58g Hybrid Modeling and Multi-Objective Optimization of an Industrial Hydrocracker

Naveen Bhutani, Ajay K. Ray, and Gade P. Rangaiah

Abstract

Hydrocracking is a complex catalytic cracking process that involves the cracking of relatively heavy oil fractions such as heavy gas oil and vacuum gas oil into lighter products: naphtha, kerosene and diesel, in the presence of hydrogen. Since the feed is a complex mixture of olefins, paraffins, aromatics and napthenic compounds, the rate constant for individual reaction steps are impossible to obtain. Hence, many researchers have followed pseudo-component approach which is based on classifying hydrocarbons on the basis of either structural classes (Martens and Marin, 2001) or common properties like boiling point range and specific gravity to reduce the complexity of problem. These first principle models are not satisfactory for industrial applications due to common process variations such as change in feed stock composition, operating conditions and catalyst deactivation. The main reason is the complex reaction kinetics which necessitates regular update of model internal parameters for accurate prediction.

Hybrid models which combine first principle and data-based approaches have significant advantages over the first principle model. They allow the integration of a-priori knowledge with the valuable information contained in the industrial operating data. Hence, the hybrid model structure captures underlying system characteristics better. Several hybrid model structures have been proposed in the literature (Duarte et al., 2004) These structures generally follow first principles approach for macroscopic balances (i.e. mass, energy and momentum balances) and employ artificial neural networks to model nonlinear reaction kinetics of complex chemical/biological kinetics. Application of such approaches to modeling of chemical (Hugget et al., 1999), biochemical (Psichogios and Ungar, 1992; Thompson and Kramer, 1994; Oliveira, 2004) and petrochemical processes (Bellos et al., 2005) has been studied using simulated, laboratory or plant data. However, application of hybrid models to industrial plants such as hydrocrackers has not been reported in the open literature.

There are two main approaches found in open literature for combining mechanistic models with empirical models to obtain hybrid models (Duarte et al., 2004). They are: serial and parallel arrangements of mechanistic and empirical models. Serial structure has been used to model kinetics of bioprocess (Acuña et al., 1991), industrial hydrodesulfurization reactor (Bellos et al., 2005) and yeast cultivation (Schubert et al., 1994) whereas parallel structure has been used to improve the prediction capability of mechanistic model for activated sludge process (Cote et al., 1995), model complex chemical reactor system (Su et al., 1992) and model and control a laboratory pressure vessel (Van Can et al., 1996).

Motivated by the availability of lot of industrial data, computational resources and limitations of first principle model (Bhutani et al., 2005) to fully capture uncertainties in feed stock composition, catalyst deactivation, operating conditions etc., the present work proposes hybrid models for an industrial hydrocracker where the hydrocracking reactor system is described by a set of pseudo-component mass balance equations using discrete lumped model approach (Mohanty et al., 1991; Pacheco and Dassori, 2002), and the reaction kinetics is represented by an adjustable mixture of neural network and mechanistic representations. Configuration, design and steady state data of the hydrocracking unit operation is taken from industry for a year of operation. A few hybrid modeling structures will be studied for hydrocracker simulation, with the objectives of comparing them and identifying a robust model.

A typical hydrocracker produces many valuable products such as naphtha, kerosene and diesel and low value products like light ends with utility consumption. Hence, hydrocracker optimization naturally involves multiple objectives. A hybrid model of hydrocracker and non-dominated sorting genetic algorithm (NSGA) will be employed for solving suitable multi-objective problems. Production of selected products will be simultaneously maximized with respect to decision variables such as feed flow rate, recycle gas flow, quench gas flow and inlet temperature subject to realistic constraints. Optimal solutions and the corresponding operating conditions will be presented and discussed.

References

Acuña G., Cubillos F., Thibault J. and Latrille E., Comparison of methods for training Grey-Box neural network models, Comp. and Chem. Eng., vol. 23, pp. S561, 1999.

Bellos G. D., Kallinikos L. E., Gounaris C. E. and Papayannakos N. G., Modelling of the performance of industrial HDS reactors using a hybrid neural network approach, Chemical Engineering and Process, vol. 44, pp. 505-515, 2005.

Bhutani N., Ray A. K. and Rangaiah G. P., “Modeling and Multiobjective Optimization of an Industrial Hydrocracking Reactors”, submitted to Ind. Eng. Chem. Res., 2005.

Côte, M., Grandjean B. P. A., Lessard P., and Thibault J., Dynamic modeling of the activated sludge process: Improving prediction using neural networks, Water Res., vol. 29, pp. 995 1995.

Duarte B., Saraiva P. M. and Pantelides C. C., Combining mechanistic and empirical modelling, International Journal of Chemical Reactor Engineering, vol. 2, 2004.

Hugget, A., Sébastin P., and Nadeau J. P., Global optimization of a dryer by using neural networks and genetic algorithms, AIChE J., vol.45, no. 6, pp. 1227, 1999.

Martens G. G. and Marin, G. B., AIChE J., vol. 47, no. 7, pp. 1607- 1622, 2001.

Mohanty, S., Saraf, D. N. and Kunjuru, D., Fuel Processing Technology, vol. 29, pp. 1-17, 1991.

Oliveira R., Combining first principles modeling and artificial neural networks: a general framework, Comp. and Chem. Eng., vol. 28, pp. 755-766, 2004.

Pacheco, M. A. and Dassori C. G., Chem. Eng. Comm., vol.189, pp.1684-1704, 2002.

Psichogios D. C. and Ungar L. H., A hybrid neural network-first principles approach to process modeling, AIChE J., vol. 38, no. 10, pp. 1499-1511, 1992

Schubert J., Simutis R., Dors M., Havlík I. and Lübbert, A., Hybrid modeling of yeast production processes- A combination of a priori knowledge on different levels of sophistication, Chem. Eng. Tech., vol. 17, pp. 10-20, 1994.

Thomson, M. L. and Kramer, M. A., Modeling chemical processes using prior knowledge and neural networks. AIChE J., vol. 40, pp. 1328–1340, 1994.

Van Can H. J. L., Hellinga C., Luyben K. C. A. M., Heijnen J. and Braake H. A. B., Strategy for dynamic process modeling based on neural networks and macroscopic balances, AIChE J., vol. 42, pp. 3403-3418, 1996.