

## **Retrofit Design of Chemical Processing Networks under Uncertainties: Application to Petrochemical Industry**

Min-ho Suh<sup>1</sup>, Ferenc Friedler<sup>2</sup>, Sunwon Park<sup>1</sup>, and Tai-yong Lee<sup>1\*</sup>

<sup>1</sup> Department of Chemical Engineering, Korea Advanced Institute of Science and Technology, 373-1 Kusong-dong, Yusong-gu, Taejon, 305-701, Korea

<sup>2</sup> Department of Computer Science, University of Veszprem, Veszprem, Egyetem u. 10, H-8200, Hungary

Multiscenario retrofit design of petrochemical processing networks is addressed in this paper. The combinatorial framework developed for process network synthesis can be used to resolve the computational complexity of the retrofit design. Retrofit design of Korean petrochemical industries under product demand uncertainty illustrates the efficacy of the proposed algorithm. We obtain Pareto optimal solutions of two objectives, namely expected cost and worst-case cost. The robust optimal solution of retrofit design under uncertainty can be determined among the Pareto optimal solutions.

### **1. INTRODUCTION**

Retrofit design means addition of new units and expansion of existing units to satisfy the economic needs and product demand requirements. In retrofit design of a chemical processing network, decisions on structural variables such as process network configuration and capacity expansions, have to be made under forecasted uncertain parameters, e.g., product demand and material cost data. Since these parameters usually highly affect the profitability of the system, uncertainties should be taken into account in the design. The most common way of representing the uncertainties is to specify scenarios of the expected values of the parameters. Based on the scenario-based approach, multiscenario mathematical model can be driven by the stochastic programming framework. In comparison with the deterministic model that doesn't consider the parameter uncertainty, the stochastic model forms a large-size problem due to the scenario-dependent variables and constraints. Need for an efficient solution algorithm is emphasized in design models considering uncertainties. Moreover, we need to solve the model repeatedly to obtain the Pareto optimal solutions which is an important procedure in decision making under uncertainties. Together with process network synthesis for new process design, the retrofit design of chemical processing network has common binary decision variables of unit existence. The combinatorial framework for process network synthesis was proposed by Friedler et al [1-4]. P-graph theory and combinatorial algorithms

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\* Corresponding author: tylee@mail.kaist.ac.kr

are rebuilt to adapt to the multiscenario retrofit design problem. Retrofit design of Korean petrochemical industries illustrates the efficacy of the proposed algorithm and robust design approach.

## 2. DESIGN UNDER UNCERTAINTIES

In representing the uncertain parameters, the scenario-based approach is one of the most commonly applied methods. Uncertain product demands are represented as the realizable scenarios and their probabilities in this paper. Absolute robustness concept [5] is applied to the robust optimization of retrofit design problem. The absolute robustness means the cost we accept when the worst-case scenario is realized. Consequently, the two objectives of the stochastic programming model are the expected cost and the worst-case cost. Computational aspects of multiscenario retrofit design model are addressed.

### 2.1 Mathematical model

In this multiscenario mathematical model, the expected cost is considered to be the objective function by constraining the required range of the worst-case cost. The objective is minimizing the expected cost.

$$\min EXCOST \quad (1)$$

The expected cost is calculated using  $p_s$ , the probability of scenario  $s$ .

$$s.t. EXCOST = \sum_s p_s C_s \quad (2)$$

Costs of all scenarios are constrained by the required worst-case cost,  $C^w$ .

$$C^w \geq C_s \quad \forall s \quad (3)$$

$C_s$  is the cost of scenario  $s$  and calculated as the sum of investment cost, operating cost, material cost, and transportation cost. Indices  $i, j, p$  represent processing unit, material, plant, respectively.

$$C_s = \sum_i \sum_p (\alpha_i Q E_{ip} + \beta_i Y_{ip}) + \sum_i \sum_p \delta_i W_{sip} - \sum_i \sum_p \left( \sum_{j \in J_{RP}} pr_j r a_{ij} \right) W_{sip} + \sum_{(j,p,p') \in t} tr_{jpp'} T_{sjpp'} \quad \forall s \quad (4)$$

$T_{sjpp'}$  is the transportation amount of material  $j$  from plant  $p$  to plant  $p'$  in scenario  $s$  when  $(j,$

$p, p')$  is the member of the transportation allowance set  $t(j, p, p')$ . Mass balances, operating

level limitations, and capacity limitations lead to the following constraints:

$$\sum_i r a_{ij} W_{sip} - \sum_{p':(j,p,p') \in t} T_{sjpp'} + \sum_{p'':(j,p'',p) \in t} T_{sjp''p} \geq MIN_{sjp} \quad \forall s, j \in J_p, p \quad (5)$$

$$\sum_i r a_{ij} W_{sip} - \sum_{p':(j,p,p') \in t} T_{sjpp'} + \sum_{p'':(j,p'',p) \in t} T_{sjp''p} \geq -MAX_{sjp} \quad \forall s, j \in J_R, p \quad (6)$$

$$\sum_i r a_{ij} W_{sip} - \sum_{p:(j,p,p') \in t} T_{sjpp'} + \sum_{p'':(j,p'',p) \in t} T_{sjp''p} \geq 0 \quad \forall s, j \notin J_{RP}, p \quad (7)$$

Equation (5) means that the amount of product  $j$ , to be produced at plant  $p$  in scenario  $s$ , should be at least  $MIN_{sjp}$ . Equation (6) means that the amount of raw material  $j$ , to be used at plant  $p$  in scenario  $s$ , should be at most  $MAX_{sjp}$ .  $r a_{ij}$  is the mass balance coefficient which is negative when the material  $j$  is input to the unit  $i$  and positive when the material  $j$  is output from the unit  $i$ . Equation (8) limits the operating level  $W_{sip}$  to the capacity of units  $Q_{ip}$ .

$$W_{sip} \leq Q_{ip} \quad \forall s, i, p \quad (8)$$

$Q_{ip}$  is the sum of original capacity  $QO_{ip}$  and expansion capacity  $QE_{ip}$ .

$$Q_{ip} = QO_{ip} + QE_{ip} \quad \forall i, p \quad (9)$$

$QE_{ip}$  has lower and upper bounds which linked to the binary variable.

$$QE_{ip}^{LO} Y_{ip} \leq QE_{ip} \leq QE_{ip}^{UP} Y_{ip} \quad \forall i, p \quad (10)$$

Equations (11) and (12) represent variable conditions.

$$Y_{ip} \in \{0,1\} \quad (11)$$

$$QE_{ip}, Q_{ip}, W_{sip}, T_{sjpp'} \geq 0 \quad (12)$$

## 2.2 Complexities in solving the multiscenario retrofit design model

This multiscenario model can be driven in the form of MILP with scenario-independent structural binary variables related to the process synthesis part of the design and scenario-dependent continuous variables related to the uncertainties. The large number of scenario-dependent variables and constraints makes the already complex process design problem more difficult to solve. A possible way of reducing the complexity of the problem is to exploit the combinatorial properties of feasible processing networks as done in the combinatorial framework developed for process network synthesis.

## 3. COMBINATORIAL ALGORITHM

The combinatorial framework of process network synthesis has been extended to the multiscenario retrofit design problem by adapting the combinatorial axiom system and altering the search direction on the P-graph from backward to forward direction. The basic algorithms, including the ABB (Accelerated Branch-and-Bound) algorithm have been extended to solve the multiscenario model by keeping its original efficacy.

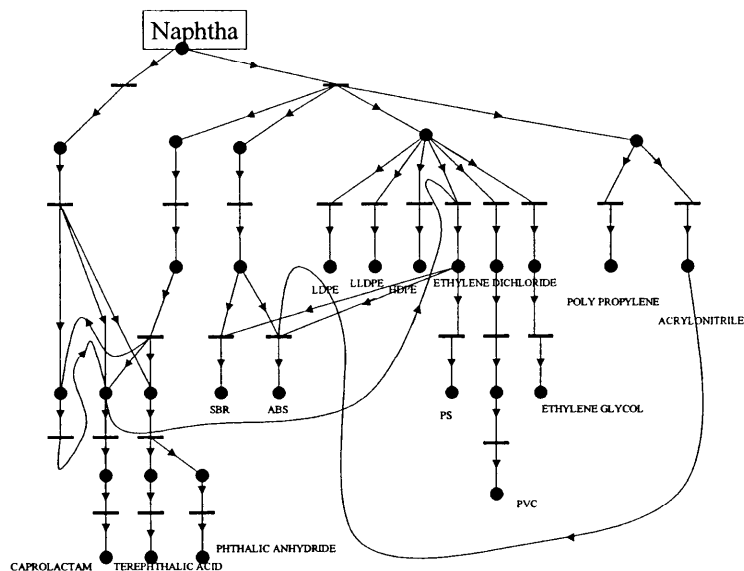


Figure 1. Maximal structure of one plant in the petrochemical processing networks.

### 3.1 Retrofit design feature

There is no difference between the retrofit design and the process network synthesis in representing the new units. Also there is no limitation on representing two or more units of which inputs and outputs are the same in P-graph representation of retrofit design. In the retrofit design, we represent extended capacities of existing units as capacities of additional units, which have the same inputs and outputs with their corresponding existing units.

### 3.2 Multiplant and transportation consideration

We represent the transportation routes of transportable materials as units with transportation cost. All the plants are regarded as a single processing network and the transportation of materials are represented by the above-mentioned method. The investment costs for units of transportation are nulls.

### 3.3 Forward direction search

It is assumed that all the products should be included in the solution networks when we carry out a process network synthesis using the P-graph theory. But in retrofit design of petrochemical processing networks, we determine the profitable products among the candidate products and some of them need not be included in the solution networks. The *potential* product concept is adopted to represent the situation of product selection in retrofit design. As shown in Figure 1, all the petrochemical products are produced from Naphtha, the main raw material. The product-oriented search algorithm of the original P-graph theory is changed to the raw- material-oriented search algorithm.

### 3.4 Computational aspect from the multiscenario point of view

The acceleration of ABB algorithm is attributable to: (i) the reduction of the initial relaxed problem to the set of combinatorially feasible structures; and (ii) the reduction in the sizes of the individual partial problems [4]. The second scheme is very effective when the ABB algorithm is applied to the multiscenario model because the reducing effect in the sizes of partial problems also is proportional to the number of scenarios.

## 4. RETROFIT DESIGN OF KOREAN PETROCHEMICAL INDUSTRIES

The new algorithm has been tested for Korean petrochemical industries under product demand uncertainty. In this retrofit design problem, various types of petrochemicals are produced from naphtha. The optimal solutions have been generated for the expected cost, the worst-case cost and the Pareto set of the two objectives.

### 4.1 Problem description

There are four petrochemical complexes which are located in Incheon, Ulsan, Yosu, and Daesan in Korea. Each plant has the same maximal structure as shown in Figure 1. Some intermediate materials can be transported from one plant to another with transportation costs. All the plants have their product demands and three demand scenarios are assumed by the forecast for petrochemical product demand of domestic, China and southeastern Asian market. Retrofit period is 10 years. Scenario 1 expects 20% annual growth rate of synthetic resin (HDPE, LDPE, LLDPE, PP, PS, etc.) market and 10% annual growth rate for the rest of the products in the market with probability of 0.3. Scenario 2 expects 15% annual growth of aromatic derivatives (PS, ABS, Caprolactam, TPA, and phthalic anhydride) and 8% annual growth rate for the rest of the products with probability of 0.3. Scenario 3 expects 10% annual growth of all the products with probability of 0.4. Basic petrochemical processing networks configuration, existing capacity and demand, and material price data are imported from Bok et al [6].

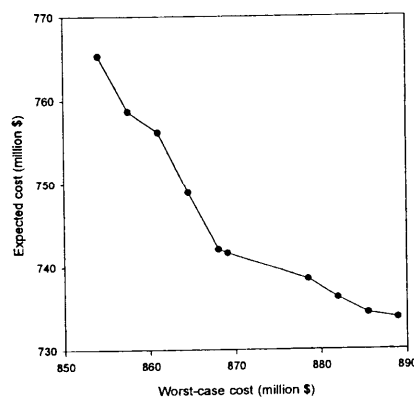
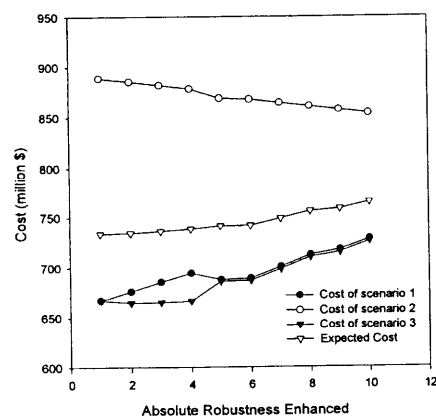


Figure 2. Behavior of robust optimal solutions. Figure 3. Pareto curve for decision making.

## 4.2 Results

The problem is solved using both the general MILP solver OSL implemented in GAMS 2.25 and the proposed algorithm implemented in C++. Computation times are 942 seconds and 133 seconds, respectively, in minimizing the expected cost without the constraint of worst-case cost requirement. The computation test was carried out on a Pentium-III, 550 MHz. Robust optimal solutions are obtained by constraining the required worst-case cost as shown in Figure 2. Instead of increasing like the costs of scenario 1 and 3, the worst-case cost of scenario 2 decreases as the absolute robustness is enhanced. Figure 3 shows the Pareto curve for the expected cost and the worst-case cost. Decision maker can determine the best design solution to be invested with his or her preference to the worst-case risk and expected cost over the uncertainty.

## 5. CONCLUSION

Combinatorial algorithm for multiscenario retrofit design of petrochemical processing networks was proposed. Retrofit design of Korean petrochemical industries was carried out using the proposed algorithm and robust optimal design method. This industrial scale problem illustrated the efficacy of the proposed method. Often the long-term design problem of chemical processing networks can be modeled as a multiperiod design model. Our future research will be focused on the extension of the algorithm to the multiperiod model with keeping the efficacy of the combinatorial framework.

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