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Review: Integrating Optimization Module into Chemical Process Simulation

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Abstract: The chemical industry has undergone significant transformation during the past 25 years due to the increased cost of energy, increasingly stringent environmental regulations and global competition in product pricing and quality. The main objective of a process design is to create a process that is economical, safe, and environmentally benign throughout the whole lifetime of the plant. One of the most important engineering tools for addressing these issues is optimization. Modifications in plant design and operating procedures have been implemented to reduce costs and meet constraints, with an emphasis on improving efficiency and increasing profitability by using computer integrated manufacturing, or CIM. To apply optimization effectively in processing plant, both theory and practice of optimization must be understood. Appropriate meshing of the optimization technique and the model are essential for success in optimization. Over the last 10 years much effort has been devoted to the study of optimization strategies of either selected sections or entire chemical plant involving both continuous and integer variables. Several algorithms have been proposed and large numbers of research applications have been presented. However, only a few applications have been reported with process simulation. This study presents a review of the concepts/application of optimization techniques. In addition, it discusses optimization software and process simulator that offers the most potential for successful and reliable results.

Key words: Process optimization, process simulation, constraints, objective function, process synthesis, process system engineering

INTRODUCTION

Chemical industry plays an important role in the daily life of our society. The purpose of a chemical process is to convert some (cheap) materials into other desirable and valuable products. Innovation in chemical process design is a key issue in today's chemical industry. Process synthesis is an important part of the overall chemical innovation process which starts with identification of the process needs prior to construction and operation of the process plant. Conceptual design is the initial stage of chemical process design where the conceptual synthesis of a process flowsheet is developed. Chemical process synthesis is an important activity to the industry and academia as it deals with the problem of how to develop and integrate flowsheets to search for the best design alternative for chemical product manufacturing processes (Alqahtani, 2008).

Optimization is the use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process. This technique is a major quantitative tool in industrial decision making regarding problems in the design, construction, process operation, plant, company level etc. (Edgar *et al*., 2001). It deals with finding the optimum design parameters for maximizing the profit or minimizing the total investment on a process plant with trade-offs between capital and operating costs (Alqahtani, 2008). As the power of computers has increased, optimization technique has been expanded and applicable for more complex problems.

Operational optimization of either a section or the entire chemical plant starting from the design stage has been a task of growing interest in the chemical industry. Traditionally, it has been performed using the standard optimization tool of commercial flowsheeting program or through an optimizer-simulator program (Diaz and Bandoni, 1996). The optimal design of chemical plant involves discrete and continuous choices. The selection of the process unit among a number of possible alternatives as optimization variables is a discrete choice. Continuous choice refers to the selection of the optimal size and the operating conditions (temperature, pressure, flowrates, compositions, conversions, etc.) of the selected process unit as the optimization variables (Lee *et al*., 2003). The applications of optimization have been mainly accomplished by using continuous choice while the

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flowsheet topology (discrete choice) has been kept fixed. The combination of discrete and continuous choices can be done but the optimization problem will become more complex and difficult to solve. Therefore, to apply optimization effectively in the chemical industries, both the theory and practice of optimization must be understood.

THE NATURE OF OPTIMIZATION

Optimization concepts: Optimization has become a major enabling area in Process System Engineering (PSE). It has evolved from methodology of academia interest into a technology that has and continues to make significant impact in industry (Biegler and Grossmann, 2004). PSE has been evolving into a specialized field at the interface between chemical engineering, applied mathematics and computer science with specific model-based methods and tools as its core competencies to deal with the inherent complexity of chemical processes and the multi-objective nature of decision-making during the lifecycle of the manufacturing process of chemical products (Klatt and Marquardt, 2009). Typical problems in chemical process design or plant operation have many possible solutions. Optimizations have been implemented to find the values of variables in the process that yield the best value of the performance criterion.

Every optimization problem contains three essential features which are (1) at least one objective function to be optimized, also known as economic model, (2) equality constraints and (3) inequality constraints. Features 2 and 3 constitute the model of the process or equipment (Edgar *et al*., 2001). Optimization solutions must not only satisfy all of the constraints, but also must achieve the objective function. In mathematical term, optimization problem can be represented by this notation:

$$\begin{array}{lll} \text{Minimize:} & f(x) & \text{objective function} \\ \text{Subject to:} & h(x) = 0 & \text{equality constraints} \\ g(x) \geq 0 & & \text{inequality constraints} \end{array} \quad (1)$$

where, x is a vector of n variables ($x_1, x_2, \ldots, x_n$), h(x) is a vector of equations of dimension m_1, and g(x) is a vector of inequalities of dimension m_2. The total number of constraints is $m = (m_1 + m_2)$.

The formulation of the objective functions is one of the crucial steps in the application of optimization. In the chemical industries, the objective function often is expressed in units of currency (cost) because the goal of the enterprise is to minimize costs or maximize profits subject to a variety of constraints. The objective function can also be expressed in term to solve the problem in maximization of the yield of component or minimization of the use of utilities or minimizing difference between a model and some data and so on (Edgar *et al*., 2001). Mass and energy balances are written as equality constraints while inequalities constraints are represented by the design specifications and logical constraints (Diaz and Bandoni, 1996).

Classification of problem types, variable types and equations: Optimization can be classified in terms of continuous and of discrete variables regardless of the solution methods. The major problems for continuous optimization include Linear Programming (LP) and nonlinear programming (NLP), with important subclass of Linear Complementarity Problem (LCP) for LP, while for NLP includes Quadratic Programming (QP) and semidefinite programming (SP). As for discrete problem, they are first classified into Mixed-Integer Linear Programming (MILP) and Mixed-Integer Nonlinear Programming (MINLP). For the former an important particular case is when all variables are integer, which gives rise to an Integer Programming (IP) problem. Regarding to the formulation in (1), algebraic form correspond to mixed-integer optimization problems have the following general form with *x* are continuous variables which generally correspond to state variables, while y are the discrete variables which generally are restricted to take 0-1 values to define for instance the assignments of equipment and sequencing of tasks:

$$\begin{array}{ll} \text{Minimize:} & f(x,y) \\ \text{Subject to:} & h(x,y) = 0 \\ & g(x,y) \geq 0 \\ & x \in X, y \in \{0, 1\}^m \end{array} \quad (2)$$

An MIP problem corresponds to a MINLP when any of the functions involved in optimization problem are nonlinear. If all the functions are linear it corresponds to a MILP. If there are no 0-1 variables, the MIP problem reduce to a NLP or LP depending on whether or not the functions are linear (Alqahtani, 2008; Biegler and Grossmann, 2004).

Caballero *et al.* (2007) had classified the different types of variables arise in an optimization problem and also differentiated two classes of equations. Implicit equations are equations that are solved by each modules in the process simulator, or any other third party module added to the model, while External/explicit equations are the equations over which user have complete control, include dependent and independent variables. Design or independent variables in a chemical process simulator are the variables that must be specified to converge the flowsheet. The number of such variables matches the degrees of freedom in the flowsheet. Variables calculated by the simulator (or in general by any implicit model) is the variable calculated by the simulator. The user has no direct control over these variables but in some simulator it is possible to force these variables to take specific value through auxiliary calculation blocks that change some of the design variables until the specification is met. In optimization the system, it is faster and usually numerically more reliable to introduce these specifications as constraints to the model. Variables that must be fixed in a given topology of the flowsheet is refer to a subset of variables that must be fixed in a given iteration when solving a NLP problem with a given topology and a given set of fixed binary (Boolean or integer) variables. Lastly are the variables that do not appear at the flowsheet level (or in other implicit block of equations) but appear in explicit external constraints. No special treatment of these variables is required.

General step to solve optimization problems: Edgar *et al.* (2001) lists six general steps for the analysis and solution of optimization problems. It may not be necessary to follow the cited order exactly, but should cover all steps eventually. Shortcuts in the procedure are allowable and the easier steps can be performed first.

- Analyze the process so that the process variables and specific characteristics of interest are define; that is make a list of all the variables
- Determine the criteria for optimization and specify the objective function in terms of the variables defined in step 1 together with coefficients
- Using mathematical expressions develop a valid process/equipment model that relates the input-output variables of the process and associated coefficients include both equality and inequality constraints. Identify the dependent and independent variables to get the number of degrees of freedom
- If the formulated problem is too large in its scope:
  - Break it up into manageable part or
  - Simplify the objective function and model
- Apply a suitable optimization technique to the mathematical statement of the problem
- Check the answer and examine the sensitivity of the result to changes in the coefficients in the problem and the assumptions

Applications: In practice, optimization can be applied in numerous ways to chemical processes and plants. Typical example in which optimization has been include are (1) determining the best sites for plant location, (2) routing tankers for the distribution of crude and refined products, (3) sizing and layout of a pipeline, (4) designing equipment and an entire plant, (5) scheduling maintenance and equipment replacement, (6) operating equipment such as tubular reactor, columns and reactor, (7) evaluating plant data to construct a model of a process, (8) minimizing inventory charges, (9) allocating resources or services among several processes and (10) planning and scheduling construction (Edgar *et al.*, 2001).

Table 1: Applications of mathematical programming in process systems engineering

	LP	MILP	QP, LCP	NLP	MINLP	Global	SA/GA
Design and synthesis							
HENS	x	x		x	x	x	x
MENS	x	x		x	x	x	x
Separations		x			x		
Reactors	x			x	x	x	
Equopment design				x	x		x
Flowsheeting				x	x		
Operations							
Scheduling	x	x			x		x
Supply chain	x	x			x		
Real-time optimization	x		x	x			
Control							
Linear MPC	x		x				
Nonlinear MPC				x		x	
Hybrid		x		x	x		

Optimization methods take advantage of the mathematical structure of the economic and the process models to locate the optimum. The method chosen for any optimization purposes depends primarily on the character of the objective function and whether it is known explicitly, the nature constraints and the number of independent and dependent variables (Alqahtani, 2008). Mathematical programming and optimization in general have found extensive use in process system engineering. Referring to Table 1, as for specific areas, process design problems tend to give rise to NLP and MINLP problems, while scheduling and planning problems tend to give rise to LP and MILP problems. The reason for this is that design problems tend to rely more heavily on predictions of process models, which are nonlinear, while in scheduling and planning the physical predictions tend to be less important, since most operations are described through time requirements and activities. In the case of process control the split is about even (Biegler and Grossmann, 2004).

RECENT WORK: OPTIMIZATION INTEGRATED WITH PROCESS SIMULATOR

The goal of process engineers it to find among the large number of alternative flowsheets, the least expensive one and to evaluate whether or not this alternative is profitable. A synthesis approach can utilise the availability of effective design methods aided by powerful simulation tools and other third party software for flowsheet optimization, sizing and cost estimation.

Costa *et al.* (2005) present the utilization of a process simulator in the operation and capacity expansion of Prosint Quimica plant, the largest Brazilian methanol producer. The process constitutes process line, fuel system and steam system which consist substantial models. Process data necessary for the process simulation from plant was accessed using Exaquantum software (Plant Information Management System-PIMS tool) which can act as Excel plug in when it is activated in a spreadsheet. Then the data collected will be transport from Excel file to Aspen file (simulator) where simulation can be executed through OLE links (object linking and embedding) previously establish between the files. The results obtained are then transferred to an output Excel file also using the OLE capabilities for several data presentation.

Subawalla *et al.* (2004) presented a multivariable optimization (MVO) as a powerfull nonlinear steady-state flowsheet simulation technique in the methylamines facilities to optimize plant performance by increasing plant capacity and/reducing energy consumption. The MVO process flowsheet involves three steps before it can be implemented in plant. First, develop models for individual unit operations and build process flowsheet. Then, validate the process flowsheet and the individual models with plant and laboratory data to minimize the error between model predictions and plant data. The last step is to create MVO flowsheet which involves defining the variables and their upper and lower limits, the constraints (include equipment operating limits) and the objective function. Common optimization variables include feed and recycle flow rates, distillation mass and energy flows and flow rates of other energy stream. They used Aspen-Plus® Simulator for the simulation.

Mahmood and Chng (2009) discussed the used of integrated HYSYS model with Excel-based spreadsheet in debottlenecking and optimization of oil and gas facilities. The debottlenecking study was split into three distinct phase: (1) develop a HYSYS fully integrated facilities model and calibrate against actual operating conditions, (2) collate design data for input into Meascap Capacity models, (3) checking Meascap results and input data particularly for items with Utilisation Factor > 100%. *Meascap* is a simple Excel-based spreadsheet tools which extracts the process data generated by a HYSYS simulation and uses it to calculate the actual design capacity (Capacity) and required capacity (Demand) of the equipment items using Capacity Models. Utilisation Factor for each piece of equipment is to indicate, in percentage, how close the equipment is required to operate compared to its design capacity.

Caballero *et al.* (2007) addressed the design and optimization of chemical processes using Chemical Modular Process Simulator that include state of the art models, including discontinuous cost and sizing equations. Using this modular framework, the problem is formulated as a generalized disjunctive programming problem and reformulated and solved as a mixed-integer nonlinear programming problem. Different algorithms (branch and bound, outer approximation, and LP/NLP based branch and bound) have been adapted to deal with implicit equations and their capabilities have been studied. These studies relies on three steps which are (1) set up the process flowsheet (Aspen HYSYS® simulator), determine the degrees of freedom and decide which of the independent variables in the flowsheet are among the available options, (2) write the mathematical programming model that includes explicit constraints (sizing and cost models), third party implicit models (other input-output models not included in the process simulator). These new constraints can be only in term of the independent and/or dependent variables that previously appear in the flowsheet and also in terms of new external variables and (3) connecting the process simulator with the rest of the model using a client-server application through the windows component object model (COM) interface. All the steps are controlled from MATLAB®, where the different algorithms were implemented. NLP sub-problems and Master problems are solved using TOMLAB-MATLAB-an interface for accessing state of the art NLP or MILP solvers.

Medeiros *et al.* (2004) analyzes HDT-LUB, aiming to optimize the process and operational aspects under the constraints of product specifications. The HDT-LUB was approached on three levels: (1) development of a steady state simulator to predict the final state of the product and hydrogen and utilities consumption from process variables, (2) definition of the economic objective, taking into account realistic aspects of process costs and the need to achieve product specification. The installed costs (ISBL, US$) were determined by the Guthrie models for year 1988 using the corresponding Marshall-Swift (M and S) index. Annual operational costs (UTIL, US$/year) were defined based on respective consumption of utilities and (3) optimization of design and operation. The HDT-LUB process was optimized using the SIMPLEX Nelder-Mead method in MATLAB R12 environment.

Goel *et al.* (2002) presents an optimization framework to identify an optimal process flowsheet structure and optimal equipment availability requirements at the conceptual design stage. It is possible to decompose the big synthesis, reliability and maintenance optimization problem into manageable sub-problems: reliability optimization and process synthesis, and maintenance and design optimization problems. In the first sub-problem, efforts are focused on optimizing the inherent availability and obtaining the optimal structure and optimal level of inherent availability required for equipment in the final optimal structure. Once the optimal structure and optimal availability of components have been obtained, detailed process models together with detailed maintenance models using time dependent reliability functions, can be used to obtain the optimal design parameters and a detailed maintenance schedule. The effectiveness and usefulness of the proposed optimization framework is demonstrated for the synthesis example of a HDA process.

Lee *et al.* (2001) illustrates a study project that initiated to develop a realistic simulation of an FCC and its upstream gas oil hydrotreater (HTR). The overall objective was to create a tool from which multiple case studies could be easily developed to study the effects of varying hydrotreater severity and FCC conversion on the product yields, properties and economics of the hydrotreater/FCC complex. The final objective was the optimization of the entire operation. For the purpose of the study, the individual HTR-SIM and FCC-SIM reactor models were first separately tuned and calibrated to match typical commercial unit operations. Calibration was required to allow a first principles reactor model to match an observed unit's performance. The matching was accomplished by adjusting model parameters tied to the installed catalyst's activity, selectivity and stability. Also captured during the calibration are non-idealities in the reactor system, such as divergence from plug-flow (e.g., hydrotreater bed channeling). Then the entire gas plant is simulated using the unit operations of HYSYS. Refinery including detailed tray-to-tray fractionators, heat exchangers, absorbers and the like. In situations in which the separation section was at or near constraints, this detail may very well be necessary, as these considerations may limit the reactor's window of operations. In order to demonstrate the full capabilities of HYSYS. Refinery, an optimization case was created to maximize the HTR/FCC complex as an integrated economic unit.

CONCLUSION

The reviewed highlighted the basic concepts that must be understood before applying the optimization. The used of readily available process simulation software as an interface to structural and continuous optimization is possible and promising strategy. The used of Excel unit operation in iCON® simulation process that allows the user to embed Microsoft Excel spreadsheets directly into the flowsheet and allows easy two-way data transfers between the softwares helps to simplify the development of optimization tools. In the future work, this research aim to generate and simulate different process flowsheets at several levels of complexity. The proposed flowsheets are then be evaluated to determine the optimal design condition and perform economic evaluation via Excel spreadsheet using VBA. The results will be validated with existing optimizer software.

FUTURE WORK

The used of cheap and readily available process software as an interface to optimization is much desired. iCON® is a locally developed process simulator by PETRONAS with Graphical User Interface (GUI) that includes all the facilities one expects from a chemical process simulator such as unit operation forms, graphs, unit conversion and process flow diagrams. In addition, iCON® provides a powerful Excel unit operation that allows the user to embed Microsoft Excel spreadsheets directly into the flowsheet and allows easy two-way data transfers between the softwares. This new approach allowed the process information from process design simulator to be extracted and used in optimization problems. The data such as pressure, temperature, flow rate and composition are extracted from iCON process simulator using the Microsoft Excel spreadsheets which is already built-in in this simulator software to optimize chemical process plant based on continuous parameters. In addition, ICON®-Excel® allows two-way data transfers that enable a cyclic optimization assessment procedure. Research is currently on-going to develop the entire framework in Fig. 1.

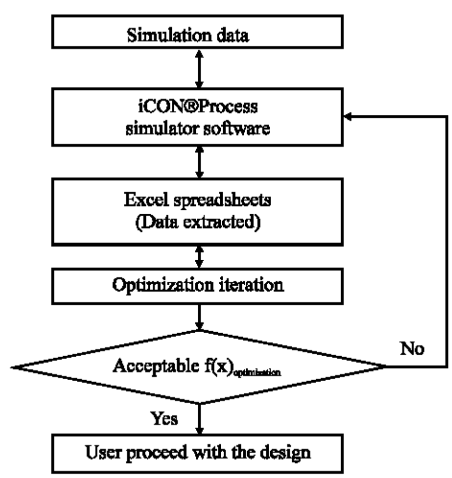

Fig. 1: Optimization framework

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