

A Method for the Petroleum Products Quality Estimation in Advanced Software Simulation Schemes

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Due to the high-order costs implied by the online analyzers, nowadays research and industry offer some alternative methods for the products quality estimation. This work focuses on one of these methods, by using a dynamic software simulator with integrated modules for quality estimation. It proposes a mathematical model to calculate the initial and final boiling temperatures for a petroleum fraction, using an algorithm based on the experimental True Boiling Points (TBP) curve determination methodology. The model is validated by its integration as a part of the software simulator for an industrial crude oil processing plant. The simulation results prove a good accuracy, this way the method becoming an interesting subject for a real industrial implementation.

Keywords: products quality, software simulation, crude oil plant

The current tendency of integrating the advanced control structures practically in any refinery plant always encounters the same problem – the online determination of products quality indicators [1-4, 10, 11]. Classically, it can be firstly solved by using the well-known product analyzers, with excellent results in terms of accuracy, but with high investment and exploitation costs. Moreover, speaking about the advanced product quality control, the measurement procedure may face some serious problems when the process intrinsic dynamic characteristics give it a higher speed compared with the analyzers' cycle [1]. This is why a second variant may be taken into account, one that is being represented by using a process mathematical model, which could give the appropriate quality parameter as normal output [12]. Of course, such a software online analyzer always raises three important questions:

- does such a (dynamic) model for the studied process exist?
- does such a software simulator which works in perfect synchronism with the process exist?
- is the result accuracy by the inferential calculus method (an approximate one) for the quality indicators affected?

Of course, when the answers to these questions satisfy the user, the much lower costs can be added on the *positive facts*. Obviously, this case represents an ideal one, when a minimum investment could yield the same results like using the complex online analyzers.

Such a case is illustrated by this work, which concerns the product quality estimation for a classical crude oil unit. The theoretic principles are presented, as well as the associated mathematical model. The software analyzers are integrated and tested in a more complex simulation platform (subject to our previous works [5-8]), with good results compared to the real ones, obtained from a dedicated hardware analyzer.

Products quality indicators for a crude oil unit

The crude oil, as well as its associated distillation products, are very complex mixtures, with a big number of pure components, very hard to predict in terms of appearance and percentage. This is why a different

approach was adopted, these mixtures being characterized by their distillation curves, which make a logical connection between the distillation temperature and the total amount of the distilled product (expressed as a percentage).

Figure 1 shows the three curves used in the industry to characterize an arbitrary petroleum product: True Boiling Points (TBP), American Society of the International Association for Testing and Materials (ASTM) and Equilibrium Flash Vaporization (EFV). All these curves are directly connected between them, this is why some well-known transformations are presented in [1, 2].

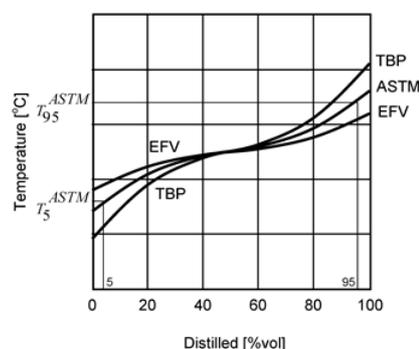


Fig. 1. Distillation curves – TBP, ASTM and EFV

From the practical point of view, these curves allow in fact the same product characterization by its boiling points. As *safety* measure, the complete non-distillate (0%) and distillate points (100%) are replaced, for instance, by T_5^{ASTM} and T_{95}^{ASTM} (associated with more feasible practical limits of 5 and 95% distillate, respectively). These temperature points give a clear indication of light and heavy components presence (and proportion) in the characterized mixture, while the temperature associated with 50% distilled represents its *medium* boiling point.

According with the petroleum market rules, in the industry, the crude oil distillation products specifications are expressed through indicators on both ASTM and TBP curves:

- the initial boiling point, T_5^{ASTM} ;
- the final boiling point, T_{95}^{ASTM} ;

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-the consecutive products gap,

$$T_{5 \text{ heavier product}}^{ASTM} - T_{95 \text{ lighter product}}^{ASTM}$$

-the consecutive products superposition,

$$T_{100 \text{ lighter product}}^{TBP} - T_{0 \text{ heavier product}}^{TBP}$$

Although not so often remarked on normal specifications, the consecutive products gap and superposition reflect a fine observation on the distillation process performance, with three situations:

- good separation (positive gap, zero superposition);
- poor separation (positive gap, positive superposition);
- unsatisfactory separation (negative gap, positive superposition) [1-3].

This work proposes a direct calculus method for the petroleum products quality indicators estimation. Instead of using a direct connection with the high-cost process analyzers, this pertinent approach takes the output signals offered by an online computer, which simulates the related plant in a perfect synchronism. In this case, the simulator output of interest are the products initial and final boiling temperatures (as aggregated quality indicators), extending the simulation applicability from a theoretical approach in the plant study to a direct method used in process control [9].

The initial and final boiling point indicators estimation

It is given a petroleum fraction characterized by NC number of pseudo-components (including water as the last component, NC), having as concentrations x_1, x_2, \dots, x_{NC} mole fractions. The $NC-1$ hydrocarbon pseudo-components (usually determined from the associated TBP curve) have the temperatures $T_1 < T_2 < \dots < T_{NC-1}$ as true boiling points. From these input data we want to obtain the product initial and final boiling points on the TBP curve.

Due to the fact that only the hydrocarbon pseudo-components count when calculating these indicators, the first step is to re-calculate the other $1, 2, \dots, NC-1$ mole fraction from the dry product, in this way the "water" being eliminated. The following relation takes this phenomenon into account:

$$x'_1 + x'_2 + \dots + x'_{NC} = 1, \quad x'_{NC} = 0. \quad (1)$$

The hydrocarbon pseudo-components remain in the same quantities in the dry product, so the new $1, 2, \dots, NC-1$ mole fractions are calculated by:

$$x'_i = \frac{x_i}{\sum_{j=1}^{NC-1} x_j}, \quad i = \overline{1, NC-1}. \quad (2)$$

At first glance, the initial boiling point corresponds to T_1 , while the final boiling point is associated with T_{NC-1} , these temperatures being the extreme boiling points for pseudo-components in the considered mixture. But this quick answer is wrong, as long as the components mole fractions are not yet taken into account.

In order to determine a suitable mathematical model for this problem, the author of this work proposes the same typical reasoning, which happens when interpreting the data collected during the experimental TBP curve fitting for a hydrocarbon mixture. Such a process suggests a small distillate accumulation (a drop) for the initial boiling point determination, the same fact being true for the final boiling point calculation. For our problem, considering a molar quantity equal to 1 is supposed to be distillate, the requested

minimum quantity will be the sum $\sum_{j=1}^k x'_j$ that satisfies the

relation $\sum_{j=1}^k x'_j \leq \varepsilon_1 < \sum_{j=1}^{k+1} x'_j$, ε_1 being a constant (considered

as parameter) which represents the minimum significant distillate quantity. The initial boiling point is now T_j , corresponding to the j pseudo-component. A similar reasoning may be applied for the final boiling point estimation, the parameter ε_2 being the largest quantity of distillate (when considering the distillation naturally ends). The following relations apply:

$$T_{INITIAL} = T_k \mid \sum_{j=1}^k x'_j \leq \varepsilon_1 < \sum_{j=1}^{k+1} x'_j, \quad (3)$$

$$T_{FINAL} = T_k \mid \sum_{j=1}^k x'_j \leq \varepsilon_2 < \sum_{j=1}^{k+1} x'_j. \quad (4)$$

These temperatures (being the boiling points for a $NC-1$ number of pseudo-components) have discrete values, while the *software analyzer* should have a continuous indication for both indicator outputs, $T_{INITIAL}$ and T_{FINAL} . Consequently, the author of this work used a values correction, so $T_{INITIAL}$ and T_{FINAL} are calculated by linear interpolation between T_k and T_{k+1} , the new relation being as follows:

$$T_{INITIAL} = T_k \mid \sum_{j=1}^k x'_j \leq \varepsilon_1 < \sum_{j=1}^{k+1} x'_j + \left(\varepsilon_1 - \sum_{j=1}^k x'_j \right) \frac{T_{k+1} - T_k}{\sum_{j=1}^{k+1} x'_j - \sum_{j=1}^k x'_j}; \quad (5)$$

$$T_{FINAL} = T_k \mid \sum_{j=1}^k x'_j \leq \varepsilon_2 < \sum_{j=1}^{k+1} x'_j + \left(\varepsilon_2 - \sum_{j=1}^k x'_j \right) \frac{T_{k+1} - T_k}{\sum_{j=1}^{k+1} x'_j - \sum_{j=1}^k x'_j}. \quad (6)$$

The mathematical model for the software analyzer is represented by equations (2), (5) and (6). Obviously, this form does not reflect the dynamic behavior of the real analyzer (as a dead-time element), but we consider that it is only a small flaw. In fact, comparing the analyzer dead-time (a few minutes) with the transient time characteristic for the mass transfer process (usually a few hours for the real plants in the industry), this drawback is not significant at all.

Moreover, the software analyzer mathematical model being the result of physical processes study and not obtained by modeling any particular analyzer, it gives the equations (2), (5) and (6) a large covering area, with pragmatism and robustness. This has been proven (in our case) by integrating the mathematical model into the large dynamic model, which simulates a real-scale crude oil plant [5-8].

The ε_1 and ε_2 practically represent the software analyzer tuning elements, which normally should be practically determined. The author suggests a continuous comparison between the results from equations (5) and (6) and the laboratory analysis and the iterative adjustment of ε_1 and ε_2 until there are pertinent calculated values of the initial and final boiling points. These fine-tuning aspects are quite problematic, but they could be addressed by a very careful constant parameters choice.

Using the software analyzer to estimate the crude oil plant products quality

The mathematical model presented here in equations (2), (5) and (6) was integrated as a special component in the crude oil plant simulator presented in detail in our previous works [7-9]. In fact, for all five products (gasoline,

Component	Boiling point at 760 mmHg [°C]	Component	Boiling point at 760 mmHg [°C]	Component	Boiling point at 760 mmHg [°C]
1	100.025	13	266.910	25	440.239
2	112.689	14	280.770	26	468.194
3	126.632	15	294.640	27	496.088
4	141.351	16	308.531	28	523.978
5	155.770	17	322.461	29	551.906
6	169.706	18	336.384	30	579.736
7	183.637	19	350.305	31	606.183
8	197.574	20	364.231	32	634.124
9	211.476	21	378.098	33	671.969
10	225.346	22	391.929	34	720.116
11	239.205	23	405.764	35	768.645
12	253.057	24	419.619	36	892.754
				WATER	100.000

Table 1
THE PSEUDO-COMPONENTS BOILING POINTS

% vol. distilled	T[°C] (GASOLINE)	T[°C] (NAPHTHA)	T[°C] (KEROSENE)	T[°C] (LGO)	T[°C] (HGO)
1	100.025	114.775	141.429	185.726	222.098
5	100.025	156.226	200.217	242.313	280.831
10	100.346	167.818	215.526	256.963	300.375
30	113.454	188.695	238.913	282.201	333.186
50	127.800	203.447	251.019	298.567	348.347
70	144.553	217.848	263.011	315.847	360.738
90	166.640	236.002	279.401	339.509	376.565
95	176.124	244.104	288.538	348.984	385.193
98	187.674	255.050	301.356	363.837	397.011

Table 2
PRODUCTS TBP DATA (AT 760 mmHg)

naphtha, kerosene, light gas oil - LGO - and heavy has oil - HGO) five independent software analyzer modules were used. For all these, a large number of simulations were performed in order to validate the model, in fact to determine the tuning parameters ε_1 and ε_2 .

For the above-mentioned crude oil plant, there were separated NC=37 pseudo-components on TBP curve, included water. Their boiling points at 760 mmHG are presented in table 1.

By using these values, the following data were obtained for the side-products TBP curves (table 2).

By applying the mathematical model from equations (5) and (6), taking into account the re-calculated concentrations from equation (2) for every product (gasoline, naphtha, kerosene, LGO and HGO), the author identifies the values $\varepsilon_1 = 0.01700$ and $\varepsilon_2 = 0.99999$, as the best fit, both with theoretical and practical results (less than 0.8% error when calculating $T_{INITIAL}$ and T_{FINAL} for every product around the column normal operating regime, where we have an extended report over practical column configuration). It is also significant the fact that for every side-product, the values of ε_1 and ε_2 were the same (which practically is completely normal, judging from the process phenomenology above discussed).

As an observation, when seriously deviating from the normal operating point (a quite hard to believe situation for a crude oil unit) the software analyzers' answers are a bit affected by errors (max 4% in $T_{INITIAL}$ and T_{FINAL} indications),

denoting the future need of adapting the equations (5) and (6) for the process high nonlinearity.

The following example shows how the software analyzers work when considering the crude oil unit around its normal operating point [9]. The plant has in service only the pressure controller, as well as the level controllers for the main column, the sidestrippers and the reflux tank.

For instance, after a 10% increase in naphtha flowrate, the main column internal reflux will lower and, as a consequence, the components with higher boiling temperatures are more present in the affected part of the column. In this respect, the sidedraws to the sidestrippers have an increasing proportion of heavy components and, normally, the stripped products final boiling points go up, as it can be seen in figure 2.

All products obtained from stripping the sidedraws (naphtha, kerosene, kerosene, LGO and HGO) are affected, the final boiling points increasing by 3, 4, 5, and 10°C respectively. Nevertheless, this effect is unidirectional (as known from the operating theory and practice) as long as the gasoline final boiling point remains unchanged.

At the same time, this lowering in the main column internal reflux has only a slight influence on the products initial boiling points, as it is shown in figure 3.

The initial temperature points increase by 1.5°C (kerosene), 2°C (LGO) and 5°C (HGO), practically having the half amplitude as the final boiling points variation. At

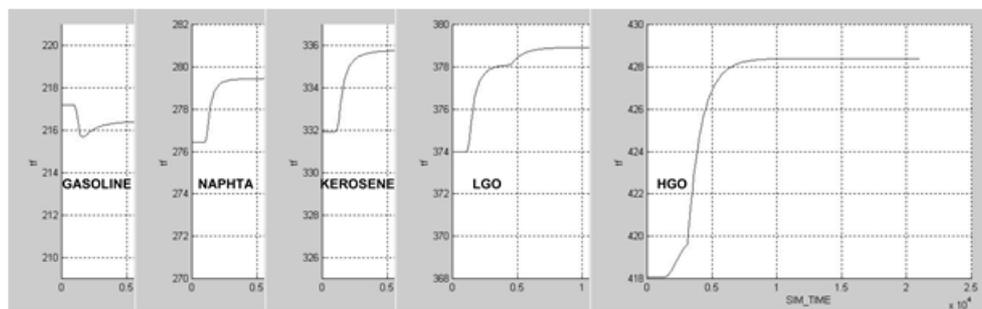


Fig. 2. The products (gasoline, naphtha, kerosene, kerosene, LGO and HGO) final boiling points variations, when the naphtha flowrate increases by 10%. The temperature values are given in [°C], and the simulation time in [s × 10⁴]

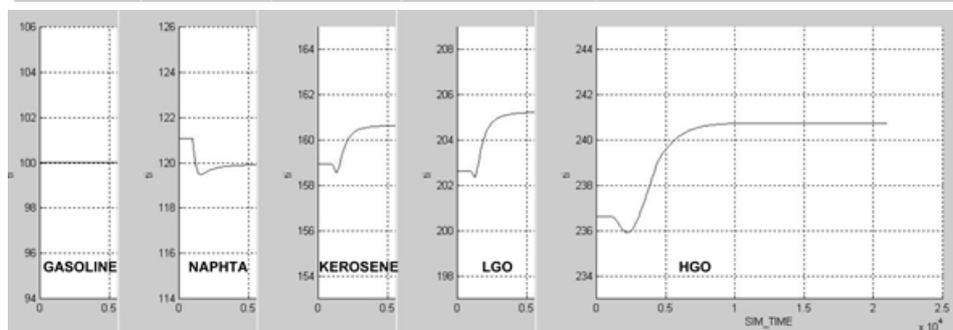


Fig. 3. The products (gasoline, naphtha, kerosene, kerosene, LGO and HGO) initial boiling points variations, when the naphtha flowrate increases by 10%. The temperature values are given in [°C], and the simulation time in [s × 10⁴].

the same time, the naphtha initial boiling point lowers by 1°C while the gasoline remains unchanged from this point of view (its initial boiling point being given by the lightest pseudo-component into the system). As a remark, the simulated crude oil unit is characterized by an inverse response for the initial boiling points of kerosene, LGO and HGO, exactly like the real plant [9].

All these results, based on the industrial operating reality and also on the engineering common sense, prove both the assumptions made and the implementation of these software product quality analyzers (applied for the crude oil unit). This is why an interesting experiment has to be done in the industry, trying to replace the hardware online analyzers with their corresponding software implementation.

Conclusions

This work has focused on how to estimate the product quality indicators – as it was applied on a crude oil plant (used just as a very complex example). The proposed mathematical model for calculating the initial and final boiling points was analytically obtained, following the principles used in products TBP curve determination. Although the method has to be improved in order to address high process nonlinearities, this approach brings more

generality and pragmatism than only modelling a particular online hardware analyzer.

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Manuscript received: 8.04.2016