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Modular Integrated Framework for Process Synthesis and Optimization Based on Sequential Process Simulator

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A novel modular integrated framework is developed in this work to perform process synthesis and optimization based on a sequential process simulator. The modular integrated framework consists of three platforms: simulation, parameter and optimization platforms. This framework integrates process simulator, interface program, optimization algorithm to form a multi-platform environment integrated system. In the framework, the alternative processes models are firstly established through a process simulator (Aspen Plus).After that, parameter extraction and processing are implemented by Excel with the interface (Aspen Simulation Workbook). And then the MINLP problem of process synthesis is solved by the multidisciplinary integration software (Isight). The rigorous models of chemical processes or units, regarded as “Black box”, are solved by the process simulator, rather than shortcut or aggregated models in the form of equations. Therefore, not only is the process synthesis problem simplified but also does improve the accuracy of the solution. Several examples are provided to illustrate the effectiveness of the proposed method.

1. Introduction

Process synthesis has a significant impact on development, design and operation of petro-chemical processes. It can be considered as the cornerstone of a process design activity. Conventionally, the synthesis problem can be described as follows: given a set of feedstocks and a set of desired final products with specifications, the topology (unit selection and interconnection) and operating parameters (temperature, flow, pressure, etc.) are optimized to achieve optimal objectives (to maximum yield, energy efficiency, profit, etc). Generalized disjunctive programming (GDP) and mixed integer nonlinear programming (MINLP) have been proved to be powerful tools in the synthesis and design of subsystems such as heat exchanger networks, mass exchanger networks, distillation sequencing, and utility systems. However, in order to avoid complex numerical solving problems, it is common to use shortcut or aggregated models rather than rigorous models in large scale chemical production process. The shortcut or aggregated models reduces the precision of the process models, and hence may predict unreliable results. On the other hand, chemical process simulators (such as Aspen Plus, Hysys, Pro II, etc.) have become reliable tools that are widely used in process engineering (Lam et al., 2010). Process simulators contain strict models for most chemical process units, tailored numerical algorithms for particular units, and large databases of physicochemical thermodynamic and transport properties. The capability of process simulators can make modelling and optimization of the process more easily. Although most of process simulator contains some optimization tools, the optimization capability is limited to the fixed topology structure, and cannot be directly applied in the process synthesis problems. Therefore, it is desired to construct process synthesis capability based on a process simulator.

2. Process synthesis based on process simulators

Recently, process synthesis based on process simulators has attracted increasing attentions. According to the types of modular environment, the research can be divided into two fields: equation-oriented and sequential modular environment. Kravanja and Grossmann (1990) first implemented a modelling and decomposition strategy in equation-oriented simulator PROSYN (the successor is called MipSyn), and developed an automated topology and parameter process synthesizer. Kravanja (2010) reviewed the capabilities of MipSyn and the challenges in sustainable integrated process synthesis, and pointed out that the future research would

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be oriented towards the development of an even more advanced and robust synthesizer that can be applied in large-scale sustainable applications in different engineering domains.

The sequential modular simulators are more desirable modular integrated tools for process synthesis and optimization because of the more extensive applications in complex chemical processes. This paper aims at the process synthesis capability based on sequential modular simulators. Diwekar et al (1992) implemented a variant of the generalized Benders decomposition (GBD) and the outer approximation (OA) algorithm in the ASPEN simulator, and proposed a two-level method that consisted of NLP subproblem (with all 0-1 variables fixed) and an MILP master problem. Several examples were presented including the synthesis of the hydrodealkylation (HDA) process and integrated gasification combined cycle (IGCC) system. Reneaume et al. (1995) presented a three-level solution strategy including superstructure level, structure level and module level. In their work, the modular simulator ProSim had been chosen since gradient information was easily accessible. The similarity between Diwekar and Reneaume methods is that the topological binary variables (y) are represented using FSPLIT blocks by varying the flow fraction between 0 and 1. So their methods cannot be used to handle the situation with more than three alternatives. Gross and Roosen (1998) put forward an optimization method that integrated evolutionary algorithms with Aspen Plus, and presented the applications in synthesis of separation sequences and overall process synthesis with limited degrees of freedom. Although the optimization was time consuming, the easy formulation of the optimization task saved preparation time owing to the use of the reliable process simulator. Leboreiro and Acevedo (2004) provided an optimization framework for the synthesis and design of complex distillation sequences, in which a modified genetic algorithm (GA) were coupled with Aspen plus to obtain the combined capability of solutions with complex non-convex mathematical problems and the formulation of rigorous models. The method was applied to the synthesis and design of extractive distillation systems and the optimization of a superstructure involving several variations of heat-integrated columns. Caballero et al. (2005) presented a superstructure-based optimization method that combined the capabilities of commercial process simulator Hysys and generalized disjunctive programming (GDP). The operational conditions (reflux and reboil ratios, recoveries, etc.) and structural parameters (number of trays, location of feed and product streams, etc.) were simultaneously optimized for the rigorous design of distillation. The same method was also used to achieve the flowsheet optimization for the selection of different equipments which were given in a set of alternatives with complex cost and size functions (Caballero et al., 2007). All aforementioned researches aimed at single objective synthesis problem and had to circumvent the "implicit constraint problem" (black-box) in process synthesis based on process simulators. To meet the requirement of the sustainable system, multi-objective process synthesis has also drew a lot of attentions. Xu and Diwekar (2005) proposed the multi-objective process synthesis problem for the environmentally friendly solvent and the separation of in-process solvents, and the multi-objective optimization framework was composed of simulated annealing algorithm, process simulator Aspen plus and external FORTRAN routine. The better and more Pareto solutions than the conventional heuristic scheme were obtained for the CH_3COOH-H_2O azeotrope system. Yue et al. (2009) proposed a three-level strategy of multi-objective process synthesis based on modular simulator that integrated the process simulator Aspen Plus, multi-objective genetic algorithm (NSGA II) and hybrid coordination strategy.

The abovementioned process synthesis methods based on modular environment are appropriate for the specific simulation system and algorithm. Due to the complexity and diversity of chemical process, application fields will be subject to certain restrictions. So it is necessary to propose such a general modular integrated and optimization approach.

3. Modular integrated framework for process synthesis and optimization

A novel modular integrated framework is developed in this work to perform process synthesis and optimization based on a sequential process simulator. The modular integrated framework integrates process simulator (Aspen Plus in this paper), interface program, optimization algorithms to form a multi-platform environment integrated system including simulation, parameter and optimization sub-platforms (as shown in Figure 1). In the framework, the alternatives (feedstocks, processes and products) are simulated as an Aspen simulation superstructure model. The extraction and processing of necessary data (decision, constraint, objective variables, etc.) is then implemented by Excel with the interface (Aspen Simulation Workbook). Finally the MINLP problem of process synthesis is solved by multidisciplinary integration software (Isight). The rigorous models of chemical processes or units, regarded as "Black box", are solved by the process simulator, rather than shortcut or aggregated models in the form of equations. Therefore, not only is the process synthesis problem simplified but also does improve the accuracy of the solution.

(1) Simulation Platform

Aspen Plus and Hysys have been widely applied in industrial and academic process simulation and design for cogeneration plants, Petroleum refining, biomass gasification system, etc. The key equipments such as heat exchangers and distillation columns can be rigorously sized or rated within the simulation environment (Lam et al., 2010). Aspen Plus is chosen to illustrate the simulation platform in this study. Simulations and models can be developed by various researchers using different software packages such as Aspen Plus and Aspen Custom Modeler. The alternatives identified are used to construct a superstructure simulation model in the same file, or the superstructure approaches to process design can also be implemented in the optimization platform using the logical workflow blocks which allow for error checking and process configuration changes. In the former method, Fsplit and Mixer blocks in simulation platform are treated as logical nodes in MINLP process synthesis but not topological binary variables. The topological binary variables are defined in the following parameter platform so that more than three alternatives can be handled in our method. This is different from the work of Diwekar and Reneaume.

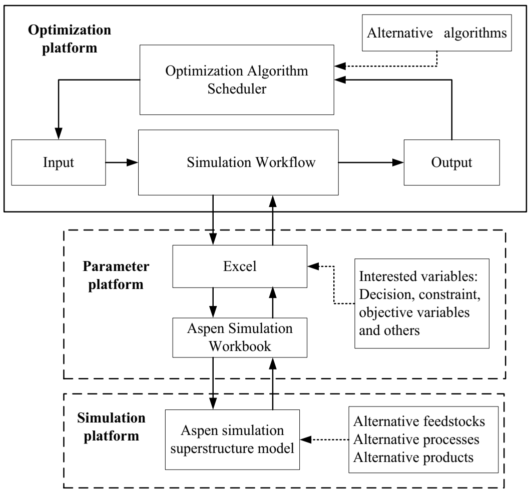

Figure 1: Modular integrated framework for process synthesis and optimization

(2) Parameter Platform

The key for the proposed modular integrated framework for process synthesis and optimization is the data exchange between modular simulation environment and optimization algorithms. The specified and calculated variables extracted from the simulation platform together with user-defined binary variables are transformed to the decision variables, constraint variables and objective variables in MINLP problem. Excel is used as the data processing platform in this study. There are several ways for data exchange between Excel and Aspen Plus. One of them is to use VBA (Visual Basic for Application) programming language. A standard simulation interface (sinter) is developed by the U.S. department of energy in conjunction with Excel and Aspen Plus. Another way is to use ASW tool for interfacing AspenTech's process simulation models with Excel worksheets. In terms of compatibility and applicability, it is a better way to exchange data between simulation platform and parameter platform. In accordance with the principle of generality, ASW is more appropriate for modular integrated optimization framework because programming is not required. The binary variables are defined in parameter platform, and slack variables (SK), multiple choice variables (MS) and conditional selection variables (CS) are also defined so that binary variables are associated with continuous variables. Taking flow as an example, the definition formulas Eqs.(1)-(3) are formulated as:

$$SK_i = F_i - F_{\max} y_i \tag{1}$$

$$MS = \sum y_i \tag{2}$$

$$CS = y_i - y_k \tag{3}$$

$$y_i \in \{0,1\}, i = 0,1,...,n$$

(3) Optimization Platform

The ranges of variables are specified in optimization platform. It is necessary to integrate various optimization algorithms in optimization platform for solving different process synthesis. The multidisciplinary design optimization software Isight is used as optimization platform. Isight has built-in Excel standard interface to transfer information between optimization platform and parameter platform, and it also provides a series of optimization algorithms for different situations. Single and multi-objective algorithms for discrete and continuous variables including genetic algorithms, simulated annealing and particle swarms as well as a number of simpler algorithms are all included in Isight. So the proposed modular integrated framework for process synthesis and optimization can be applied to single objective process synthesis as well as multi-objective process synthesis.

4. Case Study

4.1 Selection optimization of the boilers

The proposed modular integrated framework is applied to the selection of boiler operation. The steam utility system is composed of three boilers, each of which has featured efficiency, fuel cost and overhead cost. The objective is to determine the most economical use of each boiler for the given steam demand (14,400 t/h). This case includes the optimal configuration and operation condition of boilers and is typical MINLP problem.
A superstructure simulation model is built in Aspen Plus simulation platform (as show in Figure 2). The boilers are modelled as simple heaters, and STEAMNBS is chosen as property method. Specify a pressure drop of 0 kPa for each boiler. All necessary data for the case is given in Table 1.

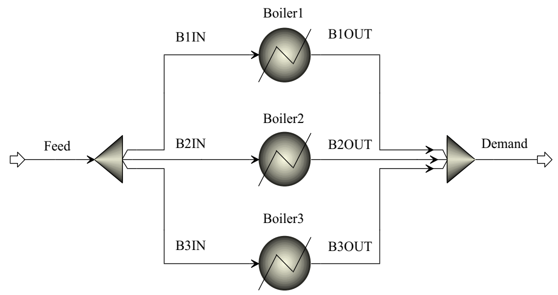

Figure 2: ASPEN PLUS superstructure representation for steam utility system

Table 1: Featured data for the boilers

	Boiler1	Boiler2	Boiler3
Eff_{Max} (%)	85 %	87 %	90 %
$Flow_{Max}$ (kg/s)	1.8	2.2	1.6
$Flow_{Max-5\%}$ (kg/s)	3.0	3.8	2.5
Fuel ($/MJ)	0.008	0.0085	0.0088
OverHead ($/h)	30	29	25
Inlet Temperature (°C)	21.3	21.3	21.3
Outlet Temperature (°C)	350	350	350
Pressure (kPa)	4,101.3	4,101.3	4,101.3

The efficiency and actual heat flow for each boiler are calculated within the parameter platform. The efficiency of the three boilers are characterized by the following relationship Eq.(4):

$$Eff = Eff_{Max} - 5\% \times \left(\frac{F - F_{Max}}{F_{Max-5\%} - F_{Max}} \right)^2 \tag{4}$$

where *Eff* is the efficiency of boiler, Eff_{MAX} is the maximum efficiency of boiler, *F* is the inlet mass flowrate of boiler, $Flow_{MAX}$ is the inlet mass flowrate of boiler at maximum efficiency and $Flow_{MAX-5\%}$ is the inlet mass flowrate at an efficiency 5 % less than the maximum efficiency.
Then, the actual heat duty is calculated from the following equation Eq.(5):

$$Q_{act} = Q \times \frac{100}{Eff} \tag{5}$$

where Q_{act} is the actual heat duty of boiler and *Q* is the heat duty of boiler calculated in Aspen Plus.
The operating cost for each boiler is the sum of fuel consumption cost and overhead cost associated with the operation status. When the boiler is operating, it incurs overhead cost. The total operating cost (*TOC*) is defined as the additive operating costs of each boiler Eq.(6):

$$TOC = \sum_{i \in B} (Q_{act} \times F_{cost} + OH \times y)_i \tag{6}$$

where B is a boiler, F_{cost} is the fuel cost and *OH* is the overhead cost.
The parameters extracted from Aspen simulation model include the inlet mass flowrate and heat duty of each boiler, while the slack variables and multiple choice variables have been defined in Eqs.(1) and (2).
The inlet mass flowrates of Boiler1 and Boiler2 (*F1* and *F2*) and binary variables *y* are chosen as decision variables, then the ranges of variables are specified in optimization platform. The mathematical formulation of the MINLP problem can be stated as Eq.(7):

$$
\begin{aligned}
&\text{Min } TOC \\
&\text{s.t. } 0 \le F_i \le 14400 \\
&\quad 0 \le Q_{act,1} \le 12500 \\
&\quad 0 \le Q_{act,2} \le 9500 \\
&\quad 0 \le Q_{act,3} \le 13500 \\
&\quad 1e^{-6} \le SK_i \le 0 \\
&\quad 1 \le MS_i \le 3 \\
&\quad y_i \in \{0,1\}
\end{aligned}
\tag{7}
$$

MISQP (Mixed Integer Sequential Quadratic Programming) algorithm is used to solve aforementioned process synthesis problem. The result shows that the minimum operating cost is $486,450 when Boiler1 is operating at 8,011.95 t/h and Boiler3 at 6,388.05 t/h.

4.2 Flowsheet optimization with cost and size functions

The proposed integrated framework can be also applied to the flowsheet optimization with discontinuous cost and size functions. The case adapted by Caballero consists of a small heat exchanger network, as shown in Figure 3. Although the topology optimization is not addressed in this case, the cost of each heat exchanger is given by a discontinuous cost function associated with the heat transfer area (*A*). It is still a typical MINLP problem. All necessary data for the case is given in Table 2.

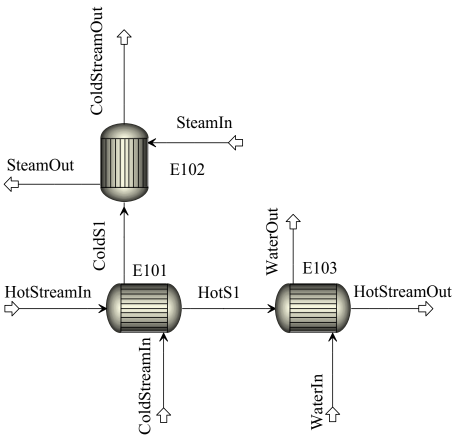

Table 2: Data for Case 2

Stream	Composition	Flow (kmol/h)	T_{in} (K)	T_{in} (K)	Cost $/kWy
Hot	DiPhenylC3	120	500	340	
Cold	Glycerol	100	350	560	
Cooling water	H_2O		323	363	20
Steam	H_2O		600	557	30
Heat exchanger	Overall heat transfer coefficient (W/m^2•K)				
E101		1,500			
E102		500			
E103		1,000			

Figure 3: Network structure for case 1

The objective function includes both the investment and utility costs. The mathematical formulation of the MINLP problem can be stated as (Eq.(8)):

$$
\begin{aligned}
&\text{Min: } TAC = \sum_{\mathrm{j \in HE}} IC_{\mathrm{j}} + Cost_{\mathrm{steam}} \times Q_{\mathrm{Steam}} + Cost_{\mathrm{water}} \times Q_{\mathrm{water}} \\
&\text{S. T.} \\
&\begin{bmatrix} IC = 2750A^{0.6} + 3000 \\ 0 < A \le 10 \end{bmatrix} \vee \begin{bmatrix} IC = 1500A^{0.6} + 15000 \\ 10 < A \le 25 \end{bmatrix} \vee \begin{bmatrix} IC = 600A^{0.6} + 46500 \\ 25 < A \le 50 \end{bmatrix} \\
&\Delta T = T_1 - T_2 \ge 10
\end{aligned}
\tag{8}
$$

where HE is short for heat exchanger, *IC* is the annualized investment cost of each heat exchanger and *Q* is the heat load supplied/removed by steam or water. T_1 and T_2 is the temperature of HotS1 and ColdS1 (in Figure 2).

There is only one degree of freedom in this case, and the heat exchange area of E101 (A_1) is selected as decision variable. The areas of E102 and E103 are calculated according to Eq.(9):

$$
A = \frac{Q}{\Delta T_{LMTD} U} \tag{9}
$$

All necessary parameters extracted from simulation platform include A_1, the log mean temperature difference (ΔT_{LMTD}) of E102 and E103, Q_{steam} and Q_{water}. The case is solved by using the adaptive simulated annealing algorithm (ASA). ASA algorithm greatly accelerates the search and improves the quality of the optimal solution through adjusting the temperature and the Increment. The discrete relationship between the annual total cost and decision variable can be observed in Figure 4. Table 3 shows a summary of the optimal results.

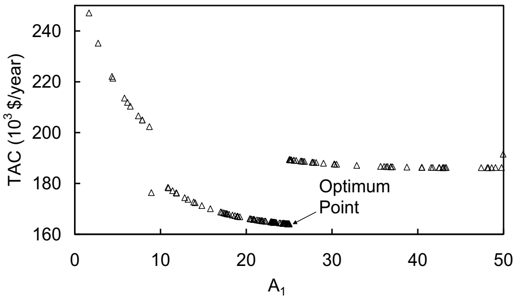

Figure 4: Impact of the heat exchange area A_1 on the annual total cost TAC

Table 3: Result for Case 2

	Area (m^2)	Investment Cost ($/y)
E101	25.0	2,5347
E102	21.5	2,4458
E103	27.9	50,923
	Power (kW)	Cost ($/y)
Heat utility	545.6	43,648
Cold utility	986.6	19,732
TAC		16,4107
	Temperature (K)	
T_1	423.4	
T_2	492.9	

5. Conclusion

In this paper, a novel modular integrated framework is proposed to perform process synthesis and optimization. In the modular framework, process simulator, interface program, and optimization algorithms are integrated to a multi-platform environment integrated system including simulation, parameter and optimization sub-platforms. The superstructure models of chemical processes or units are established in process simulator, rather than shortcut or aggregated models in form of equations. The process synthesis problems are simplified and the accuracy of the solution can also be improved. Future research will aim at a larger number of academic and industrial cases such as heat integrated complex distillation system synthesis.

References

Caballero, J.A., Milán-Yañez, D., Grossmann, I.E., 2005, Rigorous design of distillation columns: integration of disjunctive programming and process simulators. Industrial and Engineering Chemistry Research, 44, 6760-6775.

Caballero, J.A., Odjo, A., Grossmann, I.E., 2007, Flowsheet optimization with complex cost and size functions using process simulators. AIChE Journal, 53, 2351-2366.

Diwekar, U.M., Grossmann, I.E., Rubin, E.S., 1992b, An MINLP process synthesizer for a sequential modular simulator. Industrial and Engineering Chemistry Research, 31, 313-322.

Gross, B., Roosen, P., 1998, Total process optimization in chemical engineering with evolutionary algorithms. Computers and Chemical Engineering, 22, Supplement 1, S229-S236.

Kravanja, Z., 2010, Challenges in sustainable integrated process synthesis and the capabilities of an MINLP process synthesizer MipSyn. Computers and Chemical Engineering 34, 1831-1848.

Kravanja, Z., Grossmann, I.E., 1990, Prosyn — an MINLP process synthesizer. Computers & Chemical Engineering, 14, 1363-1378.

Lam, H.L., Klemeš, J.J., Friedler, F., Kravanja, Z., Varbanov, P.S., 2010, Software tools overview: Process integration, modelling and optimisation for energy saving and pollution reduction, Chemical Engineering Transactions, 21, 2010, 48 7-492 DOI: 10.3303/CET1021082

Leboreiro, J., Acevedo, J., 2004, Processes synthesis and design of distillation sequences using modular simulators: a genetic algorithm framework. Computers AND Chemical Engineering, 28, 1223-1236.

Reneaume, J.-M.F., Koehret, B.M., Joulia, X.L., 1995, Optimal process synthesis in a modular simulator environment: new formulation of the mixed-integer nonlinear programming problem, Industrial and Engineering Chemistry Research, 34, 4378-4394.

Xu, W., Diwekar, U.M., 2005, Environmentally Friendly Heterogeneous Azeotropic Distillation System Design: Integration of EBS Selection and IPS Recycling, Industrial & Engineering Chemistry Research, 44, 4061-4067.

Yue, J. C., Zhe, S. Q., Han, F. Y., 2009, Strategy of multi-objective process synthesis based on modular simulator, CIESC Joural, 1, 177-182.