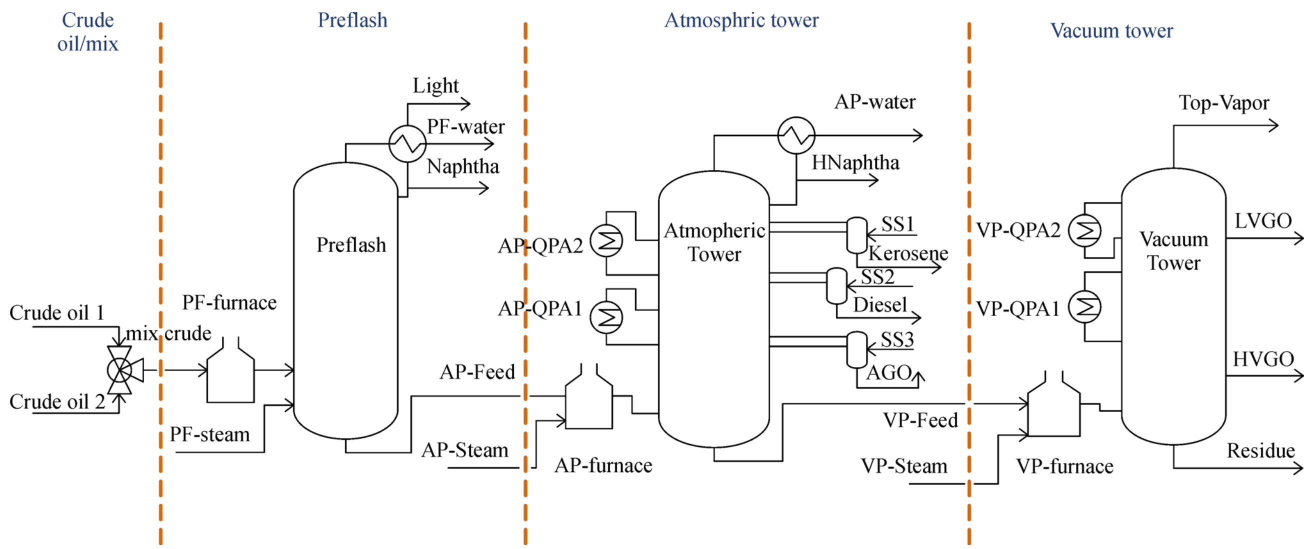

Fig. 2 Sample CDU

addition, the model includes material and energy balances around each distillation tower.

Fu et al. (2016) showed that the hybrid CDU model predicts 95% points on the product TBP curves of most products with errors of 0.3% or less. An exception is vacuum pipestill products, for which their model achieves relative errors of 0.1% to 0.9%. The cumulative error for all products leaving the atmospheric pipestill is 0.3%. The reader is referred to the original article for details about the hybrid CDU model.

3 Swing cut + bias CDU model

In this section, the procedure of swing cut size and bias calculation is described in detail. Two different feedstocks, called "crude oil 1" and "crude oil 2," are used. These feedstocks are representatives of light crude and heavy crude, respectively; their properties are shown in Table 1. We assume that the preflash and vacuum towers operate with fixed operating conditions to simplify the analysis of the results. By contrast, atmospheric pipestill can operate at different conditions to process crude oil in a manner best fitted to the product demands. Four different sets of operating conditions or modes of operation are employed for the atmospheric tower for each type of crude oil; these modes are: base case, max heavy naphtha, max kerosene, and max diesel. Each mode is described by a set of constraints on the TBP curves of the products from atmospheric pipestill, as shown in Table 2.

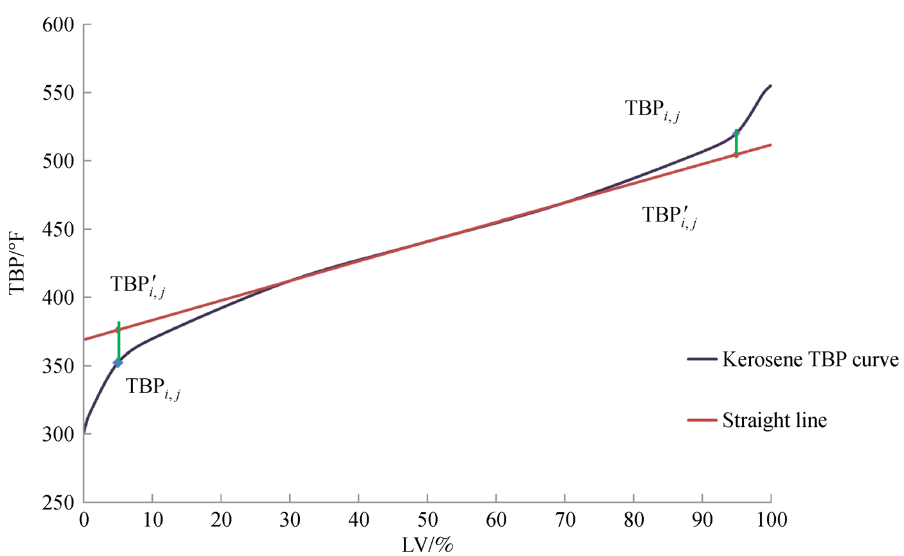

Fig. 3 Predicting the kerosene TBP curve

Table 1 Properties of crude oil 1 and crude oil 2

TBP	Unit	Crude oil 1	Crude oil 2
1	F	–32.0	–17.5
5	F	96.9	94.9
10	F	196.0	183.4
30	F	402.8	413.4
50	F	567.0	626.9
70	F	771.8	865.9
90	F	1143.2	1232.7
95	F	1331.7	1396.4
99	F	1531.9	1545.6
API		34.2	32.0
Sulfur	wt%	2.4	2.3

The yields of each product based on the equidistance assumption are shown in Table 3. The volumetric transfer ratio proposed by Li et al. (2005) is used to determine the size of each swing cut. The results are shown in Table 4. The plant operating data (Table 5) are generated using the rigorous CDU model in Aspen Plus as a surrogate. The data in Table 5 are used to calculate the yield biases for the model, which uses the equidistance assumption. The results are shown in Table 6.

The average of the biases shown in Table 6 is used as the bias for correcting the yields obtained by using the equidistance assumption. All other conditions are exactly the same, including models of the downstream processing units, product demands, inventory constraints, and objective function (minimizing total cost). The resulting biases have the largest error for yields of diesel (1.4%) at "max diesel" operating mode, which is greater than the error of the hybrid CDU model (–0.4%) at the same operating mode.

The key advantage of the hybrid CDU model over the swing cut + bias CDU model is its capability to predict CDU operation under any set of operating conditions. On the other hand, the swing cut + bias CDU model is calibrated for specific operating modes. Thus, if the optimum operation lies between predetermined operating conditions or modes, then the hybrid CDU model can take advantage of such operation. In addition, the hybrid CDU model is able to predict correctly the outcome of processing crude feedstock (operating conditions and product yields and qualities) which has not been previously processed in the plant.

4 Production planning outcomes with different CDU models

The refinery model used in this study is shown in Fig. 4. The crude unit is modeled either by the swing cut + bias or hybrid CDU model described previously. The catalytic reforming unit is represented by two instances, so that the optimization algorithm in each period can select two different modes if the demand pattern requires more than one operating mode in a given period. Similarly, fluid catalytic cracking (FCC) is represented by two instances, whereas hydrocracking (HC) is represented by three. The refinery produces two grades of gasoline, kerosene, and two grades of diesel and has a capacity

Table 2 Product TBP specifications for different operating modes

Op. mode	HNaphtha 95	Kero 95	Diesel 95	Kero 05	Diesel 05	AGO 05
	F	F	F	F	F	F
Base case	360	520	640	350	460	540
Max HNaphtha	380	520	640	360	460	540
Max Kerosene	340	540	640	330	470	540
Max Diesel	360	520	660	350	460	560

Table 3 Product yields (% of CDU feed) based on equidistance assumption

CDU feed	Op. mode	HNaphtha /%	Kerosene /%	Diesel /%	AGO /%
Crude oil 1	Base case	6.08	13.55	8.50	17.62
	Max HNaphtha	6.96	12.68	8.49	17.62
	Max Kerosene	4.74	16.06	7.31	17.64
	Max Diesel	6.08	13.39	10.64	15.64
Crude oil 2	Base case	4.74	10.06	7.65	12.86
	Max HNaphtha	5.64	9.19	7.63	12.86
	Max Kerosene	3.68	12.05	6.70	12.88
	Max Diesel	4.74	9.89	9.74	10.93

Table 4 Swing cut sizes (% of CDU feed) using the volumetric transfer ratio method

CDU feed	HN	Naphtha/Kero	Kero	Kero/Diesel	Diesel	D-A	AGO
Crude oil 1	4.74	2.23	12.68	1.15	7.31	2.18	15.46
Crude oil 2	3.68	1.95	9.19	0.92	6.70	2.12	10.75

Table 5 Product yields (% of CDU feed) from rigorous simulation

CDU feed	Op. mode	HNaphtha/%	Kerosene/%	Diesel/%	AGO/%
Crude oil 1	Base case	5.62	16.95	10.72	12.47
	Max HNaphtha	6.71	15.74	10.86	12.45
	Max Kerosene	4.32	20.80	7.61	13.02
	Max Diesel	5.62	16.83	13.12	10.18
Crude oil 2	Base case	4.35	12.76	9.51	8.69
	Max HNaphtha	5.30	11.70	9.64	8.67
	Max Kerosene	3.25	15.92	7.02	9.12
	Max Diesel	4.35	12.65	11.60	6.71

Table 6 Yield biases (% of CDU feed): swing cut vs. rigorous model

CDU feed	Op. mode	Heavy naphtha	Kerosene	Diesel	AGO
Crude oil 1	Base case	–0.46	3.40	2.21	–5.15
	Max HNaphtha	–0.25	3.06	2.37	–5.17
	Max Kerosene	–0.42	4.74	0.30	–4.62
	Max Diesel	–0.46	3.44	2.48	–5.46
	Average	–0.40	3.66	1.84	–5.10
Crude oil 2	Basic	–0.39	2.71	1.86	–4.17
	Max HNaphtha	–0.33	2.51	2.02	–4.19
	Max Kerosene	–0.43	3.87	0.32	–3.76
	Max Diesel	–0.39	2.75	1.86	–4.22
	Average	–0.39	2.96	1.51	–4.09

of 100000 barrels/day. The model is written in GAMS and solved by the ANTIGONE global solver.

Two period planning models are used for the case study to ensure that the global optimum can be computed. A small number of periods in a planning model, which optimizes the operating conditions and inventories, is consistent with the inventory pinch approach to production planning (Castillo and Mahalec, 2014). Once the optimal conditions are computed, they are used in a lower level fine-grid multiperiod model to determine the amount to produce in each period, identify the operating modes, and compute the blend recipes. In this example, each period corresponds to one day (It can correspond to a week, a month, or three months etc.) in order to be able to relate the results easily with typical operational numbers.

The product demand pattern has been specified such that all demands can be met with any of the CDU models. Three crude oil mixes are used.

The refinery model shown in Fig. 4 was created in GAMS and was optimized using ANTIGONE. Three cases were run, each of them with a fixed composition of the CDU feed. The optimal amounts of the feed to each of the operating modes of the processing units have been computed for the swing cut + bias CDU model. On the other hand, instead of using fixed operating modes, the optimal operating conditions have been computed for the hybrid CDU model. Table 7 shows that both refinery planning models with different crude unit models (swing cut + bias and hybrid) can meet the product demands, which would also be the case in industrial practice, where model accuracy varies from one planning model to another. Nevertheless, all of these models would compute some solutions which planners would consider feasible.

If the refinery models were used to determine which crude oil mix to process for a given product demand pattern, then the conclusions would be as follows:

• Use 80% of crude oil 1 and 20% of crude oil 2 if the swing cut + bias CDU model is used.

• Use 20% of crude oil 1 and 80% of crude oil 2 if the hybrid CDU model is used.

Notably, in our case study the optimal solution determined via the hybrid CDU model is the most

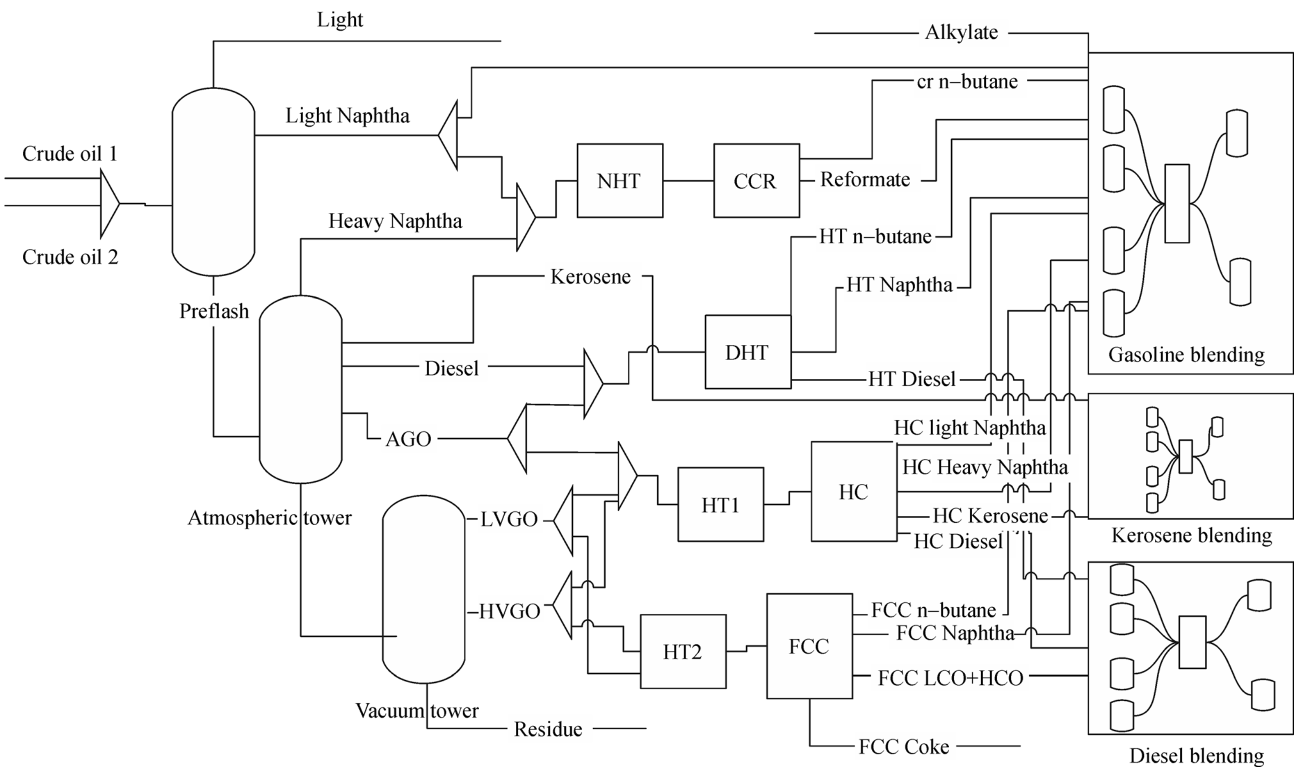

Fig. 4 Sample refinery flowchart

expensive solution computed by the model that employs the swing cut + bias CDU model.

The differences between the two options for CDU modeling lie in the amounts of the feeds to the downstream processing units, which lead to different operating costs and different blend recipes. Taking "Mix #3 as an example, the swing cut + bias CDU planning model uses (4.33%, and 4.33%) of the AP feed as the feeds to the FCC and (25.90% and 25.90%) of the AP feed as the feeds to the HC unit in periods 1 and 2. On the other hand, the planning model with hybrid model of the CDU uses (4.33% and 4.33%) of the AP feed as the feeds to the FCC and (21.41% and 23.33%) of the AP feed as the feeds to the HC unit in periods 1 and 2, respectively. The main difference between the two models is the amount of the material processed by the HC unit. Given that the swing cut + bias CDU model predicts a high amount of feed to the HC unit, the corresponding refinery model identifies that the feed mixture rich in crude oil 1 is more advantageous than that with crude oil 2 although it contains more sulfur than the latter. The hybrid CDU model predicts a high yield of diesel, thereby reducing the need for processing via the HC unit and leading to the conclusion that the feed mixture rich in crude oil 2 is a better choice than the mixture rich with crude oil 1. Given that the hybrid CDU model predicts the yield of diesel with higher accuracy than the swing cut + bias CDU model, we conclude that the result computed by the refinery model employing the hybrid CDU model is

Table 7 Total cost using different CDU models

Crude oil 1	Mix #1		Mix #2		Mix #3	
	0.2	0.2	0.5	0.5	0.8	0.8
Crude oil 2	0.8	0.8	0.5	0.5	0.2	0.2
CDU model	Swing cut + bias	Hybrid	Swing cut + bias	Hybrid	Swing cut + bias	Hybrid
Regular gasoline	42	42	42	42	42	42
Premium gasoline	48	48	48	48	48	48
Kerosene	25	25	25	25	25	25
Diesel 0	0	0	0	0	0	0
Diesel 1	14	14	14	14	14	14
Cost, 10^3 \$/day	8032.1	7237.1	7224.7	7475.7	6411.2	7711.6

more accurate than that computed by the refinery model employing the swing cut + bias CDU model.

As long as downstream units have sufficient capacities to process any feed computed by the CDU model, the influence of different CDU model versions leads to different processing routes within the refinery and different blend recipes. Refinery optimization can lead to different feed mixes which are deemed to be optimal depending on the accuracy of the CDU model. An inaccurate CDU model will make the refinery process the available crude feedstocks in a suboptimal manner and incur significantly higher operating costs than necessary.

This can sometimes lead to vastly different costs (Table 7). In the case of Mix #3, the refinery will incur additional operating costs of approximately $1 million/day because of the suboptimal routing of intermediate streams.

If downstream units do not have sufficient capacity to process the inaccurate amounts of feeds predicted by an erroneous CDU model, then the planning model will be infeasible for a given crude oil mix and the refinery will adjust the operation on the basis of what they see as the actual yields or will erroneously conclude that they have to change the crude oil mix. This situation will have a significant influence on the profitability of the refinery. By contrast, the refinery will make such a decision only when it is actually required if the CDU model is accurate.

Notably, the hybrid CDU model predictions can be improved by adding a bias, similar to the swing cut + bias CDU model. Given that the hybrid CDU model employs the operating variables as the decision variables, such bias term can be related to the plant operating conditions instead of only averaging over all ranges of operations. This case will be investigated further in our future work.

5 Conclusions

The case studies presented in this work show that using an accurate CDU model leads to substantially different refinery production plans than those computed by the current best model (swing cut + bias) used in industrial practice. Refinery planners do not necessarily realize that the production plans based on erroneous CDU models are suboptimal because refineries have many degrees of freedom. In practice, planning model inaccuracies are difficult to detect because the operating instructions for the CDU are frequently expressed as, e.g., "produce yield of *xx* % of product P, subject to 95% point being less than *yy* °F." From experience, the planner or scheduler knows that instructions should be phrased as illustrated above to ensure that they lead to a feasible operation. The optimal operation may in fact be to draw the product P exactly at 95% point, but inaccurate CDU models do not allow for such a conclusion.

As illustrated by the case studies, inaccurate CDU models may lead to substantially different costs in refinery operation. These results indicate that the refiners can gain substantial financial benefits by using accurate CDU models in refinery-wide optimization models.

Acknowledgements This work has been supported by the Ontario Research Foundation, McMaster Advanced Control Consortium, and Imperial Oil.

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