Mathematical Modeling and Global Optimization for Planning and Scheduling of Petrochemical Processes, and Natural Gas to Liquid Fuel Energy Systems

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In the last twenty years, the petrochemical industry has succeeded by creating markets and supplying them with suitable products used to create goods such as plastics, cosmetics, lubricants, and paints. Petrochemical production begins in a refinery that separates crude oils mainly into lighter components such as naphtha, light naphtha, top oil, and liquid fuels including gasoline, diesel and jet fuel. The lighter components are further processed into various petrochemicals such as ethylene, propylene, butadiene, benzene, toluene, xylol and some other high-valued products via cracking, butadiene extraction, hydrotreating, etherification, and polymerization processes. Nowadays, tighter competition, strict environmental regulations, and lower-margin profits, drive the petrochemical industry to apply new technologies to improve their planning operations.

In this presentation, detailed nonlinear models are first proposed to predict product yields and properties in production units including crude distillation unit, vacuum distillation unit, hydrocracking units, catalytic cracking units, ethylene-cracking units and other processing units present in a petrochemical plant. The yield and property prediction models for crude distillation and vacuum distillation units are developed using swing cut theory based on crude assay data. Empirical non-linear models are developed for other processing units, including bilinear, trilinear, quadratic, polynomial, and exponential terms. Parameter estimation for all of the developed models is performed by globally minimizing the least squares error between the parametric models and real production data. Moreover, property indices in blending units are linearly additive and calculated on weight or volume basis, which introduce bilinear and trilinear terms. We also introduce binary variables to denote different operation modes for several production units.

The entire planning model is a non-convex mixed integer nonlinear optimization model (MINLP). To solve this large-scale nonlinear model, we propose an optimization-based procedure to obtain the tightest lower and upper bounds for variables especially the variables involving nonlinear terms. Then, we incorporate those tightest lower and upper bounds into commercial solver ANTIGONE to obtain ε-global optimality. Finally, a user-friendly platform is developed to allow the user to modify the planning model by updating model parameters when new data is available, product demands and specifications, cost parameters and many more. Several large-scale industrial examples are solved to illustrate the efficiency of our proposed model and global optimization approach.