Challenges in the Development of the Mathematical Modeling of a Delayed Coking Process

Cláudio N. Borges[1,2], Maria Anita Mendes[1] and Rita M. B. Alves[1]

(1) University of São Paulo, Polytechnic School, Department of Chemical Engineering, São Paulo, Brazil.

(2) Refinery Presidente Bernardes – RPBC, Petrobras, Cubatão, Brazil.

claudio.neves@petrobras.com.br; rmbalves@usp.br

Abstract

The Delayed Coking Unit is a thermal conversion process used in many refineries to convert vacuum residue into lower molecular weight high-value products (gases, coker naphtha and coker gas oil) and petroleum coke. A slight increase of liquid yield of delayed coking could bring very considerable economic benefits, especially liquid distillate. Market competition, restrictions on product specifications and operational bottlenecks require better control of production planning. Therefore, developing new strategies and mathematical models focused on operational optimization of industrial processes and formulations of products is essential to achieve better yields and more accurate product quality monitoring.

Usually, this process is composed by three main equipments: the main fractionator, the coking furnace and at least two coke drums, which work batch due to need of removing the accumulated petroleum coke. The main fractionator has as main purposes: fractionating the effluents of the coke drums and the fresh feed from the vacuum tower distillation. In the coking furnace, heating and thermal cracking reactions of the feed are carried out. While in the coke drum, thermal cracking reactions and coke formation as well as the vapor-liquid equilibrium occur.

Constraints in carry out modeling and simulation in good adherence to the industrial plant, which is empirical, are data quality and degree of detail of the models used.

When complex kinetic models are not used to represent the industrial plant data, molecular information is masked due to the absence of physical and chemical properties, which are beyond the definition of the lump considered, since the chemical structure is not well known.

For the development of rigorous models including more details of chemical reactions kinetics, the feedstock and products composition, and, so their molecular structure, are required. Molecules are the common foundation for feedstock composition, property calculation, process chemistry, and reaction kinetics and thermodynamics. Rigorous

modeling that allow reaction of complex feeds and prediction of molecular properties require an unprecedented level of molecular details.

Two factors have supported modeling at the molecular level becoming feasible: (1) recent development in analytical chemistry allows assessing the measurement of the complex structure of the vacuum residue, directly or indirectly; (2) use of advanced computational methods.

The proposed model is based in lumped kinetic scheme and vapor-liquid equilibrium conditions in the furnace and coke drum. This work is based on the experimental data analysis and operating conditions from an industrial delayed coking unit. Therefore, the aim is to discuss the main challenges in the development of mathematical model of the furnace and coke drum such as rigorous molecular characterization of the vacuum residue and products, to find out parameters that affect coke morphology, to detail reaction zones inside the coke drum, to select correlations for critical properties and formation enthalpy of pseudo components.