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Industrial Application of Surrogate Models to Optimize Crude Oil Distillation Units

Lluvia M. Ochoa-Estopier[a,*], Víctor M. Enríquez-Gutierrez[a], Lu Chen[a], José M. Fernández-Ortiz[b], Lorenzo Herrero-Soriano[b], Megan Jobson[c]

[a] Process Integration Limited, Station House, Stamford New Road, WA14 1EP, Altrincham, UK.
[b] Compañía Española de Petróleos, S.A.U., Refinería La Rábida, Pol. Ind. Nuevo Puerto s/n - Palos de la Frontera, Aptdo. 289 – 21080, Huelva, Spain.
[c] Centre for Process Integration, School of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, M13 9PL, Manchester, UK.
lluvia.ochoa-estopier@processint.com

This work presents a new approach to optimize existing crude oil distillation systems. The main features of this approach are its ability to provide key insights of the main factors affecting product yields and energy consumption; and the consideration of system limitations, such as crude oil changes, column flooding, heat transfer bottlenecks and product quality specifications. The new approach showcases sophisticated and systematic modelling and optimization methodologies, namely artificial neural networks and simulated annealing. The approach has been applied successfully in a debottlenecking study for yield optimization of a medium-scale Spanish refinery. The implementation of the optimization results was carried out successfully in the refinery; initial projections confirm predicted benefits of $7.2 million per year.

1. Introduction

Distillation units are the first processing units in petroleum refineries; they separate the crude oil feedstock into petroleum fractions that are further processed in downstream operations. Due to their size, high energy requirements and position in the process sequence, the operation of crude oil distillation units (CDUs) has a significant impact on the overall refinery yields, operating costs and carbon dioxide emissions. The configuration of a crude oil distillation system typically consists of a pre-flash or pre-fractionator unit, atmospheric and vacuum distillation units, and a heat exchanger network (HEN). To maintain profitable and safe operation, the CDU operating conditions need to be continuously adjusted to accommodate changes in crude oil properties and flow rate, changes in the prices of crude oil, refined products and of utilities; varying product quality specifications, plant aging, etc. Systematic and sufficiently accurate approaches to identify optimal operating conditions for existing industrial crude oil distillation systems are currently lacking.

For existing crude oil distillation systems, retrofit projects and operational optimization can be undertaken to improve the separation and energy performance of the system. Retrofit optimization has more potential to improve energy recovery and yields than operational optimization, as structural modifications requiring capital investment can be performed to increase the system's flexibility and overcome existing bottlenecks (e.g. coolers, pumps and column stages operating at maximum capacity). Instead, operational optimization offers the advantage of delivering significant economic benefits without capital investment or downtime, as only operational variables are considered (e.g. flow rates and temperatures). Thus, the best strategy to capitalize on existing resources and minimize economic risks whilst improving the performance of the distillation system is to implement operational optimization before considering retrofit.

The operational optimization problem is highly constrained, which means that models need to incorporate sufficient detail and accuracy (Smith et al., 2013) to provide meaningful estimations. Surrogate models can provide a suitable alternative to first-principle models, as they can capture process details accurately, whilst being simpler, faster and more robust than first-principle models (e.g. rigorous process simulation models). Surrogate models applied to optimize crude oil distillation units include support vector regression models (Yao

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et al., 2012), polynomial models (López C. et al., 2013), and neural network models (Motlaghi et al., 2008; Ochoa-Estopier et al., 2015; Ibrahim et al., 2018).
This work builds on the methodologies of Ochoa-Estopier et al. (2015) and Jobson et al. (2017), which employ artificial neural network (ANN) models and data analysis to find operating conditions that maximize the yields of valuable distillation products while minimizing energy consumption. Such methodology has been extended to include crude oil flow rate as an optimization variable. This paper presents the successful application of this approach to a challenging industrial case, i.e. yield optimization of a Spanish refinery which was highly constrained – hydraulically and energetically – as a result of operating the plant at 40 % above design capacity.

2. Methodology

The main features of this approach are the development of surrogate models to represent the distillation process and the implementation of such models in an overall framework for simultaneous operational optimization of the distillation process and heat exchanger network. The heat exchanger network is simulated using in-house software i-Heat™ of Process Integration Limited. This work extends the approach of Ochoa-Estopier et al. (2015) for modelling the distillation process, to include the crude oil flow rate as an optimization variable and to incorporate data analysis (Jobson et al., 2017) into the overall optimization procedure. The new methodology can further exploit the balance between “quantity” and “quality” (i.e. the production of valuable products vs. the sharpness of the separation) and provides useful insights into the process behavior (i.e. dominant constraints and variables, and their bounds) that significantly reduce the search space for optimization and increase the chances of finding a global optimum.

2.1 Understanding the process

The first step consists of defining the objective, scope and required level of detail of the optimization problem. In industrial applications, defining these aspects not only determines the duration of the study, but can also be critical in the success of the study. The best strategy for defining these aspects early in the study is to carry out a pre-assessment, incorporating the experience and understanding of plant operators. In this pre-assessment, the product ‘gaps’ and ‘overlaps’, and the furnace inlet temperature and outlet temperatures are compared with a benchmark to reveal the main opportunities for improvement. The gaps/overlaps help to identify which separations need further improvement, while the furnace temperatures indicate how much energy is recovered in the heat exchanger network, and whether the distillation feed temperature is appropriate for the type of crude oil. Discussions with the refinery engineers reveal the main operational problems (e.g. key bottlenecks) and provide insights on the current flexibility of the system (e.g. which pump-arounds flow rates can be varied; how easily product specifications are met). That information helps to focus the optimization (e.g. energy minimization, yield optimization), the units to be considered and main process constraints. By understanding the process at the earliest stage of the study, it is possible to tailor the complexity of the optimization problem to include only those issues that are most relevant to the project.

2.2 Data collection and reconciliation

In the next step, establishing the base case, historical data are checked for consistency and used to tune rigorous simulations (e.g. by adjusting tray efficiencies and heat exchanger fouling coefficients) for the selected representative operating scenarios. Reconciling historical data with rigorous simulation results is useful to identify measurement errors, to check the consistency of mass and energy balances and to identify how many scenarios to consider. A heuristic rule for refineries that process a range of crude oils and blends is to consider at least two representative crudes for optimization (e.g. one light and one heavy crude oil) and verify the optimizer results with one or two additional crudes/blends. These rigorous simulations will be used to create the surrogate models and to validate the optimization results before and after on-site implementation.

2.3 Sampling and sensitivity analysis

The next step extracts data from the validated rigorous models to develop the surrogate models and identify underlying trends that help guide the optimization. The sampling approach of Ochoa-Estopier et al. (2015) is extended in this work to consider the crude oil flow rate as a degree of freedom for optimization. Each sample is generated using rigorous models; the simulation results are extracted and analyzed (Jobson et al., 2017). Dimensionless normalized values are introduced to represent flow rates. Table 1 illustrates the normalized variables used in this work, where m_{crude}^{0} is the crude oil flow rate of the base case. The normalized variables are used to create the latin hypercube sampling plan and are included in the sensitivity analysis. The advantage of using normalized values, compared to using other techniques such as principal component analysis, is that these normalizing implicitly captures mass and energy trade-offs while also preserving their

physical meaning. As a result of this analysis, the dominant optimization variables and constraints are identified and the bounds of the optimization variables are adjusted to narrow the search space for optimization, which significantly increases the chances of finding a global optimum. Sampling and analysis are repeated until an appropriate number of samples is obtained to regress the ANN model (e.g. 1,000 samples).

Table 1: Normalized variables used in this work

Variable(s)	Description	Dimensionless variable(s)
m_{crude}	Crude oil flow rate	$m^*_{crude} = m_{crude}/m^0_{crude}$
m_p	Flow rates of distillation products, pump-arounds and reflux	$m^*_p = m_p/m_{crude}$
$m_{s,i}$	Flow rate of stripping steam used for distillation product *i*	$m^*_{s,i} = m_{s,i}/m_{p,i}$

2.4 Surrogate modelling and optimization

The samples from the rigorous simulations are used to regress the surrogate models for use in the optimization. The artificial neural network modelling approach and optimization framework of Ochoa-Estopier et al. (2015) are used in this work. The ANN model comprises a set of feed-forward networks, one network per output, with hyperbolic tangent functions in the hidden layers and identity functions in the output layer. The ANN model inputs – which are also the optimization variables – include furnace outlet temperatures, the normalized flow rates in Table 1, and pump-around return temperatures (or duties). The ANN model outputs are used to simulate the HEN, to check that process constraints are met and to calculate the objective function during optimization. These outputs include variables related to product quality (e.g. ASTM D86 temperatures, flash points), stage temperatures, % column flooding, and HEN stream data (i.e. inlet and outlet temperatures, enthalpy change and heat capacity flow rate). The ANN model is validated using data from rigorous simulations and implemented in the optimization framework, as illustrated in Figure 1.

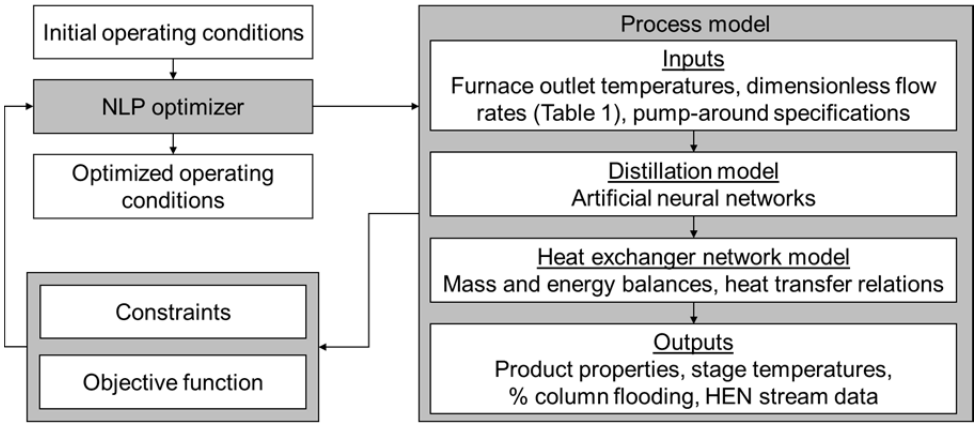

Figure 1: Optimization framework. NLP: nonlinear programming.

The optimization problem is formulated as a nonlinear programming problem solved using a simulated annealing algorithm. Objectives that can be considered in the problem include to maximize net profit (*net profit = product revenue – operating costs*), to minimize energy consumption or to maximize product revenue. The constraints considered in the optimization problem include the lower and upper bounds of the optimization variables, product quality specifications, top stage temperatures (to prevent corrosion), hydraulic limits (i.e. column flooding) and heat exchanger approach temperatures. Only operational variables are optimized: the configuration of the distillation towers and HEN are fixed. The optimization is run several times to check the consistency of the solutions. The best solution is selected and validated with the rigorous simulation model.

2.5 Implementation strategy

The next step is to implement the optimization results on-site. This work starts by adjusting the variable that is expected to bring the most benefit, then waiting until the distillation operation stabilizes again (around 1–3 hours), and then continuing with the second-best variable, and so on. The waiting periods allow a smooth transition from one state to another, which is especially important for highly bottlenecked processes; plant measurements can indicate that a steady state is reached and are useful for determining the benefits realized, with respect to the optimization objectives, after each operational change.

3. Implementation and Results

The methodology presented in Section 2 has been implemented in a Spanish refinery to maximize the yields of the most valuable products and to mitigate the effects of severe heat transfer and hydraulic bottlenecks. The crude oil distillation system was designed for a processing capacity between 80,000-90,000 bbl/d (530 to 600 m^3/h), using two different types of crudes (i.e. a heavy and a light blend) as base cases. The distillation system comprises crude oil desalters, one flash drum, one atmospheric distillation unit (ADU), one vacuum distillation unit (VDU) and a heat exchanger network. The HEN has 12 process-to-process exchangers (24 shells), with split streams, water and air coolers, and two furnaces. The ADU produces six products, namely naphtha, jet fuel, kerosene, diesel, atmospheric gas oil (AGO) and atmospheric residue (AR). The VDU separates the residue into four products, namely light vacuum gas oil (LVGO), medium vacuum gas oil (MVGO), heavy vacuum gas oil (HVGO), and vacuum residue (VR). The diesel and LVGO products are blended into a single product, so they are considered as the same product with the same price. Similarly, the AGO, MVGO and HVGO products are blended into a single product with the same price.

3.1 Understanding the process

The refinery processes more than 20 types of crude oil divided into two categories: lighter low-sulphur (LS) and heavier high-sulphur (HS) crudes. LS crudes are processed 60 % of the time. At the time of the study, the refinery was processing ~115,000 bbl/d (760 m^3/h) of crude oil, which represents an operation 30-40 % above design capacity, leading to severe heat transfer and hydraulic bottlenecks. In particular, the ADU condenser struggled to satisfy cooling requirements of LS crudes, the ADU and VDU furnaces typically operated at the maximum capacity, and flooding was frequent in the diesel and LVGO/MVGO sections of the columns. Moreover, as two pump-arounds served other processing units, these pump-around flow rates could not be varied, reducing the flexibility of the distillation system. Tight product quality specifications on the most valuable products also constrained the flexibility of the distillation system. Nevertheless, the pre-assessment study indicated that maximizing the yields of the most valuable products was a more economically attractive objective than minimizing energy consumption. Thus, the study focused on optimizing the product yields and debottlenecking the distillation units.

3.2 Base case, sampling and sensitivity analysis

Historical data were collected to set up the base case. Two representative crude oils, one for each type of crude, were selected to account for all the crudes and blends processed in the refinery. The collected data were checked for consistency and used to set up one rigorous simulation in UniSim® for each crude. The two reconciled UniSim® simulations were connected to a MATLAB® code to perform sampling and sensitivity analysis. Twenty-eight independent variables (i.e. normalized flow rates, furnace outlet temperatures, pump-around duties) and sixty-two distillation constraints (e.g. product quality, % flooding, top and bottom stage temperatures) were initially considered in the study. The results of the sensitivity analysis shown in Figure 2 illustrate how trends in product quality (Figure 2a) and flooding (Figure 2b) are useful for setting the bounds of the optimization variables. In addition, the sensitivity analysis provided valuable insights to the process behavior prior to optimization, for example:

- Diesel and LVGO are the products with the highest potential to deliver economic benefits.
- The light components in the AGO stream need to be recovered in lighter products such as diesel.
- Two main operational changes are needed: 1) adjusting the ADU furnace outlet temperature, 2) increasing the stripping steam flow rate to the AGO stripper.
- Of all the product quality constraints considered in the study, the dominant constraints correspond to the jet fuel flash point temperature and the kerosene boiling range (ASTM D86 T5% and T95%).
- Of the 62 constraints initially considered, only 15 needed to be included in the optimization problem.

These observations served to simplify the formulation of the optimization problem and guided the optimization algorithm: new bounds of the optimization variables were defined, irrelevant process constraints were not included in the formulation, weighted penalties were applied to the dominant optimization constraints and optimization solutions were analyzed against the sensitivity analysis results.

3.3 Surrogate modelling and optimization

The sampling and sensitivity analysis steps were repeated until a representative number of samples was obtained to regress the surrogate ANN models. One ANN distillation model was developed for each type of crude. The inputs of the model are the independent variables considered in the sensitivity analysis (28 variables), while the outputs correspond to the 15 constrained variables, and stream data needed to simulate the HEN (90 variables). The ANN models were validated against a new set of data from rigorous simulations, showing very good agreement. The ANN models were implemented in the optimization framework described

in Section 2. Several optimization runs were performed for each type of crude oil, the best solution per crude was selected from these runs and was validated with the rigorous simulations. The main operational changes proposed by the optimizer for both scenarios are summarized in Table 2. For reasons of commercial sensitivity, detailed information cannot be shared. Note that the optimization results for the diesel and AGO flow rates, and the ADU furnace outlet temperatures are consistent with the findings of the sensitivity analysis. Table 2 shows the net profit estimated from operating the LS crude 60 % of the year and operating the HS crude 40 % of the year, which amounts to $4.1 million for the entire year. These economic benefits are dominated by an increase in product revenue; the increase in operating costs is insignificant.

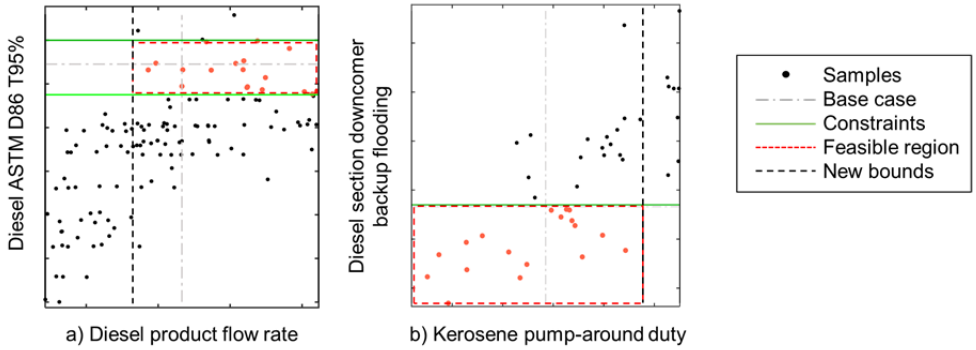

Figure 2: Scatter plots show interdependence of independent variables on product quality and flooding.

To mitigate the effects of heat transfer and hydraulic bottlenecks, the optimizer suggested shifting the loads between the ADU and VDU according to the type of crude oil. As shown in Table 2, for the LS crude, the AR flow rate increases, shifting separation load from the ADU to the VDU. This change reduces the liquid-vapor traffic in the ADU, reduces the condenser duty and alleviates flooding in the diesel section. Similarly, to mitigate flooding problems in the LVGO/MVGO section when processing HS crudes, the optimizer suggested reducing the AR flow rate, i.e. processing less of the feed in the VDU tower. This load shifting was facilitated by the problem formulation – namely considering diesel and LVGO as the same product.

Table 2: Optimization results showing the change from the base case for each type of crude oil

Item	Units	LS crude	HS crude	Overall
ADU furnace outlet temperature	°C	+0.5	+0.9	
Diesel flow rate	t/h	+0.8	+1.5	
AGO flow rate	t/h	-6.4	-1.2	
AR flow rate	t/h	+3.0	-1.3	
LVGO flow rate	t/h	+2.1	+0.5	
Operating costs	Million $/y	+0.081	+0.005	+0.086
Product revenue	Million $/y	+2.834	+1.395	+4.315
Net profit	Million $/y	+2.753	+1.390	+4.143

3.4 Implementation

These results were implemented on-site on two occasions, one for each type of crude oil. The implementation plan in both cases consisted of adjusting the ADU furnace outlet temperature first, increasing the stripping steam flow next (AGO stripping steam for the HS crude oil, and AR and AGO steam streams for the LS crude oil), and then making the remaining modifications suggested by the optimizer. The refinery also decided to keep the Advanced Process Controller in operation, to automatically adjust product flow rates.

- *Implementation for the HS crude oil*. The optimization proposed increasing the column feed temperature. However, heat transfer limitations in the ADU furnace did not allow such an increase unless the feed flow rate was decreased (by 3 %). This operational change led to increased revenue from valuable products, mainly diesel, while meeting the heat transfer constraints of the furnace. Based on plant measurements after this change, revenue associated with valuable products increased by $3.5 million per year. The next most beneficial solution found by the optimizer was to increase the flow rate of AGO stripping steam, to aid recovery of diesel from AGO. However, this change had little effect on performance, since most of the diesel was already recovered from AGO after the first modification.
- *Implementation for the LS crude oil*. When the implementation started, the ADU furnace outlet temperature was being operated 5°C above the optimal value. To reach the optimal furnace outlet

temperature, the throughput was increased by 4 % while keeping the ADU furnace operating at maximum capacity. This change slightly compromised the separation sharpness, while increasing product flow rates, and increasing the net profit by $2.2 million per year. The next most beneficial operational change, to increase the stripping steam flow to the ADU, further helped to vaporize light components. The third best operational change was to increase AGO stripping steam, to improve diesel recovery from AGO. After these changes were implemented, the net profit for the LS crude increased by $3.7 million per year, relative to when the implementation started.

Due to unexpected equipment malfunction in both implementations (coking in the VDU furnace, one air cooler and the HVGO pump-around pump breaking down, etc.), it was not possible to implement the remaining modifications suggested by the optimizer. However, even though the operating scenarios at the implementations were very different from the base case used to carry out the study, the main operational changes identified in the sensitivity analysis and in the optimization were still relevant, applicable and able to deliver significant economic benefits during implementation. For both representative crude oils, plant measurements were used to calculate the expected net profit of on-site implementation of operational changes. The projected increase in net profit of $7.2 million per year is achieved mainly by ajdusting the ADU furnace outlet temperature and stripping steam flow rates to increase distillation yields – without any capital investment.

4. Conclusions

A new approach for operational optimization of crude oil distillation systems has been developed that uses sensitivity analyses, artificial neural networks and stochastic optimization. The approach was extended in this work to include the crude oil flow rate as an optimization variable. The methodology, developed and tested in academic case studies, has been applied to optimize yields of the bottlenecked crude oil distillation system of a Spanish refinery. The study showed that optimization was crucial to identify the right balance between capacity and separation efficiency to maximize profit, which was achieved by manipulating the crude oil flow rate, furnace outlet temperatures, and stripping steam. On-site implementation indicated that relatively minor operational changes in the product yields can increase profit by $7.2 million per year, with realtively no impact on energy costs. A new academic-industry project is under way to extend the methodology to use historical plant data, together with first-principles models, to develop surrogate models for real-time optimization.

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