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Theoretical Sensitivity Analysis of Fully Integrated Crude Fractionation Unit

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Abstract

Integrated distillation systems reduce the energy consumption of industrial processes, so the use of integrated units in modern large-scale refineries is a matter of current interest. On the other hand, thermal and mechanical integration along with the complexity of multicomponent mixtures cause simulation and control difficulties. The objective of the research is to study energy efficiency and parametric sensitivity of the fully integrated crude fractionation unit (FI CFU, Petlyuk column). This type of column was designed to maximize diesel recovery and ensure that the fraction recovered meets the key specifications for diesel. We also selected the most suitable control parameters and specified the reflux rate areas of potential unstable operation.

Keywords: *Energy saving; Oil refining; Integrated distillation systems; Multicomponent mixture; Sensitivity analysis.*

1. Introduction

Oil refineries are a major consumer of industrial energy: according to U.S. Energy Information Administration, they account for about 8% of total energy consumption [1]. Crude Distillation Units (CDU) or Crude Fractionation Units (CFU) separate oil into a number of distillates. With their maximum capacity, the units consume a lot of energy – equivalent to 2% of the total oil processed [2]. Thus, even a moderate decrease in energy consumption makes economic sense, especially for large-scale industries. At the same time, its thermodynamic efficiency is no larger than 12%, and researchers see a room for significant improvement of the process [3]. For example, 5% of thermodynamic improvement may lead to 39% reduction in utility cost [4]. Also, the global need for better sustainability gives an additional incentive to the development of novel distillation concepts.

All innovative principles applied in distillation process and equipment design are presented by heat pump assisted technologies (vapor compression (VC), mechanical vapor recompression (MVR), thermal vapor recompression (TVR), absorption heat pump (AHP), compression-recompression heat pump (CRHP), thermo-acoustic heat pump (TAHP), and heat integrated distillation column (HIDiC)), cyclic distillation, reactive distillation (RD), thermally coupled (Petlyuk) and dividing-wall columns (DWC). The latter integrates two Petlyuk columns in a single shell [3].

A great number of studies have focused on the development of integrated distillation schemes, their efficiency and controllability. It is worth noting that the application of integrated distillation schemes includes the separation of different mixture types – from binary and ternary to multicomponent and continuous.

In his thesis, Rijke [5] presented an extensive analysis of different distillation schemes and their efficiencies. He compared traditional distillation sequences, sequences with heat pump and integrated distillation for separation of propane-propylene fraction. The calculations showed that traditional distillation requires 2-10 times more energy than an integrated system. Kaibel *et al.* [6] focused their study on the separation of three and four component mixtures in a dividing-wall column and reported about 10 – 40% energy savings in comparison with the conventional scheme. Hernandez *et al.* [7] performed thermodynamic analysis of the

Petlyuk column for a ternary mixture and predicted the energy savings of up to 50% if the integrated technology is implemented on the industrial scale. Caballero and Grossmann [8] consider the development of energy-efficient integrated distillation schemes for multicomponent fractioning (5 and more components) and point out that the integration reduced the energy consumption by about 30%. The advisability and practicability of integrated systems for multicomponent mixture separation was shown by Jana and Mali [9]. Furthermore, Lee *et al.* [10] demonstrated investment savings and reduction in energy consumption when integrated distillation was used for multicomponent mixtures, as illustrated by aromatic recovery from catalytic reforming products.

The next step of research in this field is supposed to include advanced separation of continuous mixtures. Although the cost efficiency of integrated distillation systems can be considered a generally accepted fact, even the latest research has mainly focused on advanced distillation of three or four-component mixtures [11]. Our paper aims to fill this gap and estimate the energy efficiency of oil separation in the Petlyuk column.

Atmospheric crude oil fractionation produces three and more products, so this makes considerable profit for large-scale refineries. However, consistent and in-depth studies of strengths and shortcomings of CFU integrated schemes are currently in very short supply [12].

It is commonly accepted [13-14] that industrial application of integrated schemes is limited due to their complicated modeling and control, especially in the case of multicomponent and continuous mixtures, not least because of the possibility of multiple steady states [15-16]. Another control problem of thermally coupled distillation systems is highlighted by Miranda-Galindo and Segovia-Hernandez [17], who concluded that integrated systems are far less controllable under at optimal conditions than under non-optimal ones. Jia *et. al.* [18] considered the convenient control structure of the three-product Petlyuk column using only temperature controllers. However, temperature control scheme fails to handle the disturbances for more complex cases. For instance, Qian *et. al.* [19] investigated pressure-compensated temperature difference control for four-product extended Petlyuk dividing-wall columns and suggested to employ pure temperature controllers as more recommended than composition controllers in the industrial process. However, pure temperature and pressure control schemes still require laboratory testing of product quality and composition. Virtual analyzers significantly reduce the number of tests, but their existing types calculate the flow composition and qualities based on temperature and pressure dependences and only function adequately within a narrow range of parametric variation [20]. The accuracy and prediction ability of virtual analyzers could be improved by a substantial mathematical model based on MEH equations. Therefore, for a multicomponent integrated distillation, it is worth developing a fundamental mathematical model, appropriate for direct quality control under optimal operating conditions and suitable for multiplicity analysis.

Wang *et al.* [16] link unstable operation with the parametric sensitivity of the system. Hence, further development of control schemes and selection of appropriate manipulated inputs require quantitative evaluation of parametric sensitivity.

Some sensitivity tests were carried out by Mali and Jana [21] and Tavan [22] for reactive distillation columns. They plotted controlled variables, such as energy consumption, product purity, temperature profiles and so on, against design and operating variables to find out optimal integrated schemes simulated in Aspen. These studies were solely based on step-by-step changes in manipulated variables and observation of subsequent changes in controlled ones. None of these studies used sensitivity analyses to estimate the comparative level of influence from each variable. Smith *et al.* [23] highlighted some aspects of sensitivity analysis applications, such as the choice of operating point and manipulated variables. The authors showed a number of techniques for analyzing parametric sensitivity using simple model examples that are far from the topic of our work.

All the works above contain many useful principles for sensitivity analysis but it is still challenging to find a practical study focused on certain regions of high parametric sensitivity as a source of potential control problems. Since industrial implementation of advanced distillation is an important strategic objective, we consider it reasonable to implement sensitivity analysis to real FI CFU based on an adequate mathematical model. We suppose that the analysis enables one to operate the column in the optimal region without sacrificing controllability. We find it possible to reveal regions with high parametric sensitivity using RSF (Relative Sensitivity Functions). Ranjbar *et al.* [24] highlighted a prominent role of RSF for determining the optimum operating conditions of the unit.

In the present work, we simulate a fully integrated crude fractioning column (Petlyuk column) with a capacity of 18.5 t/h in Aspen HYSYS^{TM} and evaluate its energy consumption compared to a conventional one. We propose parametric sensitivity analysis of control parameters based on developed fundamental mathematical model. As a result, we specify the most appropriate control parameters and their values corresponding to stable operation and desirable diesel quality.

A solution to the control problems that we are searching for in this study will help accelerate the implementation of the Petlyuk column in the oil refining industry. The approach is implementable for a wide range of advanced distillation units, including non-atmospheric FI CFU, dividing-wall columns, and reactive distillation columns.

2. Materials and methods

2.1. Simulation and comparison of conventional and fully integrated units

The conventional and fully integrated schemes of CFU are presented in the Figs. 1, 2.

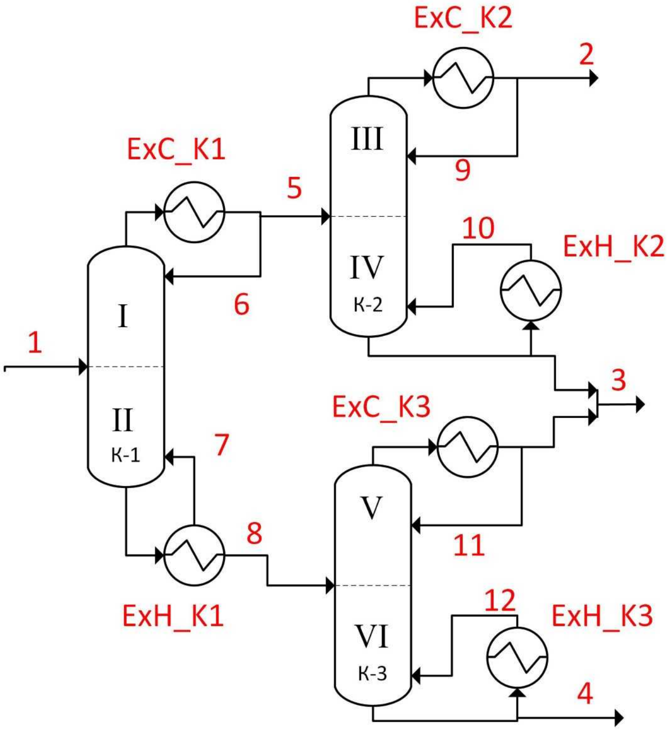

Fig. 1. Conventional crude fractionation unit

Streams are marked with Arabic Figs: 1 – oil; 2 – straight-run gasoline; 3 – diesel (side stream); 4 – oil residue; 5 – liquid-vapor mix to K-2 (feed K-2) from K-1; 6 – reflux K-1; 7 – boilup K-1; 8 – liquid-vapor mix to K-3 (feed K-3) from K-1; 9 – reflux K-2; 10 – boilup K-2; 11 – reflux K-11; 12 – boilup K-3. Heat flows: ExC_K1: -1.273 MW; ExC_K2: -0.911 MW; ExC_K3: -0.688 MW; ExH_K1: +0.889 MW (+0.407 MW for heating stream 8 before K3); ExH_K2: +0.438 MW; ExH_K3: +0.215 MW

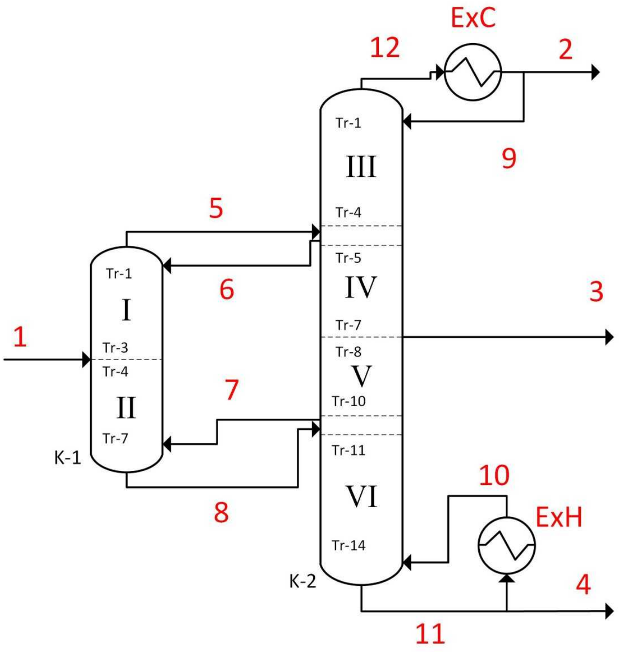

Fig. 2. Fully integrated scheme of oil distillation (Petlyuk column)

Streams are marked with Arabic Fig.s: 1 – oil; 2 – straight-run gasoline; 3 – diesel (side stream); 4 – oil residue; 5 – vapor from K-1; 6 – reflux K-1; 7 – vapor from K-2; 8 – liquid from K-1; 9 – reflux K-2; 10 – boilup.
Heat flows: ExC: -1.065 MW;   ExH +1.778 MW

Both conventional and fully integrated CFUs were simulated in Aspen HYSYS^{TM}. They were divided into six sections restricted by inlet and outlet flows, namely feeds and products, as assumed by Proios and Pistikopoulos [25]. The number of trays in each section was equal for both schemes. Loads, feed compositions, product temperatures and compositions were the same (or very close) for both schemes (Tables 1, 2).

Table 1. Design variables of CFUs

Parameter	CFU without integration	Petlyuk
Number of trays per section (without condensers and reboilers)		
Section I	3	3
Section II	4	4
Section III	4	4
Section IV	3	3
Section V	3	3
Section VI	4	4

Table 2. Feed and product composition data

Parameter	CFU without integration	Petlyuk
load	K-1 kmol/h 95 t/h 18.5	K-1 kmol/h 95 t/h 18.5
Feed composition, vol.%	IBP 53 10 % 110 50 % 318 90 % 450 EBP 533	IBP 53 10 % 110 50 % 318 90 % 450 EBP 533

Parameter	CFU without integration	Petlyuk
Distillate composition, vol.%	K-2 IBP 53 10 % 64 50 % 119 90 % 172 EBP 217	K-2 IBP 53 10 % 64 50 % 119 90 % 170 EBP 194
Side stream composition, vol.%	Res K-2 + dist K-3 IBP 150 10 % 195 50 % 228 90 % 296 EBP 364	K-2 IBP 164 10 % 194 50 % 239 90 % 322 EBP 364
Residue composition, vol.%	K-3 IBP 293 10 % 348 50 % 389 90 % 495 EBP 533	K-2 IBP 352 10 % 371 50 % 399 90 % 502 EBP 533

Fig. 3 summarizes the comparison of energy efficiency for conventional and fully integrated structures.

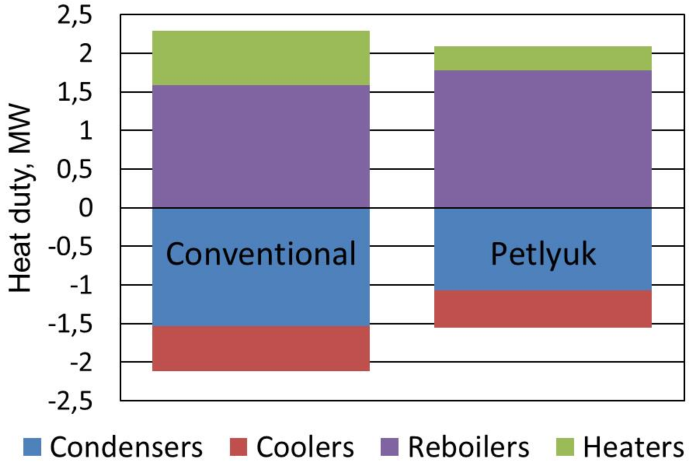

Fig. 3. Energy consumption of the conventional CFU and the Petlyuk column

Fig. 3 was based on the following assumptions:

1. Initial temperature of crude oil is 12°C.
2. Temperatures of gasoline, diesel fraction and residue, directed to the product storage, are 30, 60 and 90°C, respectively.
3. The heat of product streams from the top of the columns is used for crude oil and bottom heating. Thus, because heat flows in Fig. 3 account for the internal flows of the process flow diagram, they differ from the data shown in Fig. 1, 2 by the values of the internal heat flows. The values of preheat and intermediate heating are not shown in Fig. 1, 2 but are taken into account in Fig. 3.

Energy savings (%) were calculated as:

[total (conventional) – total (Petlyuk)]/ total (conventional)

The results demonstrate 8.7% saving in terms of heat supply and 2.4% saving in terms of heat removal.

2.2. Parametric sensitivity analysis

The main goals of control are to maintain recovery and product specifications in the operation region. Since integrated CFU was found more effective, it is important to evaluate the effects of different parameters on aimed (controlled) variables.

The method of research includes calculations of the relative parametric sensitivity function (S_E^F) and the analysis of the variable parameter vs. relative parametric sensitivity function.

Relative sensitivity of function *F* to parameter *E*, evaluated at the operating point, was given in many studies [23, 26].

$$S_E^F = \frac{\partial F}{\partial E} \cdot \frac{E^0}{F^0} \tag{1}$$

2.2.1. Selection of input and controlled variables

The purposes of the newly developed CFU are to provide the maximum recovery of light fractions and to follow the key specifications for diesel. Recovery can be estimated by the presence of light components in the residue.

Product composition completely specifies its quality [27]. The key specification for diesel, along with sulfur content, is a cetane number or cetane index; you can easily derive one from the other using aniline point [28].

ASTM (ASTM-D4737 2009) recommends calculating the cetane index by four variables: density and temperature values of 10%, 50%, 90% fractions recovered. Thus, the components with NBPs corresponding to the desirable cetane index are the appropriate variables for diesel quality control.

Diesel fraction with a cetane index of more than 45 requires the following NBPs: T10≤195, T50≤235, T90≤345. We used the hypothetical fractions given by HYSYS with NBPs T10≤193, T50≤235, T90≤335 as control parameters, and our calculations showed the cetane index of diesel fraction to be equal to 45.969 in this case.

The main aim of further studies is quality control of diesel fractions recovered by the side stream of K-2 (see Fig. 2). Given that the vapor flow is more difficult to manipulate both in the main column (K-2) and between the main column and the prefractionator (K-1) than the liquid flow [29], we considered the sensitivity of diesel fraction specifications to the liquid flow.

The list of controlled variables in the corresponding flow of the product (see Fig. 1) taken from the Hysys model is presented in Table 3.

Boilup and reflux rates are in routine use as manipulated inputs, which specify temperature and rate profiles. Vapor split (R_V) as an additional degree of freedom was applied for the operation of a divided wall column by Dwivedi *et al.* [30] (where R_V ≡ fraction of vapor boilup sent to prefractionator from the main column). In our case, vapor split (R_V) and liquid split (R_L) served as inputs in sensitivity analysis (R_V, R_L ≡ fractions of vapor boilup and liquid reflux, sent to prefractionator from the main column, respectively). The function was used to analyze the sensitivity of the product quality and recovery in an integrated CFU.

Table 3. Controlled variables

№	Variable/Hysys	Flow symbol	Controlled property
1	IBP-NBP 193	3	diesel quality
2	IBP-NBP 235	3	diesel quality
3	IBP-NBP 335	3	diesel quality

2.2.2. Operating point conditions

The model developed in Aspen Hysys^{TM} enabled us to obtain operating point (OP) conditions. In the process of relative sensitivity calculations, the splits, reflux and boilup rates were varied under the conditions of mean temperatures, pressures and equilibrium constants for every section. OP conditions for all manipulated inputs are listed in Table 4. Inputs varied from 50 to 150% from OP numerical values in the process of calculation.

Table 4. OP conditions

Input	Numerical value	Input	Numerical value
B	72 kmol/h	R_V	0.7
R	140 kmol/h	R_L	0.1

2.2.3. Relative sensitivity calculation

The relative sensitivity calculation implies an explicit form of a controlled variable through the inputs, so the equations of component material balance for the main column were developed using the approach reported in [26].

$$X_{jSS} = \frac{X_{jn}}{\frac{R\cdot(1-R_L)-SS}{R\cdot(1-R_L)}\cdot\left(\sum_{i=0}^{n-1}\left(\frac{R\cdot(1-R_L)-SS}{R\cdot(1-R_L)\cdot K_j}\right)^i+\left(\frac{R\cdot(1-R_L)-SS}{R\cdot(1-R_L)\cdot K_j}\right)^n\right)} \qquad (2)$$

Following the approach described by Samborskaya *et al.* [26], we were able to obtain a rapid evaluation of the impact of control and design parameters on the process on a wide variability interval. Besides, the model forms the basis of optimization, multiplicity and parametric sensitivity analysis. The model includes equilibrium constants calculated at mean temperatures in the sections. Non-ideal behavior of the mixture could also be taken into account but it can be neglected in the case of hydrocarbon mixtures.

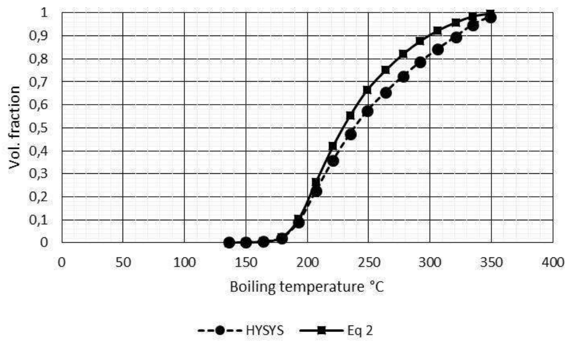

Fig. 4. Side stream compositions

The method is verified using the composition and specifications of diesel fuel as an example. Fig. 4 shows the compositions obtained by HYSYS and the described method. The cetane indexes corresponding to both calculation approaches differ by less than one point (46.3 – HYSYS, 45.7 – equation (2) [26]).

HYSYS–hysys-calculated composition; Eq. 2–composition calculated using equation (2).Sensitivity coefficients S_E^F are calculated and normalized by means of MathCad. As a result, the sensitivity coefficients vs. inputs rates were studied within the operating range framework.

3. Results and discussion

The authors have studied the parametric sensitivity of side stream composition in section V to locate the region of operational stability, where *F* is the product stream composition and *E* denotes the reflux, or liquid split residue rates. Side stream is commonly used as a diesel motor fuel, so its composition is strictly regulated. The relative sensitivities calculated for section V (Figs. 5, 6) enable us to recommend the appropriate operation conditions and control loop.

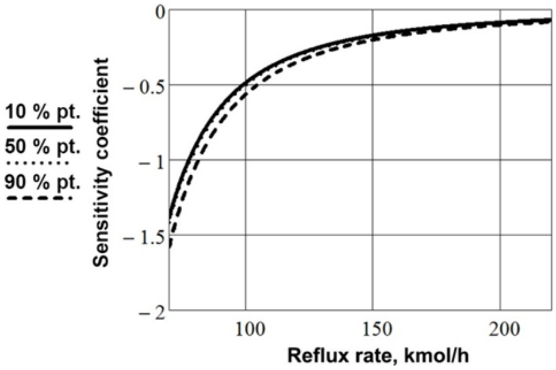

Fig. 5. Parametric sensitivity of controlled variables in section V to reflux rate

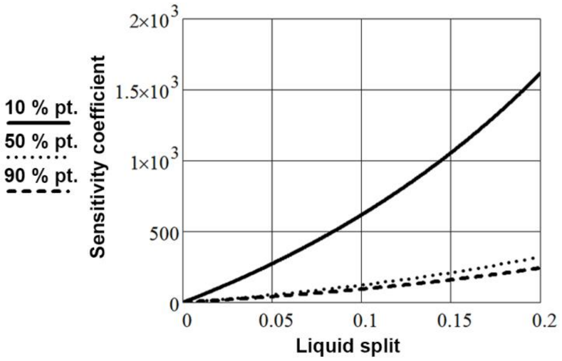

Fig. 6. Parametric sensitivity of controlled variables to liquid split (section V)

As Fig. 5, 6 show, the sensitivity of diesel specifications to the liquid split is significantly higher than their sensitivity to the reflux rate. The measurement scales of the vertical axes indicate the difference between and to be several orders of magnitude. The particular diversity in sensitivity coefficients within section V is presented in Table 5.

Table 5. RSFs for control variables

E	S_E^{10}	S_E^{50}	S_E^{90}
R_L (0.05 -0.15)	275 – 1050	50 – 200	50 – 150
R (70 - 210)	(-1.4) – (-0.07)	(-1.4) – (-0.07)	(-1.6) – (-0.08)

The ranges of liquid split and reflux rate were taken considering the percentage of variation (50–150%) around the operating point (Table 4). According to Table 5, the liquid split fluctuations can lead to unstable operation of the column. In order to find the areas of unstable operation, we expanded the interval of reflux rate variation from 30 to 220 kmol/h and did calculations under slight deflections of the split rate related to the operating point. The most essential results for low reflux rates are similar for all NBPs. The summary picture is reproduced in Fig. 7.

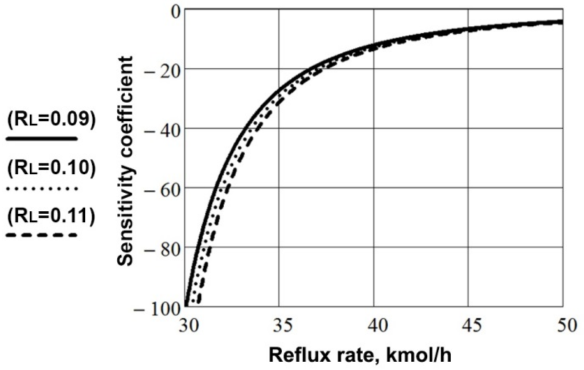

Fig. 7. Parametric sensitivity under different liquid splits

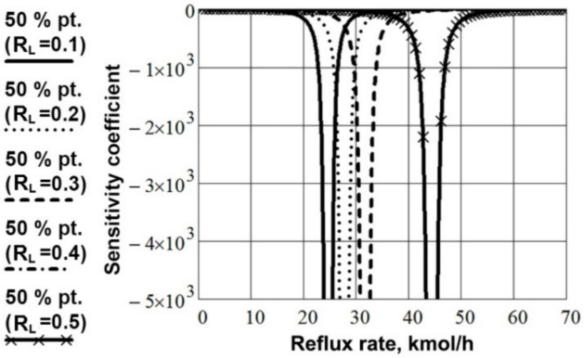

Fig. 8. Parametric sensitivity of temperature of 50% fractions recovered under different liquid splits (significant deviations)

Obviously, slight fluctuations of the split rate lead to unstable operation of the column under reflux rate R=50 kmol/h. The difference in behavior before and after the point R=50 kmol/h most likely stems from the weakening role of the split with an increase in R. When R is comparatively low, slight split fluctuations lead to temperature changes, which obviously affect equilibrium constants and product composition. An increase in R gradually negates the influence of split on the composition, and at $R \geq 50$ product quality is determined by reflux rate only. In the region of slight fluctuations of split over the OP = 0.1 (R_L = (0.09–0.11)), all controlled variables show remarkably high sensitivity. More significant changes in the split rate confirm that conclusion (the example for under R_L = (0.1–0.5) is given in Fig. 8).

For clarity, the region of the reflux rates under study has been shifted to the zone of minimal R (0–70) kmol/h. Sensitivity coefficients under major changes of liquid split are dramatically high for R = (20–50). This fact confirms the recommendation not to reduce reflux rate lower than 50 kmol/h.

On the other hand, it could be problematic to avoid undesirable regions of manipulated parameters, especially during startup and shutdown operations. The values of liquid split and reflux rate are in direct correlation: the lower the reflux rate, the lower the liquid split. For example, according to Fig. 8, if the reflux rate in an unstable region R = (40–50), the liquid split should be $R_L \leq 0.4$. Thus, we identified the intervals of stable operation of the Petlyuk column (in relation to the diesel specifications).

In summary, the presented approach to sensitivity analysis is suitable for different multicomponent integrated systems in accordance with standards and technical requirements for the desired product.

4. Conclusion

Current environmental challenges call for the use of advanced crude oil fractioning technology on an industrial scale. Our calculations have proved that oil refineries will gain energy benefits if they switch to advanced oil distillation. This paper views mathematical modeling as a way to overcome control difficulties of the FI CFU (Petlyuk column) given the multicomponent character of crude oil and complex interactions between internal flows in integrated systems. Sensitivity analysis enables us to avoid regions of unstable operation and maintain product quality at a required level.

The most significant results of the study are:

- The energy efficiency analysis of the FI CFU in comparison with conventional refinery unit has shown that the FI CFU column saves 8.7% in terms of heat supply and 2.4% in terms of heat removal.
- Sensitivity of diesel specifications to the liquid split is higher than their sensitivity to the reflux rate, and fluctuations in the liquid split rate can lead to the unstable operation of the Petlyuk column.
- The composition of diesel fraction is better controlled by the reflux rate. The reflux rate areas of potential instability are specified (R=20–50). Operation in the unstable region requires the liquid split to be kept as low as possible.

The proposed mathematical model is fundamental and can be implemented for sensitivity and multiplicity analysis of various integrated systems (for example, dividing-wall column and reactive distillation). On the other hand, the model is appropriate for steady state operation only, and the development of a dynamic model is a matter of further studies.

The described method of theoretical sensitivity analysis makes it possible not only to specify the best control parameters, but also to develop predictive controllers and virtual analyzers of stream composition and product specifications, which facilitates the industrial application of integrated schemes.

Symbols:

B	*boil-up rate, kmol/h;*
CDU	*crude distillation unit;*
CFU	*crude fractionation unit;*
E	*variable;*
ExC	*condenser;*
ExH	*reboiler;*
F	*function dependent on E;*
FI CFU	*fully integrated crude fractionation unit;*
IBP	*initial boiling point;*
K	*equilibrium constant;*
MEH	*material, energy and heat balances;*
n	*number of trays;*
NBP	*normal boiling point;*
R	*reflux rate, kmol/h;*
R_L	*liquid split rate, kmol/h;*
RSF	*Relative Sensitivity Function*
R_V	*vapor split rate, kmol/h;*
$\boldsymbol{S_E^F}$	*relative coefficient of function F parametric sensitivity to the variable E.*
SS	*side stream rate, kmol/h;*
x, y	*liquid and vapor molar parts respectively;*

Indexes:

0 – operating point;
SS –side stream concentration;
j – component number.

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Declarations of interest: none.

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