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Review

Simulation and characterization in the refining industry: A review

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Oil refining is one of the most complex chemical industries; the objective of refinery operations is to generate as much profit as possible by converting crude oils into valuable products. The current trend toward processing petroleum needs sufficient compositional information to understand the chemistry of reactions that are involved. The objective of the present paper is to review the simulation technologies and characterization techniques which have been used in refining industry. It is found that simulation can be used in crude oil scheduling, predicting wax precipitation, asphaltene deposition, and for fractionation of crude oil based on equilibrium stage relations. The review on characterization methods clearly illustrates that the spectroscopic techniques (IR/FTIR, NMR, NIR); chromatographic techniques; true boiling point; solvent precipitation; refractive index; differential scanning calorimeter and thermogravimetry; and near- infrared region are mostly used in characterizing crude oil.

Key words: Simulation, oil refining, crude oil characterization, true boiling point.

INTRODUCTION

Oil refining is one of the most complex chemical industries, which involves many different aspects and complicated processes with various possible connections. The objective in refinery operations is to generate as much profit as possible by converting crude oils into valuable products such as gasoline, jet fuel, diesel, and so on (Zhang and Zhu, 2000; Gary and Handwerk, 2001).

In recent years, the requirements for large quantities of liquid hydrocarbons, part–icularly gasoline and diesel fuels have increased and will continue to escalate, which will necessarily cause steady rise in production volume of the refining industry. The International Energy Agency in its World Energy Outlook 2008 is predicting the increase in yearly oil use to be 1.3% until 2020 and 1.0% from 2020 to 2030 (Muzic et al., 2011).

Various processes are applied in order to separate a mixture, including extraction, crystallization, semi-permeable membranes, etc.; but distillation has been found to be having substantial advantages over other processes. As a rule, it is the most cost-effective process, so it may be used for mixtures with very diverse properties (Buckley et al., 1985).

Distillation is the oldest and the most universal process

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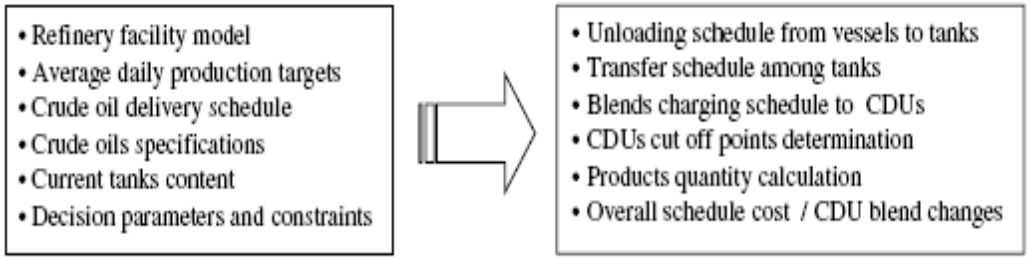

Figure 1. Software system's input/output information.

of chemical technology and other branches of industry incorporating separation of mixtures. In petroleum refineries, there are many distillation columns that are presently working satisfactorily well. There are also several others that are not working well, and at least a few that function very poorly, or not at all. Failure to obtain the specified and required performance is due in many cases to faulty or inadequate control system design. Troubleshooting of columns that are already in operation is frequently necessary, but practical considerations usually limit corrective measures to relatively minor items. Proper original design is by far the best way to guarantee satisfactory operation and control (Buckley et al., 1985).

Simulation is presently a mature well tested technology and it is widely used for a variety of purposes, including design, control, test, optimization, and integration of process plants (Denn et al., 2004). Simulations can save a lot of time and money which gives a pre-assessment for the real refining processes. More-over, they are a lot cheaper and much faster than running series of experiments. To establish the simulation, both the operating variables (input specifications) and the definition of the mixture (characterization) have to be specified first (Leelavanichkul et al., 2004; Eckert and Vanek, 2005). This paper gives a review on the simulation technologies and characterization techniques which have been used in refining industry.

Simulation

Simulation is widely used in petrochemical industry. Many models have been proposed in the past for predicting wax precipitation (Lira-Galeana and Firoozabadi, 1996; Casavant and Cote, 2004; Pan et al., 2009). Compare numerous studies have been reported in asphaltene deposition and asphaltene molecular and colloidal structures (Hirschberg et al., 1984; Kawanaka et al., 1991; Andersen and Speight, 1999; Mullins, 2008; Mullins et al., 2012).

Kumar et al. (2001) have developed a steady state multi component distillation model based simulator particularly suited for fractionation of crude oil based on equilibrium stage relations. Results of such a simulator gave complete true boiling point (TBP) curves for all the products that can be used to predict other product properties such as Reid vapor pressure (RVP), flash point, pour point, etc (Kumar et al., 2001). Motlaghi et al. (2008) have designed an expert system of a crude oil distillation column to predict the unknown values of required product flow and temperature in required input feed characteristics. The system was also capable to optimize the distillation process with minimizing the model output error and maximizing the required oil production rate with respect to control parameter values (Motlaghi et al., 2008).

Chryssolouris et al. (2005) have proposed a simulation-based approach to the refinery operation which addressed primarily the scheduling of a refinery importing various types of crude oil. Figure 1 illustrates software system's input/output information. The study show that the proposed approach compared with manual spreadsheet-based calculations, may accelerate the scheduling process, proposing alternative solutions of comparable quality while increasing the accuracy of computations and allowing the investigation of what-if scenarios (Chryssolouris et al., 2005).

Pan et al. (2009) have presented a new approach for crude oil scheduling (Figure 2) which can avoid composition discrepancy without using iterative algorithm and find better solution effectively. They have used a new mixed integer non-linear programming (MINLP) for crude oil scheduling firstly, and then proposed some heuristic rules collected from expert experience to linearize bilinear terms and prefix some binary variables in the MINLP model (Pan et al., 2009). Robertson et al. (2011) suggested a multi-level simulation approach for the crude oil loading/unloading scheduling problem. They have used the nonlinear simulation model for the process units to find optimized refining costs and revenue for a blend of two crudes. Results showed that this integrated approach can lead to a decrease of production and logistics costs or increased profit, provide a more intelligent crude schedule, and identify

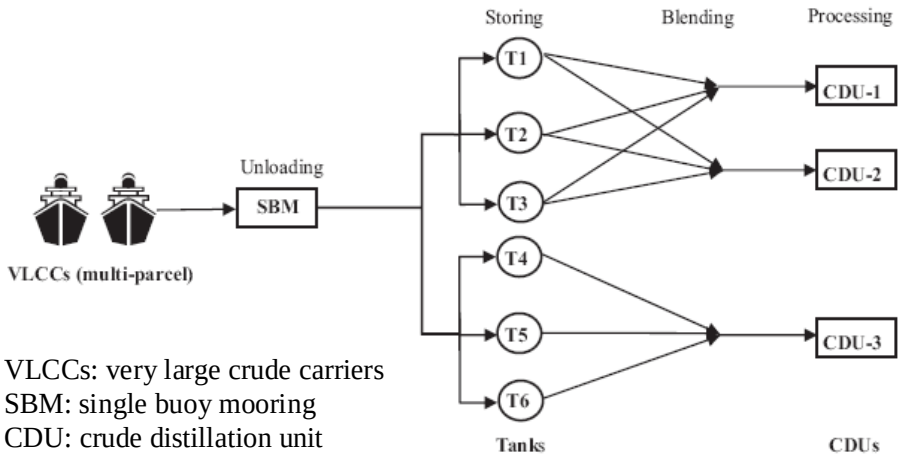

Figure 2. Schematic of crude oil scheduling (Pan et al., 2009).

production level scheduling decisions which have a tradeoff benefit with the operational mode of the refinery (Robertson et al., 2011).

Oil characterization

Characterization of complex mixtures is a common tool especially in the oil processing industry. To establish the simulation both the operating variables (input specifications) and the definition of the mixture have to be specified first (Leelavanichkul et al., 2004; Eckert and Vanek, 2005). A method widely used for characterizing crude oil (hydrocarbons) is the true boiling point (TBP) curve. TBP distillation is a widely used batch distillation process for the characterization of crude oils, traditionally mainly for marketing and refining purposes. The TBP curve is obtained by plotting the cumulative mass or volume distillation fraction with increasing temperature. The shape of these curves is dependent on the volatility of components in a given crude oil. As such, these curves give a “footprint” of the composition of crude oils.

Behrenbruch and Dedigama (2007) proposed a new method of characterizing crude oils based on the shape of TBP distillation curves using a two parameter form of the gamma distribution from statistics. The proposed method was found to describe experimental data very well with just two parameters, and as such offers a very practical approach in terms of classifying crude oils (Behrenbruch and Dedigama, 2007).

Gas chromatography (GC) is an analytical technique that is broadly used for characterizing crude oil (hydrocarbons), and numerous advances in this method have originated in petroleum industry laboratories (Gautam et al., 1998; Barman et al., 2000). Moreover, its use has markedly increased in the last few years with the progress in instrumentation and the relatively low cost of the equipment (Durand, 2000).

Barman et al. (2000) have provided a broad overview of major chromatographic techniques that have been applied to the characterization of petroleum and related products. They have discussed the scope, applicability, and versatility of individual techniques such as gas, liquid, supercritical fluid, thin-layer, and size-exclusion chromatography. They have found that analytical approaches vary widely depending on the chromatographic technique, instrumentation, minimum detection limit, and sample type. Several techniques such as open-column liquid chromatography, medium pressure liquid chromatography, high-performance liquid chromatography (HPLC), and supercritical fluid extraction provided separation of compound classes for subsequent characterization by higher resolution chromatography, spectroscopy, hyphenated or multi technique chromatographic approaches have also been described (Barman et al., 2000).

Carbognani et al. (2007) have analyzed maltene phases from deasphalting to detect SAR hydrocarbon group types using thin layer chromatography with flame ionization detection (TLC−FID). They have confirmed the validity of proposed technique (TLC−FID) by careful calibration procedures and validation with preparative group-type analysis (Carbognani et al., 2007).

Leelavanichkul et al. (2004) have characterized the crude oil using a combination of different experimental techniques including: true boiling point (TBP) distillation which was performed to fractionate the crude oils: single carbon number (SCN) fractions up to C_{25} and a residue fraction C_{25+}, solvent precipitation, refractive index (RI) measurement that was used in the determination of paraffin, naphthene, and aromatic (PNA) contents, HPLC which was employed to separate the maltene fraction of the residues into three sub-fractions based on hydrocarbon group types: saturates, aromatics, and resins (SAR), high temperature gas chromatography simulated distillation which was used for the analysis of the

light-ends contents, and the saturate and aromatic fractions collected from the HPLC fractionation, and size exclusion chromatography was used to characterize the resin and asphaltene fractions (Leelavanichkul et al., 2004).

Falla et al. (2006) have proposed a methodology for the estimation of the SimDis (Simulated Distillation) properties of crude petroleum based on Near Infrared (NIR) spectroscopy. The NIR spectral data were correlated with the SimDis curves (weight percent vaporized at a given temperature) and the salt content of the petroleum by neural network techniques. The resulted network reproduced quite accurately the SimDis curves, showing the technical feasibility of the proposed methodology (Falla et al., 2006).

Pasquini and Bueno (2007) have described an approach to predict the true boiling point (TBP) curve and to estimate the American petroleum Institute (API) gravity in order to characterize the petroleum processed in refineries by using the information presented in its absorbance spectrum obtained in the near-infrared region.

Gautam et al. (1998) have made a review on the spectrometric techniques used for characterization of the crude oil and various petroleum products. They stated that the spectrometric methods offer a great potential for fast and reliable characterization of crude oil and its products compared to conventional methods such as octane number by the American Society for Testing and Materials (ASTM) knock engine method or vapor pressure by the Gabner method are time consuming and often expensive to maintain. They have found that of the various spectroscopic techniques available, infrared (IR/FTIR) and nuclear magnetic resonance (NMR) offer the best opportunities for the characterization of crude oil and related petroleum products. Nuclear NMR had proved to be of great value in petroleum research because it can identify the chemical nature of individual types of hydrogen and carbon, even in complex organic mixtures of petroleum and its refined products. The NMR technique was found to be also useful as a means of estimating molecular weight and for studying the effects of various refining processes (Gautam et al., 1998). Kok (2011) has characterized heavy and medium grade crude oils in limestone matrix using differential scanning calorimeter (DSC) and thermogravimetry (TG-DTG).

CONCLUSION

In this review, various simulation technologies and characterization methods that have been used in refining industry were presented. It is found that simulation can be used in crude oil scheduling, predicting wax precipitation, asphaltene deposition, and for fractionation of crude oil based on equilibrium stage relations. To establish the simulation, both the operating variables (input specifications) and the definition of the mixture have to be specified first. The mixture is defined by its characterization. TBP distillation curves can be used to classify crude oils based on the curves' shape.

The chromatographic techniques vary widely depending on the sample type (gas chromatography, liquid chromatography, supercritical fluid chromatography, thin-layer chromatography, open-column liquid chromategraphy, medium pressure liquid chromatography, high-performance liquid chromatography, high temperature gas chromatography simulated distillation, spectroscopy, hyphenated or multi technique chromatographic approaches, and size-exclusion chromatography). This review illustrates that the spectroscopic techniques (IR/FTIR, NMR), solvent precipitation, refractive index, differential scanning calorimeter and thermogravimetry, and near-infrared region are mostly used in characterizing crude oil.

Conflict of Interests

The authors have not declared any conflict of interests.

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