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Long-Cycle Operation for Residue Hydrotreating Processes with Bayesian Optimization

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ABSTRACT

For the long-cycle process industry, operational cycles can be severely affected by equipment aging, catalyst deactivation, and safety limitations. As illustrated by the residue hydrotreating process, metal impurities gradually deposit on the catalyst during residue purification, leading to catalyst poisoning and eventual process shutdown. Such long-cycle processes require dynamic adjustments of operating conditions to balance immediate economics with long-term sustainability. While current practice relies on empirical tuning based on historical data, this work focuses on studying how to obtain an optimal operating trajectory to guide the monthly adjustments of operating variables. The long-cycle simulation of the residue hydrotreating process can be performed using the commercial software, PetroSIM. After adjusting the feed conditions, its embedded mechanistic model can calculate the deviation of average bed temperature from the set point and output the remaining operating time. Since Bayesian optimization (BO) is well-suited to address complex processes with unknown mechanisms and high computational costs, and can effectively seek optimal solutions, a BO framework incorporating constraints evaluated by PetroSIM is proposed in this work to optimize the monthly feed composition and maximize the total profit over the entire operational cycle. The results indicate that the total profit achieved through BO-optimized operation is 17.8% higher than that from empirical operation. The optimized strategy demonstrates practical rationality: in the early stage of high catalyst activity, more residue can be processed; in the later stage, increasing the light oil ratio helps extend the processing cycle. This strategy provides theoretical support for advancing the research toward industrial applications.

Keywords Process Operations, Derivative Free Optimization, Petroleum, Hydrotreating processes

INTRODUCTION

Residue hydrotreating (RHDT) is a process that removes sulfur and metal impurities from heavy oil via catalytic reactions [1]. As the process proceeds, the catalyst gradually deactivates until its activity drops below a specified threshold, requiring a unit shutdown and catalyst replacement [2]. RHDT therefore operates over finite operational cycles. Given the high cost of the catalyst and the time-consuming replacement procedure, it is economically imperative to purify as much residuum as possible within each cycle. The key operational variable is the residuum content in the feedstock. Increasing this fraction lowers feed costs, thereby raising short-term processing profits. However, feeding a higher-impurity feedstock accelerates catalyst deactivation, which shortens the operable duration in the future. Conversely, decreasing the fraction yields the opposite effect: it extends catalyst life and increases process sustainability at the expense of short-term operating profit. This poses a significant trade-off problem: determining how to optimize the operations each month to maximize the total profit across the entire RHDT running cycle.

In this optimization, a critical constraint is the relationship between feed composition and the remaining useful life (RUL) of the catalyst. PetroSIM, a professional software in this field, contains an RHDS module capable of simulating the long-cycle operation of residue hydrotreating [3]. This module incorporates state-space correlations to model catalyst deactivation: it predicts catalyst activity for the subsequent month based on the current state (e.g., catalyst activity) and process inputs (e.g., feed properties). Using this framework, PetroSIM calculates the minimum temperature rise required to satisfy the product composition constraint, from which the weighted average bed temperature (WABT) is determined. The distance between this value and the predefined threshold, combined with the catalyst deactivation rate, is then used to estimate the current RUL. Hence, distinct operating strategies yield different RUL trajectories. These RUL estimates are generated by the deterministic model embedded within PetroSIM. However, due to the closed architecture of this commercial software, neither the model nor its underlying database is accessible. As a result, analytical derivatives cannot be obtained. This study does not seek to construct a surrogate model for this internal relationship. Instead, we focus on solving the long-cycle operational optimization problem using this black-box simulator, and it is a scenario commonly encountered in industrial practice.

Bayesian optimization (BO) is a widely used black-box optimization algorithm grounded in Bayesian theory [4]. As an iterative framework, it integrating modeling and optimization. Specifically, the algorithm first fits a surrogate model (e.g., Gaussian process regression) for the objective function using an initial set of observed points. Based on this model, the subsequent point is selected by maximizing an acquisition function (e.g., expected improvement) that balances exploration and exploitation. Each newly evaluated sample is incorporated to update the surrogate, thereby progressively reducing uncertainty over the objective function. By repeatedly executing this 'decision-modeling' iteration, Bayesian optimization converges to the optimum with as few function evaluations as possible. Consequently, it is particularly suitable for black-box issues where evaluations are computationally expensive.

For the RHDT process, the operational optimization is conducted via the PetroSIM simulator, which is characterized by its opaque mechanisms and significant computational cost (a full-cycle simulation takes over one minute). If an evolutionary strategy (e.g., genetic algorithm) requiring numerous iterations is adopted, the optimization process becomes time-consuming—at least 16.7 hours for 1000 iterations. Thus, to minimize the number of calls to PetroSIM, this study utilizes BO method to address this operating scenario.

This section outlines the theoretical foundation and overall framework of this study. The remainder of the paper is organized as follows: Section 2 details the methodology for simulating the long-cycle RHDT process using PetroSIM; Section 3 formulates the objective of this study by defining the optimization problem, along with its associated constraints and boundary conditions; Section 4 presents the results and discusses the operational benefits achieved; Section 5 concludes this study and suggests potential directions for future research.

RHDT PROCESS SIMULATION

Process simulation of residue hydrotreating can be accomplished using the RHDS module in PetroSIM. Figure 1 shows the RHDT process flowsheet developed on this platform. Residuum and hydrogen are fed into the reactor for hydrotreating. The effluent then passes through an ideal separator (modeled as a component splitter) to simulate a high-pressure high-temperature flash drum, assuming complete separation of non-condensable gases (H_2S, NH_3) from the liquid hydrocarbons based on a defined split fraction. The Peng-Robinson (PR) equation of state with built-in binary interaction parameters is applied throughout the process, as it is widely accepted for hydrocarbon systems containing sour components (H_2S, NH_3). The liquid stream is subsequently fractionated into products of varying boiling points (gas, naphtha, diesel, and bottoms). In addition, H_2O serves as a wash water stream to rinse metal deposits from the catalyst. HPS functions as a high-pressure vent line to withdraw excess hydrogen feedstock.

Table 1: Properties of the feed oil.

Property	**Value**
Sulfur content	3.0 ~ 6.0 wt%
Conradson carbon content	11.20 wt%
Nickel content	21.80 ppmwt%
Vanadium content	64.40 ppmwt%
Nitrogen content	0.24 wt%
Distillation 1% (TBP)	273.4 °C
Distillation 5% (TBP)	349.4 °C
Distillation 10% (TBP)	384.6 °C
Distillation 30% (TBP)	459.0 °C
Distillation 50% (TBP)	523.2 °C
Distillation 70% (TBP)	597.6 °C
Distillation 90% (TBP)	694.4 °C
Distillation 99% (TBP)	722.2 °C
Specific gravity (Std. Cond.)	0.977 -
Temperature	260 °C
Pressure	101 kPa
Volume flow	535.7 m^3/h

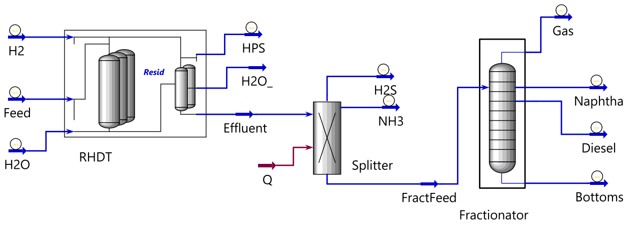

Figure 1. Flowsheet of the RHDT process in PetroSIM.

Table 1 presents the properties of the feedstock. The sulfur content is identified as the key factor responsible for catalyst deactivation. Hence, adjusting the proportion of heavy oil in the feed can be regarded as effectively modifying the sulfur content. According to the review [5], this study specifies the sulfur content of the heaviest feed as 6.0 wt% and that of the lightest feed constituents as 3.0 wt%. As the only manipulated variable, feed sulfur content dominates catalyst RUL and thus drives profitability. Fixed true boiling point (TBP) cut points minimize product yield variation from the separation system, so the ideal splitter simplification has negligible impact on economic conclusions. Due to the requirements of the downstream processes in RHDT, the sulfur content in the bottoms product needs to be maintained below 0.5 wt%, regardless of the feedstock. However, there are price variations: heavy feedstock costs about 350 USD/m³ (P_H), light feedstock costs about 600 USD/m³ (P_L), and the purified effluent is valued at approximately 800 USD/m³ (P_B).

Table 2: Parameters of the reactor.

Parameter	**Value**
WABT (Start of Run)	360 °C
WABT (End of Run)	420 °C
Number of beds	5 -
Catalyst density	493.7 kg/m³
Catalyst weight	1656.37 ton

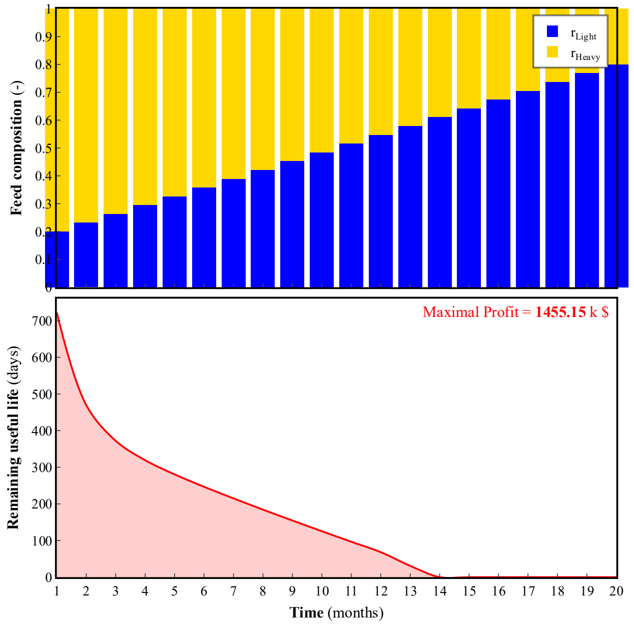

Figure 2. Feed composition and RUL trajectory under empirical operation.

In addition, the parameters of the reactor remain constant, as listed in Table 2. It can be seen that the catalyst inventory is held constant. Thus, its activity progressively decreases during residue hydrotreating. In PetroSIM, this effect is reflected by a rise in WABT, as the process must maintain the product sulfur specification. Starting from the first month (WABT=360°C), operating decisions are updated at monthly intervals. The process stops once the WABT exceeds the set value (WABT=420°C). Figure 2 illustrates an empirical operational approach: linearly increasing the light feedstock fraction from 0.2 to 0.8 to compensate for the declining catalyst activity in later periods. However, as can be seen from PetroSIM's estimation, the RUL reaches zero by the 14th month, implying that no profit can be generated from subsequent operations. Therefore, the total profit, calculated as the cumulative monthly product revenue minus feedstock costs, is 1455.15 thousand USD.

OPERATIONAL OPTIMIZATION

In this study, given that hydrogen is typically supplied in excess during industrial residue hydrotreating and its precise consumption is difficult to quantify, hydrogen-related costs are treated as fixed overheads and excluded from the objective function. Operating conditions influence utility consumption through their effect on WABT; however, the integrated value of total utility cost remains largely unchanged across different operating strategies over the entire processing cycle, allowing minor fluctuations to be neglected in the model. Moreover, catalyst are expensive and consumed in large quantities; frequent replacement not only increases operating expenses but also disrupts the refinery-wide material balance. Industrial practice therefore prioritizes the full utilization of catalyst within each operating cycle. Accordingly, this study optimizes profit over a full single catalyst cycle; as the one-time catalyst replacement cost is independent of operating decisions, it is neglected in the analysis. Based on these assumptions, the objective is to maximize the total profit by optimizing the heavy component fraction in the monthly feed. The optimization problem is expressed in Equation 1. This study sets the total duration to no more than 20 months. The heavy oil fraction in the feed for each month is represented by the set $\boldsymbol{r}_H = \{r_H^{(i)} \mid i = 1, \ldots, 20\}$. The light oil fraction is complementary, such that $r_H^{(i)} + r_L^{(i)} = 1$. A binary decision variable $z_i \in \{0, 1\}$ governs whether the monthly processing profit contributes to the total profit; its value is assigned based on the RUL estimated via PetroSIM: $z_i = 1$ when $RUL > 0$, and $z_i = 0$ when $RUL = 0$. The total feed flow rate F_{in} is set to 535.7 m³/h. The product flow rate of the bottoms $F_B^{(i)}$ is simulated by PetroSIM. P_B, P_H, and P_L correspond to the prices of the bottoms, heavy feedstock, and light feedstock. Additionally, c is defined as 24*30 (hours*days).

$$\max_{\boldsymbol{r}_H} \sum_{i=1}^{20} z_i * \left(F_B^{(i)} P_B - r_H^{(i)} F_{in} P_H - r_L^{(i)} F_{in} P_L\right) * c \qquad (1)$$

$$z_i, F_B^{(i)} = \text{PetroSIM}\left(r_H^{(i)}, r_L^{(i)}\right), i = 1, \ldots, 20$$

$$r_H^{(i)} + r_L^{(i)} = 1, i = 1, \ldots, 20$$

$$0 \leq r_{\mathrm{H}}^{(i)} \leq 1$$

$$0 \leq r_{\mathrm{L}}^{(i)} \leq 1$$

The Bayesian optimization algorithm is applied to optimize this problem. The procedure is illustrated in Figure 3. First, 30 sets of $\boldsymbol{r}_{\mathrm{H}}$ are sampled within the domain using Latin hypercube sampling, and the light feedstock fraction $\boldsymbol{r}_{\mathrm{L}}$ is derived accordingly. For each set, PetroSIM computes the corresponding $F_{\mathrm{B}}^{(i)}$ and $RUL^{(i)}$ (i.e., z_i). Subsequently, the values of the objective function are calculated, and the sample with the highest value is denoted as $\boldsymbol{r}_{\mathrm{H}}^{*}$. Gaussian process regression is utilized to fit the mapping from the decision variables to the objective function. The next point to be evaluated is determined via the expected improvement. This process iterates until a predetermined iteration count is met, at which point the optimal solution $\boldsymbol{r}_{\mathrm{H}}^{*}$ is returned.

This framework is implemented via the BoTorch library in Python, and the parameters are presented in Table 3. The RBF kernel, known for its universal approximation capability, is adopted for the Gaussian process, while expected improvement (EI) serves as the acquisition function. A total of 550 iterations are performed, with the initial samples used to initialize the Gaussian process regression constituting about 5.5% of the total iterations.

Table 3: Parameters of BO.

Parameter	Value
Gaussian kernel	RBF kernel
Acquisition function	EI
Number of initial points	30
Number of iterations	520

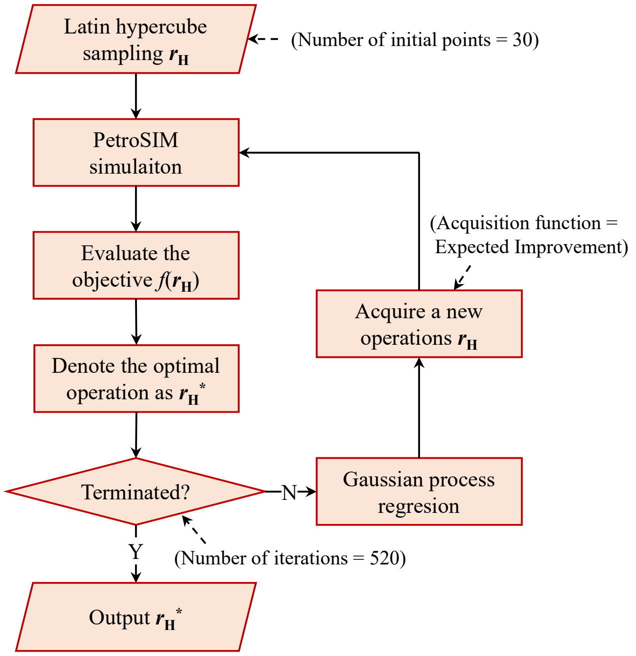

Figure 3. Workflow of the BO strategy.

RESULTS AND DISCUSSION

Figure 4 illustrates the iterative process of the algorithm. The horizontal axis represents the number of objective function evaluations, comprising 30 initial evaluations and 520 iterative evaluations. Total revenue and total cost are shown by cyan and pink bars, respectively. The difference between them, which is the total profit (i.e., objective function value), is plotted as a blue curve. In addition, the green line represents the magnitude of the acquisition function, i.e., the EI value. It is mapped to the right vertical axis, and non-zero values of this line suggest that the subsequent sampling point can improve upon the current $\boldsymbol{r}_{\mathrm{H}}^{*}$. It can be observed from the figure that the green line displays multiple peaks in the initial iterations. The BO focuses on exploring the decision space during this period. This drives the algorithm to quickly locate the promising region for the optimum. In the middle and later stages, BO emphasizes exploitation by sampling around the optimal solution, which serves to improve the accuracy of the surrogate model. The algorithm identified the optimal value at iteration 432, requiring merely 7.2 hours of runtime.

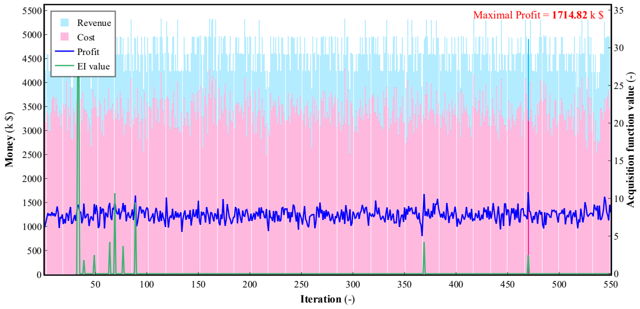

Figure 4. Iteration process of BO for Equation 1.

The bars representing revenue and cost associated with the optimal operation are highlighted in Figure 4. The total profit obtained is 1714.82 thousand USD, reflecting a 17.8% improvement over that achieved by the empirical operation. Figure 5 depicts the optimal operation and the estimated RUL. As shown, a higher fraction of heavy oil is fed during the early processing stage, thereby maintaining a lower cost level. Contrary to the empirical operation that continuously increases the fraction of light oil feed, optimized strategies recommend utilizing periods of high catalyst activity to process more residue. Subsequently, the fraction of light oil feed is progressively increased in the mid-to-late periods to prolong the processing time. Compared with the results in Figure 2, the RUL here is sustained for one additional month, resulting in additional profit.

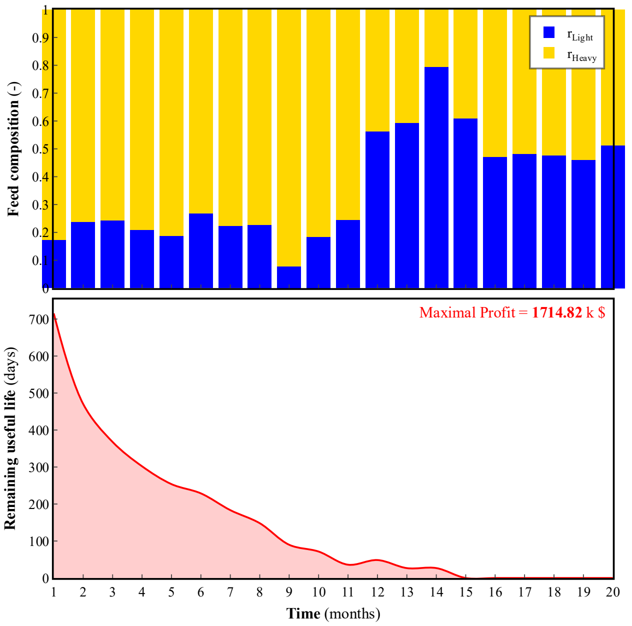

Figure 5. Feed composition (with varying $\boldsymbol{r}_{\mathbf{H}}$) and RUL trajectory after BO optimization.

Figure 6 illustrates the iterative process, showing that BO identified the optimum at a relatively early stage. This is attributed to the reduced dimensionality and simpler surrogate modeling in the single-variable problem. As shown in Figure 7, the results suggest that residue should constitute the majority of the feed. Although only 12 months of operation are valid, the profit reaches 1667.83 thousand USD, which is 212.68 thousand USD higher than that of empirical operation. However, this result is inferior to that of the free-feed optimization. The rationale lies in the fact that the optimal solution under this problem is a lower bound solution of Equation 1. Consequently, plants are advised to optimize the supply of light and heavy oils at the supply chain level.

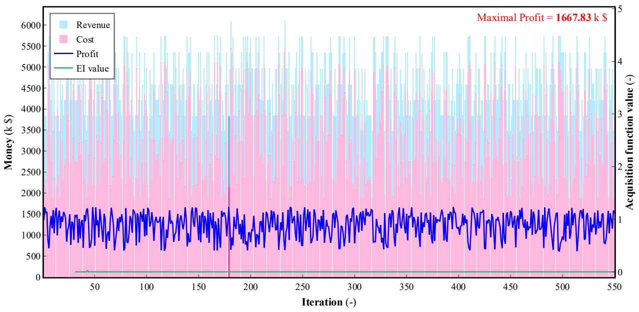

Figure 6. Iteration process of BO for Equation 1 under constant $\boldsymbol{r}_{\mathbf{H}}$ constraint.

Additionally, in practical applications, the supply of light oil often lacks flexibility. This implies that the feed composition must be predetermined prior to startup. For comparative purposes, another optimization scenario is investigated: maximizing total profit by optimizing a constant heavy oil fraction in the feed. Mathematically, this is equivalent to adding a constraint to Equation 1: $r_H^{(1)} = r_H^{(2)} = \ldots = r_H^{(20)}$.

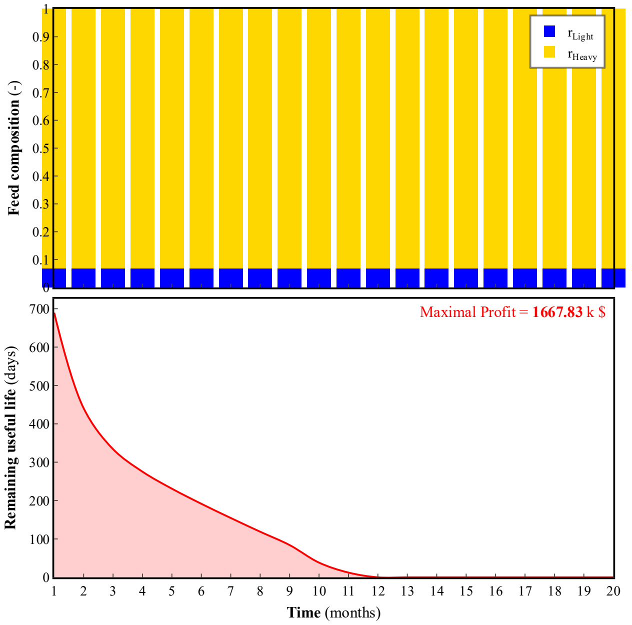

Figure 7. Feed composition (with constant $\boldsymbol{r}_{\mathbf{H}}$) and RUL trajectory after BO optimization.

CONCLUSION

The main contribution of this work lies in developing an optimization framework for long-cycle operating trajectories of residue hydrotreating based on the PetroSIM, a problem essentially characterized by high-dimensional black-box optimization. BO, leveraging a probabilistic surrogate model to actively sample and iteratively update the posterior, enables efficient optimization with minimal objective function evaluations. This study employs BO to address the problem. Following 432 iterations (7.2 hours), BO identifies the optimal solution, yielding a 17.8% profit improvement compared to empirical operation. The optimized results exhibit an operating pattern with a higher heavy oil ratio in the early stage and a higher light oil ratio in the later stage. This pattern is consistent with the decreasing catalyst activity over time and the stronger impact of feed when activity is low. This provides practical guidance: operators can initially set a high throughput and then gradually reduce it based on WABT feedback. Moreover, this study investigates a lower-bound case of the problem by optimizing with fixed operations each month. This is designed for refineries with limited flexibility in light feed supply. The results, though not as good as those from unrestricted operational optimization, still show a 14.6% increase over the unoptimized practice.

Similar optimization problems, balancing immediate economic returns and future sustainability, are prevalent in various industrial contexts. Additionally, commercial software such as PetroSIM, PRO/II, and Aspen HYSYS do not provide analytical derivatives. The proposed BO framework is general and inherently incorporates uncertainty considerations, laying a foundation for methodological innovations and adaptations to more complex industrial problems.

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REFERENCES

1. Ferreira C, Tayakout-Fayolle M, Guibard I, Lemos F. Hydrodesulfurization and hydrodemetallization of different origin vacuum residues: new modeling approach. Fuel 129:267-277 (2014). https://doi.org/10.1016/j.fuel.2014.03.056
2. Kohli K, Prajapati R, Maity SK, Sau M, Garg MO. Deactivation of hydrotreating catalyst by metals in resin and asphaltene parts of heavy oil and residues. Fuel 175:264-273 (2016). https://doi.org/10.1016/j.fuel.2016.02.036
3. Fan M, Zhao Y, Wang Y, He S. Simulation and application of fixed-bed residuum hydrotreating unit process model based on RHDS-SIM. *Chem. Ind. Eng. Prog.* 40:5514– 5522 (2021) https://link.cnki.net/doi/10.16085/j.issn.1000-6613.2020-2152
4. Frazier PI. A tutorial on Bayesian optimization. *arXiv preprint* arXiv:1807.02811 (2018) https://doi.org/10.48550/arXiv.1807.02811
5. Marafi A, Albazzaz H, Rana MS. Hydroprocessing of heavy residual oil: opportunities and challenges. Catalysis Today 329:125-134 (2019). https://doi.org/10.1016/j.cattod.2018.10.067
