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Application of Post-Optimality Analysis in Process Engineering

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Abstract The main objective of optimizing any chemical process is to find the best operation conditions that can maximize the production of the most valuable products and minimize operating costs with respecting the operational and environmental constraints. Uncertainty or variations in some parameters such as demand and supply of each processing unit or product prices can seriously affect the optimization results and lead to inefficient operation. Many techniques of stochastic programming were proposed to handle the effect of variations in process parameters in order to determine a robust operation conditions; however, applications of post-optimality analysis has received less attention especially in process engineering. This work discusses the important of post-optimality analysis and shows how it can be used to investigate the effect of such variations on the optimal solution of a petrochemical complex that is formulated as a LP model. The general objective of this study is to try to bridge the gap between the theory and practice of the post-optimality analysis in process engineering. This work attempts to use a modified method of post-optimality analysis that jointly use sensitivity relations and stability region calculations to provide the decision maker in petrochemical complex with valuable and easy-to-use information that help in handling the effect of variation in some process parameters. The results of this study can help the decision maker to identify sensitive parameters that need accurate estimate or intensive monitoring.

1 Introduction

Optimization of production levels is an essential task to maximize company profit margins and to remain in the competitive market especially with high fluctuating in the prices of raw materials and products in addition to variations in the supply and demand. Many models of petrochemical processes and optimization techniques were proposed to handle this task [1]; however, it was recognized that optimization results can suffer from the existence of uncertainty in model parameters due to inaccurate estimates of some parameters. In addition, variations in input data, such as supply and cost of raw materials, can easily affect the process profitability. Many studies were conducted to understand the effect of such uncertainty or variation on the optimized model. There are two general approaches for dealing with the existence of uncertainty in optimization problem: incorporating the uncertainty directly into the optimization problem formulation, such as stochastic programming, and analysis of the effect of uncertainty on the optimal solution, post-optimality analysis.

Many techniques of stochastic and fuzzy programming were proposed to handle the effect of variation in process parameters in order to determine a robust operation conditions [2]. In the other hand, applications of post-optimality analysis have received less attention especially in refinery industry. Post-optimality analysis can help the decision maker to determine how much actual values of parameters may differ from the estimates used in the model before the optimal results become irrelevant. Generally, post-optimality analysis can provide the decision-maker with valuable information about sensitive parameters and constraints. Despite its value, applications of the post-optimality analysis (e.g., in production planning) have received less attention compared with stochastic programming. This may be due to the challenge of studying the effect of simultaneous variations in the model parameters. In addition, current state-of-art post-optimality analysis methods for different linear optimization problems (e.g., LP and MILP) are rarely used due to the high computational complexity.

In this project, we showed how the post-optimality analysis, mainly stability analysis, can be conducive to the decision maker in any process industry. A stability analysis technique, modified tolerance approach, is applied to the petrochemical complex in order to demonstrate the use of such analysis and to determine sensitive parameters that need accurate estimate or intensive monitoring. Moreover, the approach computes the stability limits (allowable variation ranges) of coefficients of objective function and right-hand-side of LP model to help the decision maker to maintain efficient plant operation.

2 Post-optimality analysis of LP model

After the optimal solution has been computed for a given model, it is important to know how the solution behaves under different variations in problem parameters. Sensitivity analysis and stability analysis are used to evaluate the effects of variations on the optimal solution or basis of the LP problem. Consider a LP problem in form:

$$Max\ \{\ P=\mathbf{c}^{\mathbf{T}}\mathbf{x} : \mathbf{Ax} \leq \mathbf{b},\quad \mathbf{x} \geq \mathbf{0},\quad \mathbf{x} \in \mathbf{R}^{\mathbf{n}} \} \tag{1}$$

Sensitivity analysis is usually associated with the determination of the values of the Lagrange multipliers, $\boldsymbol{\lambda}$, that describe the change in the optimal solution with respect to the variations in RHS coefficients. The sensitivity relations are important and useful for the decision maker, but the major challenge is to determine when they are valid. For example, the Lagrange multiplier, λ_i, presents the increase in the optimal value for a maximization problem when the associated RHS coefficient, i.e., b_i, is increased by one unit; however, we do not know by how much the coefficient can be increased under simultaneous variations in vector $\boldsymbol{b}$ before the optimal basis changes and the value of the Lagrange multiplier becomes invalid. This shows the importance of computing stability limits for each coefficient under simultaneous variations and within which the optimal basis remains unchanged.

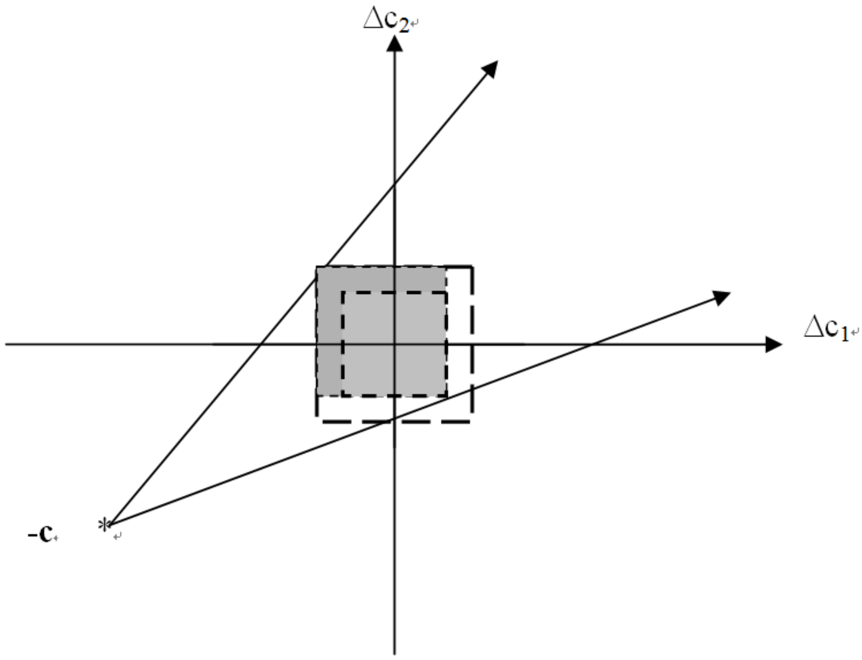

Figure 1: Obtained stability limits inside the stability cone.

During the last few decades, many stability approaches have been proposed, for variation in parameters of LP [3]. To date there is no single approach that dominates. In contrast to other approaches, the tolerance approach leads to easy-to-use results and considers simultaneous and independent variation in the problem parameters [3,4]. It basically depends on optimality conditions and uses the concept of basic and non-basic variables to modify matrix $\boldsymbol{A}$ at each iteration. In this study, the modified tolerance approach proposed by Al-Shammari [5] is used to determine the stability ranges. The proposed method provides a new perspective on the problem and has two steps for computing the stability region or limits. First, it defines the entire stability region as a cone and studies the relation between the sensitivity information, Lagrange multipliers, and model parameters. Second, it determines maximum stability limits presented by the maximum rectangular parallelepiped or hyperbox that can be built inside the cone. This hyperbox offers flexible and easy-to-use allowable variation limits as shown later on for variation in objective coefficients, i.e. prices or raw materials and products.

To demonstrate the approach, consider problem (1) that has a unique optimal solution. To define the entire stability region or stability cone for variations in the coefficients of the objective function, duality information or Lagrange multipliers are used:

$$\nabla_b \boldsymbol{P}^* = \boldsymbol{\lambda} = \boldsymbol{c}^T \boldsymbol{A}_A^{-1} \tag{2}$$

where $\boldsymbol{A_A}$ is the matrix of active constraints. By introducing the perturbations vector, $\Delta \boldsymbol{c}^T$:

$$\boldsymbol{\lambda}' = (\boldsymbol{c}^T + \Delta\boldsymbol{c}^T)\boldsymbol{A}_A^{-1} \tag{3}$$

by using the non-negativity condition on the optimal solution, there is no change in optimal solution if $\boldsymbol{\lambda}' \geq \mathbf{0}$. By substituting and rearranging:

$$-\Delta\boldsymbol{c}^T \boldsymbol{A}_A^{-1} \leq \boldsymbol{\lambda} \tag{4}$$

This inequality relation represents the stability region. This stability region can be defined as a stability cone because it satisfies the definition of a cone. In other words, the optimal solution and basis (not objective value) remain optimal under any scalar positive multiplication in the objective function. The solution remains optimal for any variations that satisfy equation (4). The stability cone is shown in Figure 1 for a maximization problem with two variables. Next step is defining the largest possible stability ranges starting with computing ordinary (individual) stability limits for Δc_i as follows:

$$\left(\max_{h} \quad \Delta\boldsymbol{c}_h = \frac{\lambda_g}{\boldsymbol{A}_{Agh}^{-1}} : \Delta\boldsymbol{c}_h < \mathbf{0}\right) < \Delta\boldsymbol{c}_h^{ord} < \left(\min_{h} \quad \Delta\boldsymbol{c}_h = \frac{\lambda_g}{\boldsymbol{A}_{Agh}^{-1}} : \Delta\boldsymbol{c}_h > \mathbf{0}\right) \tag{5}$$

where h and g are indices of objective coefficients and constraints, respectively. In Figure 2, the ordinary stability limits of the coefficient c_i are the intersections between the cone's constraints and Δc_i axis. The main challenge in LP stability analysis is the presentation of this cone to the decision maker in a simple and useful way, especially for simultaneous variations. The most useful approach is to construct the largest possible hyperbox inside the cone. Extension of stability analysis for simultaneous variations is discussed in details in Al-Shammari [5].

For variations in the RHS coefficients, a similar stability analysis is employed for the dual problem:

$$min \quad \{\boldsymbol{\lambda}^{\mathrm{T}}\boldsymbol{b} : \boldsymbol{\lambda}^{\mathrm{T}}\boldsymbol{A} \geq \boldsymbol{c}^T \;\&\; \boldsymbol{\lambda} \geq \boldsymbol{0}\} \tag{6}$$

to determine the variation limits before the optimal basis changes. In this analysis the optimal solution and slack variables are used in the same manner as the Lagrange multipliers were used in the variations analysis of vector $\boldsymbol{c}$.

3 Case study: Petrochemical complex consists of seven plants

The petrochemical complex that is used as a case study consists of seven plants: an ethylene plant, an ethylene dichloride (EDC) plant, a vinyl chloride monomer (VCM) plant, a polyvinil chloride (PVC) plant, and three different polyethylene plants (LDPE, HDPE, and LLDPE) as shown in the model representation of the site in Figure 2. The raw material for this complex is ethane which used to produce ethylene. Small quantities of some side-product hydrocarbons, such as propane, butane, and gasoline, are also produced from the ethylene plant. Produced ethylene can be delivered as a main raw material to four plants: LLDPE, LDPE, HDPE, and EDC, and/or exported based on demand and economics. The operation of the VCM plant depends on the production and price of EDC and its production can be exported or used to produce PVC. Detailed description of the plants and different technologies used in processing are presented in Meyers [6] and Rudd et al. [7]; and prices of raw materials and products are obtained from ICIS [8].

The optimization model of petrochemicals production is formulated as a LP problem:

$$\max \quad c^T x$$

$$s.t \quad \begin{aligned} & A_{ineq} x \le b_{ineq} \\ & A_{eq} x = b_{eq} \\ & x \ge 0 \end{aligned}$$

where $\boldsymbol{x} \in \boldsymbol{R}^n$ presents the production flow rate per day. The objective coefficients vector, $\boldsymbol{c}$, presents the price of products and/or raw materials, right hand side vector, $\boldsymbol{b}$, may presents the demand and supply, and matrix $\boldsymbol{A}$ usually describes plant specifications such as production yields.

The objective function of this problem is to maximize the net profit defined as the difference between sales revenue and total production costs for each product as follows:

Max net profit = (sales revenue - cost of raw materials - operating costs)

The problem constraints include inequality, equality and non-negativity constraints. The equality constraints mainly represent the mass balance around each plant and the inequality constraints represent the limitations of the process or the products, e.g., plant capacity and supply of raw materials.

4 Results and discussion

The petrochemical complex problem was solved using Matlab and the maximum profit was found to be 1,111,420 dollars per day without considering the costs of maintenance, storage, transporting and also fixed costs. Optimal solutions of key process variables and production levels are shown in Table 1. All productions of EDC and CVM are transported to the next plant to produce a more valuable product, PVC. Moreover, HDPE is not produced because is relatively non-profitable comparing with LLDPE and LDPE.

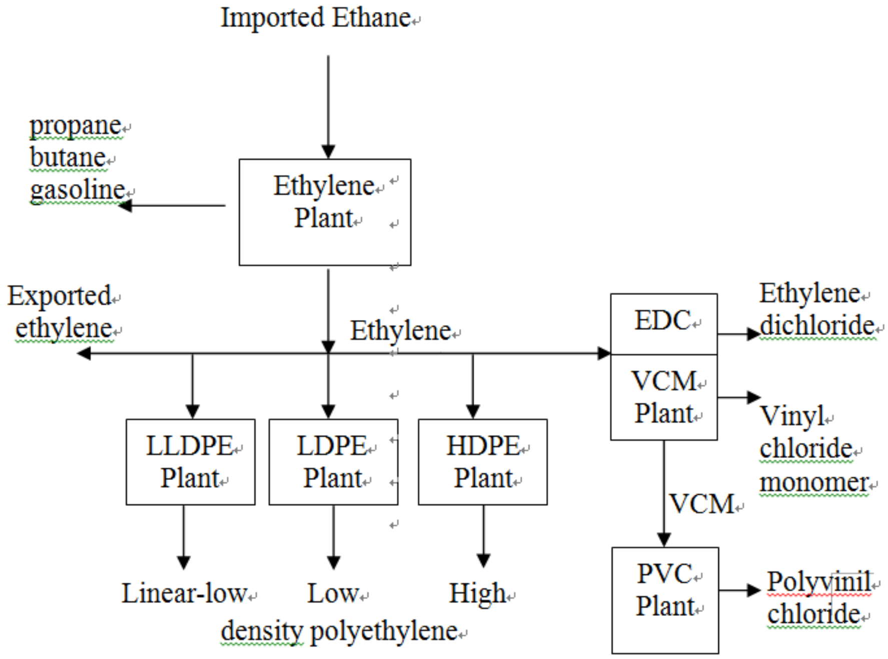

Figure 2: Model representation of petrochemical complex

Table 2 presents the results obtained from stability analysis of the objective coefficients. It shows the allowable range of price changes for raw material and each product within which obtained optimal production levels, shown in table 1, remain optimum. In other words, the optimal solution would change if the price of HDPE increased by more than 389.7 $/ton and the complex should start producing HDPE because it became relatively more valuable. Other useful information can be obtained from the data show in Table 2. Such information can help the decision maker to understand the interaction between production levels and other factors (e.g., prices); and determine when the process need to be re-optimized.

Obviously, some parameters have infinite limits in one direction of changes because they reached the maximum production limits, such as PVC, and any increase in their prices would not affect the solution. The optimal production levels are sensitive to simultaneous changes in prices of EDC, VCM, and PVC.

In contrast, individual stability limits for individual variations is greater than those for simultaneous variations since the obtained stability range for each parameter decreases with increasing the number of uncertain parameters. Presented limits of simultaneous variation were obtained using same weighting factor (k_i=1) for all parameters in Table 2; however, different weighting factors can be used based on the relative important or frequent change of each parameters. Analysis and results obtained for variations in ethane and ethylene prices and in RHS coefficients (e.g. supply and demand of materials and capacity constraints) will be discussed and presented in the extended paper.

5 Conclusion

This study presents the application of post-optimality analysis to a simplified process engineering problem formulated as LP problem, in order to investigate the effect of uncertainty or variation in model parameters, mainly objective coefficients on the optimal production levels. Modified tolerance approach was used to compute the allowable variation limits, for individual and simultaneous variations, within which the operation levels remain optimum. The main objective of the obtained results is to supply the decision maker in the plant with useful and easy-to-use information that can help to understand the interaction between production levels and other factors (e.g., prices) and to enable effective use of sensitivity information such as Lagrange multipliers.

Table 1: Optimal production levels of main variables.

Selected variables	Molar flow rate *Kmol/day*	Selected variables	Production rate *ton/day*
Ethane imported	43100	EDC exported	0
Ethylene produced	50,000	EDC to VCM	250.0
Ethylene exported	10,000	VCM exported	0
Ethylene to LLDPE	19090	VCN to PVC	240.0
Ethylene to HDPE	0	PVC exported	230.0
Ethylene to LDPE	18320	LLDPE	520.0
Ethylene to EDC	2590	HDPE	0
		LHPD	500

Table 2: Stability limits of individual and simultaneous price variations of some variables.

Selected variables	c_i $/ton	Individual stability limits, $/ton		Simultaneous stability limits, $/ton	
		lower	upper	lower	upper
LLDPE	1530.0	-379.8	65.6	-195.8	52.8
HDPE	1124.0	-1124.0	389.7	-1124.0	195.8
LDPE	1630.0	-105.4	Inf	-52.8	Inf
EDC	470.0	-470.0	43.1	-470.0	22.4
VCM	573.0	-573.0	92.0	-573.0	22.4
PVC	1720.0	-94.8	Inf	-22.4	Inf

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