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ROBUST INVESTMENT MODEL FOR LONG RANGE CAPACITY EXPANSION OF CHEMICAL PROCESSING NETWORKS USING TWO-STAGE ALGORITHM

°**JINKWANG BOK**[1], **HEEMAN LEE**[2], and **SUNWON PARK**[1]

[1]Department of Chemical Engineering, KAIST, Taejon 305-701, KOREA
swpark@convex.kaist.ac.kr Fax: 82-42-869-3910

[2]Samsung SDS CO., LTD., Seoul 135-080, KOREA

__Abstract__ - The problem of long range capacity expansion planning for chemical processing network under uncertain demand forecast scenarios is addressed. This optimization problem involves capacity expansion timing and sizing of each chemical processing unit to maximize the expected net present value considering the deviation of net present values and the excess capacity over a given time horizon. A multiperiod mixed integer nonlinear programming optimization model that is both solution and model robust for any realization of demand scenarios is developed using the two-stage stochastic programming algorithm. Two example problems are considered to illustrate the effectiveness of the model.

Keyward : Two-stage Algorithm, Long Term Planning, Robust Planning

1. Introduction

Policy making about capacity expansion timing and sizing of processing units is of importance since it requires substantial amount of investment cost with long payout time. Optimization modeling for the processing network capacity expansion problem has been studied by Sahinidis et al. (1989) in the form of multiperiod MILP model, but a serious shortcoming of their model is its deterministic nature. Real world situations are characterized by a high degree of uncertainty, and this exerts an important influence on the investment, production, and pricing decisions (Paraskevopoulos, 1991). Uncertainty involved in demand is generally focused because, in general, this parameter is the hardest to estimate accurately (Berman et al., 1994).

Solution robustness means that optimal solution from the model is almost optimal for any realization of the demand scenarios, while model robustness refers to the optimal solution which has almost no excess capacity and unmet demand. Markowitz (1975) proposed a robust optimization algorithm and Malcolm and Zenios (1994) developed a robust optimization model for the expansion of power capacity under uncertain load forecasts, and it generated capacity expansion plans that are both solution and model robust for power system.

The objective of this paper to build a robust multiperiod mixed integer nonlinear programming model which is solution and model robust under several uncertain product demand scenarios for the capacity expansion timing and sizing of chemical processing units. The proposed model features large size mixed nonlinear programming so that two stage programming algorithm is used to find better solution.

2. Theoretical Background

The basic idea of this model is the combined use of the robust scheduling algorithm and the two stage stochastic programming.

(a) Robust planning algorithm. The capacity expansion model in this study adopts the robust optimization modeling framework by Malcolm and Zenios (1994). First, two sets of variables are defined: design variables and control variables. Design variables depend only on the fixed and structural constraints which are independent of uncertain demand parameters. For the capacity expansion model of a processing network, individual process capacity at each time period belongs to design variables. Control variables could be adjusted once the uncertain parameters are observed, and their optimal values depend both on the realization of uncertain parameters, and on the value of the design variables. Variables denoting purchase/sales/production amount of each chemical at each time period are treated as these control variables. Next, a set of scenarios and the probability of each scenario are introduced. In this study only demand scenarios which represent the forecasted market demand changes during the given planning horizon are considered. The robust optimization model is then developed to maximize the expected net present value subtracted by the expected deviations from optimality and penalty term for model error which is the expected excess capacity in this problem. Constraints for the model consist of two types: scenario dependent and scenario independent constraints. For scenario dependent constraints the optimal solution set for one scenario may not satisfy the constraints of the other scenarios, and error terms as model infeasibility measure are defined. Following is the compact formulation of the robust optimization model for a capacity expansion problem.

Maximize $\Phi = E(\xi) - \lambda E((dev(\xi))^2) - \omega E(z_s^2)$ (1)

subject to: $Ax = b$:scenario independent constraints (2)

$B_s x + C_s y_s + z_s = 0 \ \forall s \in \delta$: (3)

scenario dependent constraints

where Φ: objective function of the robust optimization model

δ	:	set of scenarios
λ, ω	:	penalty parameters
ξ	:	net present value
$E(\xi)$	:	expected net present value
$dev(\xi)$	:	deviation of net present value
x	:	design variable set
y_s	:	control variable set for scenario s
z_s	:	infeasibility error for scenario s

Note that the proposed robust model features a quadrature which complicates the solution process while the classical stochastic programming without penalty terms can be modeled as linear form. To minimize the computation difficulties due to nonlinearity, the two-stage stochastic programming algorithm is used.

(b) Two stage stochastic programming. Ierapetritou et al. (1994) and Liu and Sahinidis (1996) developed a two-stage stochastic programming approach for process planning under uncertainty to minimize the computational difficulties. They decomposed the problem into the master problem and the sub problem, dealing with the capital investment decision and the operating plan, respectively. The decisions of design variables are made in the master problem whereas the control variables are considered in the sub problem. The sub problem generates the lower bound while the master problem generates the upper bound for the net present value (Liu and Sahinidis, 1996). Once the sub problem is solved with the expansion information from the initial expected-value problem, the results of the operation plan is transferred to the master problem as a parameter set. The results from the master problem is given to the next sub problem as expansion parameters. The iteration is continued until the gab of the two problems is less than tolerance.

3. Mathematical Formulation

Formulation of Robust Optimization Model

(a) Indices and sets:

i = 1, NP	Process
j = 1, NC	Chemicals
l = 1, NM	Market
s = 1, NS	Scenario
t = 1, NT	Time period

(b) Variables:

Y_{it} 0 - 1 variable to denote if the capacity of process i is expanded at time period t

Pur_{sjlt} Amount of product j purchased from market l at the beginning of time period t by scenario s

Q_{it} Total capacity of process i available in period t

QE_{it} Capacity expansion of process i to be installed in period t

$Sale_{sjlt}$ Amount of product j sold to market l at the beginning of time period t by scenario s

W_{sit} Operating level of process i at time period t by scenario s

WI_{sijt} Amount of chemical j consumed by process i at time period t by scenario s

WO_{sijt} Amount of chemical j produced by process i at time period t by scenario s

Zp_{sit} Excess capacity of process i at time period t by scenario s

ξ_s Net present value for scenario s

(c) Parameters:

a^u_{sjlt}	Upper bound for purchase of chemical j from market l at time period t under scenario s
d^u_{sjlt}	Upper bound for sales of chemical j from market l at time period t under scenario s
LB	lower bound for optimal net present value
$MAS(k)$	master problem in iteration k
NC	Number of chemicals in the network
NM	Number of markets
NP	Number of processes
NS	Number of demand scenarios
NT	Number of time periods considered
p_s	Probability of demand scenario s
Pur^k_{sjlt}	value of variable Pur_{sjlt} in the solution of the sub problem in the kth iteration of the decomposition algorithm
Q^k_{it}	value of variable Q_{it} in the solution of the sub problem in the kth iteration of the decomposition algorithm
QE^k_{it}	value of variable QE_{it} in the solution of the sub problem in the kth iteration of the decomposition algorithm
$Sale^k_{sjlt}$	value of variable $Sale_{sjlt}$ in the solution of the sub problem in the kth iteration of the decomposition algorithm
$SUB(k)$	sub problem in iteration k
QE^L_{it}	Lower bound for the capacity expansion of process i at time period t
QE^U_{it}	Upper bound for the capacity expansion of process i at time period t
W^k_{sit}	value of variable W_{sit} in the solution of the sub problem in the kth iteration of the decomposition algorithm
Y^k_{it}	value of variable Y_{it} in the solution of the sub problem in the kth iteration of the decomposition algorithm
α_{it}	Unit cost for the capacity expansion of process i at time period t
β_{it}	Fixed cost for the capacity expansion of process i at time period t
γ_{jlt}	Price of sales of chemical j in market l during time period t

Γ_{jlt}	Price of purchases of chemical j in market l during time period t
δ_{it}	Unit operating cost for process i
η_{ij}	Material balance coefficients for process i and input chemical j (zero if j is not an input to process i)
λ	Penalty term for expected deviation of net present values
μ_{ij}	Material balance coefficients for process i and output chemical j (zero if j is not an input to process i)
ρ^k_{sit}	Lagrange multiplier of constraint in the kth iteration of the decomposition algorithm
ω	Penalty term for the excess capacities by different scenarios

The MINLP model for the planning problem is as follows:

Maximize

A) Objective function
= Expected net present value - Expected square of deviation of net present value - Expected square of excess capacity

$$\Phi = \sum_{s=1}^{NS} p_s\xi_s - \lambda\sum_{s=1}^{NS} p_s\left(\xi_s - \sum_{s=1}^{NS} p_s\xi_s\right)^2 - \omega\sum_{s=1}^{NS}\sum_{t=1}^{NT}\sum_{i=1}^{NP} Zp^2_{sit} \quad (4)$$

subject to:

B) Deterministic objective function

Net present value = Profit by chemical sales - Cost of chemical purchase - Process unit operating cost - Capacity expansion cost

$$\xi_s = \sum_{j=1}^{NC}\sum_{l=1}^{NM}\sum_{t=1}^{NT}\sum_{s=1}^{NS}(\gamma_{jlt}Sale_{sjlt} - \Gamma_{jlt}Pur_{sjlt}) - \sum_{i=1}^{NP}\sum_{t=1}^{NT}\sum_{s=1}^{NS}\delta_{it}W_{sit} - \sum_{i=1}^{NP}\sum_{t=1}^{NT}(\alpha_{it}QE_{it} + \beta_{it}Y_{it}) \quad (5)$$

C) Production/Inventory capacity limitations

$$Q_{it} = Q_{i\,t-1} + QE_{it} \qquad i = 1,\ldots,NP \qquad t = 1,\ldots,NT \quad (6)$$

$$Y_{it}QE^L_{it} \le QE_{it} \le Y_{it}QE^U_{it} \qquad i = 1,\ldots,NP \qquad t = 1,\ldots,NT \quad (7)$$

D) Availability/Demand limitation of each chemical

$$Pur_{sjlt} \le a^U_{jlt} \qquad s = 1,\ldots,NS \qquad j = 1,\ldots,NC \qquad l = 1,\ldots,NM \qquad t = 1,\ldots,NT \quad (8)$$

$$Sale_{sjlt} \le d^u_{sjlt} \qquad s = 1,\ldots,NS \qquad j = 1,\ldots,NC \qquad l = 1,\ldots,NM \qquad t = 1,\ldots,NT \quad (9)$$

E) Material balance equations for each chemical in the process network

$$WI_{sijt} = \mu_{ij}W_{sit} \qquad s = 1,\ldots,NS \qquad i = 1,\ldots,NP \qquad j = 1,\ldots,NC \qquad t = 1,\ldots,NT \quad (10)$$

$$WO_{sijt} = \eta_{ij}W_{sit} \qquad s = 1,\ldots,NS \qquad i = 1,\ldots,NP \qquad j = 1,\ldots,NC \qquad t = 1,\ldots,NT \quad (11)$$

$$\sum_{l=1}^{NM} Sale_{sjlt} + \sum_{i=1}^{NP} WI_{sijt} - \sum_{l=1}^{NM} Pur_{sjlt} - \sum_{i=1}^{NP} WO_{sijt} = 0$$
$$s = 1,\ldots,NS \qquad j = 1,\ldots,NC \qquad t = 1,\ldots,NT \quad (12)$$

F) Production limitations

$$W_{sit} - Q_{it} + Zp_{sit} = 0 \qquad s = 1,\ldots,NS \qquad i = 1,\ldots,NP \qquad t = 1,\ldots,NT \quad (13)$$

G) Variable conditions

$$Y_{it} = 0 \text{ or } 1 \; i = 1,\ldots,NP \qquad t = 1,\ldots,NT \quad (14)$$

$$QE_{it}, Q_{it}, W_{sit}, Pur_{sjlt}, Sale_{sjlt}, Zp_{sit} \ge 0$$

Decomposition Algorithm

In this section, the decomposition algorithm developed by Liu and Sahinidis (1996) is applied to the robust planning model. At the first stage, decision for capacity expansion is made, (Y_{it}, Q_{it}, and QE_{it}), and at second stage operating planning is considered ($Sale_{sjlt}$, Pur_{sjlt}, and W_{sit}). At the kth iteration, the master problem and sub problem are as follows:

The sub problem SUB(k)

Maximize

objective function (4)

subject to

$$\xi_s = \sum_{j=1}^{NC}\sum_{l=1}^{NM}\sum_{t=1}^{NT}\left(\gamma_{jlt}Sale_{sjlt} - \Gamma_{jlt}Pur_{sjlt}\right) - \sum_{i=1}^{NP}\sum_{t=1}^{NT}(\alpha_{it}QE^k_{it} + \beta_{it}Y^k_{it})$$

$$W_{sit} - Q^k_{it} + Zp_{sit} = 0$$

$$Zp_{sit} \ge 0 \qquad (4)$$

constraints (8) - (12)

$$W_{sit}, Sale_{sjlt}, Pur_{sjlt} \ge 0$$

Q^k_{it}, QE^k_{it}, and Y^k_{it} are the optimal solution of the master problem in iteration k.

Chemical 1 time Chemical 2

The master problem MAS(k)

Maximize α

subject to

$$\alpha \le \sum_{s=1}^{NS} p_s\xi_s - \lambda\sum_{s=1}^{NS} p_s\left(\xi_s - \sum_{s=1}^{NS} p_s\xi_s\right)^2 - \omega\sum_{s=1}^{NS}\sum_{t=1}^{NT}\sum_{i=1}^{NP} Zp^2_{sit} + \sum_{s=1}^{NS}\sum_{i=1}^{NP}\sum_{t=1}^{NT}\rho^k_{sit}(W^k_{sit} - Q_{it})$$

$$\xi_s = \sum_{j=1}^{NC}\sum_{l=1}^{NM}\sum_{t=1}^{NT}\left(\gamma_{jlt}Sale^k_{sjlt} - \Gamma_{jlt}Pur^k_{sjlt}\right) - \sum_{i=1}^{NP}\sum_{t=1}^{NT}(\alpha_{it}QE_{it} + \beta_{it}Y_{it})$$

constraints (6), (7), and (14)

$$Q_{it}, QE_{it} \ge 0$$

ρ^k_{sit} are the Lagrange multipliers relevant to constraint (18) and $Sale^k_{sjlt}$, Pur^k_{sjlt} and W^k_{sit} are the optimal solutions of the sub problem in iteration k.

4. Test Examples

Example 1. Small size problem

The robust optimization formulation developed in section 2 is applied to the following small size problem.

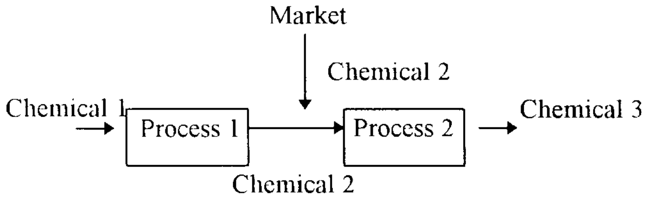
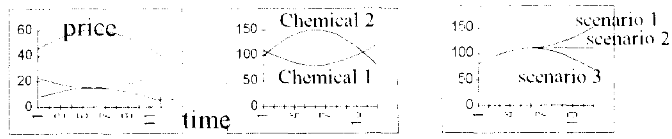


Figure 1. Chemical processing network for the test example.

Figure 1 describes the processing network for the test problem. Chemical 1 is used as a resource material for process 1. Process 1 produces chemical 2, and it is fed into process 2 to produce chemical 3. Chemical 2 can also be purchased from the market. Chemical 3 is then sold to satisfy the market demand.

Graphs in Figure 2 show the forecasted price data, availability, and demand trend of three chemicals for the next 12 time periods. It is assumed that all the price parameters have been already discounted at the specified interest rate and include the effect of taxes in the net present value. Demand of chemical 3 is uncertain, and three demand scenarios are considered. All three demand scenarios assume the same constant market growth until time period 6. According to demand scenario 1 the demand for chemical 3 is forecasted to be reduced, while scenario 2 forecasts it to be saturated and to be constant after time period 6. Demand scenario 3 assumes continuous growth of the market demand for chemical 3.



Price forecast Available chemicals Demand cenarios for chem. 3

Figure 2. Price and demand scenarios.

Table 2 shows the comparison of computational results between stochatic programming and the robust optimization technique. For various penalty sets, net present value assuming each scenario is realized, expected value and standard deviation of it, and expected excess capacity are calculated. Trade-off between solution robustness and model robustness is illustrated and gives the alternatives to the decision makers. The results of excess capacity show the proposed model is more model robust

Table 2. Computational Results

λ, ω	Realized Scenario 1	Realized Scenario 2	Realized Scenario 3	Expected Profit	Standard Deviation of Profit	Expected Excess Capacity
0.01, 0.1	30347	30461	30438	30420	65.82	205.8
0.1, 0.1	30367	30378	30376	30374	6.35	201.7
1.0, 0.1	30368	30370	30369	30369	1.15	201.3
1.0, 0.01	30755	30757	30757	30757	1.15	312.6
0.1, 1.0	28485	28506	28506	28499	12.12	68.4
Stochastic Programming	30759	32454	32112	31843	978.6	665.7

Table 3. Computational statistics

type	binary variables	continuous variables	constraints
Master problem	24	82	82
Sub problem	0	730	730

6. Conclusions

A robust optimization model for determining capacity expansion timing and sizing of chemical processing networks was presented by employing a robust optimization technique in the model. Compared with the non-robust profit maximization plan, the proposed model found more model robust and solution robust solution by incorporating penalty terms for the expected deviation of net present values and excess capacity in the objective function. The proposed model featured two-stage stochastic programming to reduce the computational difficulties. Finally, effectiveness of the model is illustrated through the test examples.

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