Robust MINLP Optimization Model for Petrochemical Network Design under Uncertainty
Proceedings of European Congress of Chemical Engineering (ECCE-6)
Copenhagen, 16-20 September 2007

Robust MINLP Optimization Model for Petrochemical Network Design under Uncertainty

A) Al-Qahtani, K.[a] B) Elkamel, A.[a*] C) Ponnambalam, K.[b]

[a]*Department of Chemical Engineering, University of Waterloo, N2L 3G1 Waterloo, Canada*
[b]*Department of Systems Design Engineering, University of Waterloo, N2L 3G1 Waterloo, Canada*

Abstract

This paper addresses the strategic planning, design and optimization of a network of petrochemical processes under uncertainty and risk considerations. The problem was formulated as a two-stage stochastic mixed-integer nonlinear programming model (MINLP) with parameter uncertainty considered in process yield, raw material and product prices, and upper and lower product market demand. Risk was accounted for in terms of deviation in both projected benefits in the first stage variables and process yield and forecasted demand in terms of the recourse variables. For each term, a different scaling factor was used to analyze the sensitivity of the petrochemical network due to variations of each component. The study showed that the final petrochemical network bears more sensitivity to variations in product demand for scaling parameters values that maintain the final petrochemical structure obtained form the stochastic model. The concept of Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) are also investigated to numerically illustrate the value of including the randomness of the different model parameters. Modeling uncertainty in the process parameters provided a more robust analysis and practical perspective of this type of problems in the chemical industry.

Keywords: Petrochemical planning, planning under uncertainty, robust optimization

1. Introduction

The Petrochemical industry is a network of highly integrated production processes where products of one plant may have an end use or may also represent raw materials for other processes. This flexibility in petrochemical products production and the availability of many process technologies offer the sense of switching between production methods and raw materials utilization. The world economic growth and increasing populations will keep global demand for transportation fuels and

* To whom correspondence should be addressed. Tel.: (519)-888-4567 ext. 37157. E-mail address: aelkamel@uwaterloo.ca.

petrochemical products growing rapidly for the foreseeable future. One half of the petroleum consumption over the period of 2003 to 2030 will be in the transportation sector, whereas the industrial sector accounts for a 39-percent of the projected increase in world oil consumption, mostly for chemical and petrochemical processes (International Energy Outlook, 2006). Meeting this demand will require large investments and proper strategic planning for the petrochemical industry.

The petrochemical industry is based on the conversion of petroleum and natural gas to chemicals. Petroleum feedstock, natural gas, and tar represent the main production chain drivers for the petrochemical industry (Bell, 1990). From these, many important petrochemical intermediates are produced including ethylene, propylene, butylenes, butadiene, benzene, toluene, and xylene. These essential intermediates are then converted into many other intermediates and final petrochemical products constructing a complex petrochemical network. This multiplicity gives rise to a highly interactive and complex structure as it involves hundreds of chemicals and processes. With such nature, the petrochemical industry requires high level planning and consideration of the different structural alternatives when considering future developments.

Considering this type of high level strategic planning models, especially with the current volatile market environment and the continuous change in customer requirements, the impact of uncertainties is inevitable. In production planning, sources of system uncertainties can be categorized as short-term or long-term depending on the extent of time horizon (Subrahmanyam et al., 1994). The short-term uncertainties mainly refer to operational variations, equipment failure, etc. Whereas, long-term uncertainty may include supply and demand rate variability and price fluctuations, on a longer time horizon (Shah, 1998). Technological uncertainty in the left-hand-side coefficients which can be viewed in the context of production planning as the variation in process yields is another important uncertainty factor.

The realization of the petrochemical planning needs along with its important impact has inspired a great deal of research in order to devise different modeling frameworks and algorithms. These include optimization models with continuous and mixed-integer programming under both deterministic and uncertainty considerations.

The seminal work of Stadtherr and Rudd (1976, 1978) defined the petrochemical industry as a network of chemical process systems with linear chemical transformations and material interactions. They showed that the model provided a good representation of the petrochemical industry and can be used as a tool for estimating the relative effectiveness of available and new technologies and their impact of the overall industry. Their objective was to minimize feedstock consumptions. A similar LP modeling approach was adapted by and Sokic and Stevancevic (1983). Sophos et al. (1980) presented a model that minimizes feedstock consumption and entropy creation (lost work). Fathi-Afshar devised a multiobjective model of minimizing cost and gross toxicity emissions. Modeling the petrochemical industry using linear programming may have showed its ability to provide relatively reliable results through different technology structures. However, the need for approximating non-linear objective functions or the restriction of process technology combination alternatives mandated different modeling techniques involving mixed-integer programming.

One of the first mixed-integer programming models that tackled this problem was proposed by Jimenez et al. (1982) and Jimenez and Rudd (1987) for the development of the Mexican petrochemical industry. The proposed models were used to plan the installation of new plants with profitable levels as opposed to importing chemical products. However, there were no capacity limitations constraints on the processes. Al-Amer et al. (1998) developed an MILP model for the development of Saudi Arabia's petrochemical industry maximizing profit. The model included minimum economic production quantity for the different processes and accounted for domestic consumption and global market exports. This model was further extended by Alfares and Al-Amer (2002) to included four main product categories: propylene, ethylene, synthesis gas and aromatics and their derivatives. They devised a non-linear objective function of production investment cost at different production levels and derived a linear representation of the function through piece-wise linear approximation. Al-Sharrah et al. (2001, 2002) presented MILP models that took sustainability and strategic technology selection into consideration. The models included a constraint to limit the selection of one technology to produce a chemical achieving a long term financial stability and an environmental consideration through a suitability objective. Sustainability was quantified by a health index of the chemicals and increasing profit was represented by the different processes added values. This work was later extended by Al-Sharrah et al. (2003) with the aim of identifying long-range and short-range disturbances that affect planning of the petrochemical industry. Al-Sharrah et al. (2006) further developed their petrochemical planning framework into a multiobjective model accounting for economic gain and risk from plant accidents. The above body of research did not account for parameter uncertainties.

Another stream of research that tackled modeling under uncertainty included the work by Ierapetritou and Pistikopoulos (1994) who proposed an algorithm for a two-stage stochastic linear planning model. The algorithm is based on design flexibility by finding feasible subspace of the probability region instead of enumerating all possible uncertainty realizations. They developed a Benders decomposition scheme for solving the problem without a priori discretization of the random space parameters. This was achieved by means of Gaussian quadrature numerical integration of the continuous density function. In a similar production planning problem, Clay and Grossmann (1996) developed a successive disaggregation algorithm for the solution of two-stage stochastic linear models with discrete uncertainty. Liu and Sahinidis (1995; 1996; 1997) studied design uncertainty in process expansion through sensitivity analysis, stochastic programming and fuzzy programming, respectively. In their stochastic model, they used Monte Carlo sampling to calculate the expected objective function values. Their comparison over the different methodologies was in favor of stochastic models when random parameters distributions are not available. Ahmed et al. (2000) proposed a modification to the decomposition algorithm of Ierapetritou and Pistikopoulos (1994). They avoided solving feasibility subproblems and instead of imposing constraints on the random space, they developed feasibility cuts on the master problem. The modification avoids suboptimal solution and a more accurate comparison cost and flexibility. Nerio and Pinto (2005) developed a multiperiod MINLP model for production planning of refinery operations under uncertain petroleum and product prices and demand. The model was solved for 19 periods and five scenarios.

The representation through risk management using variance as a risk measure was proposed by Mulvey et al. (1995) in which they referred to this approach as robust stochastic programming. They defined two types of robustness: solution robustness referring to the optimal model solution when it remains close to optimal for any scenario realization, and model robustness representing an optimal solution when it is almost feasible for any scenario realization. More recently, Ahmed and Sahinidis (1998) proposed the use of upper partial mean (UPM) as an alternative measure of variability with the aim to eliminate nonlinearities introduced by using variance. In addition to avoiding nonlinearity of the problem, UPM presents an asymmetric measure of risk, as apposed to variance, by penalizing unfavorable risk cases. Bok et al. (1998) proposed a multiperiod robust optimization model for chemical process networks with demand uncertainty and applied it to the petrochemical industry in South Korea. They adopted the robust optimization framework by Mulvey et al. (1995) where they defined solution robustness as the model solution when it remains close to optimal for any demand realization, and model robustness when it has almost no excess capacity and unmet demand. Barbaro and Bagajewicz (2004) proposed a new risk metric to manage financial risk. They defined risk as the probability of not meeting a certain target profit, in the case of maximization, or cost, in the case of minimization. Additional binary variables are then defined for each scenario where each variable assumes a value of 1 in the case of not meeting the required target level; either profit or cost, and zero otherwise. Accordingly, appropriate penalty levels are assigned in the objective function. This approach mitigates the shortcomings of the symmetric penalization in the case of using variance, but on the other hand, adds computational burden through additional binary variables.

The above discussion points out the importance of petrochemical network planning, modeling uncertainty and considering risk in process system engineering studies. In this paper we study and compare the strategic planning, design and optimization of a network of petrochemical processes under deterministic conditions, uncertainty and uncertainty with risk consideration. The problem is formulated as a two-stage stochastic mixed-integer nonlinear model (MINLP) with nonlinearity arising from modeling the risk components. Both endogenous uncertainty, represented by uncertainty in the process yield and exogenous uncertainty, represented by uncertainty in raw material and product prices, and upper and lower product market demand were considered. The considerations of uncertainty in these parameters provided a more robust and practical analysis of the problem especially at a time when fluctuations in petroleum and petrochemical products prices and demands are souring.

The remainder of the paper is organized as follows. In the following section we will explain the proposed model formulation for the petrochemical network planning under deterministic conditions, under uncertainty and with uncertainty and risk consideration. Then we will briefly explain the concept of value of information and stochastic solution, in section 3. In section 4, we will illustrate the performance of the model through an industrial case study. The paper ends with concluding remarks in section 5.

2. Model Formulation

2.1 Deterministic Model

The optimization of petrochemical network design involves a broad range of aspects varying from economical and environmental analysis, strategic selection of processes and production capacities. The general deterministic model framework presented in this paper follows closely that of Al-Sharrah et al. (2001, 2006). A set of N number of chemicals involved in the operation of M processes is assumed to be given. Let X_j be the annual level of production of process $j \in M$, F_i the amount of chemical $i \in N$ as a feedstock, and a_{ij} the input-output coefficient matrix of material i in process j, and D_i^L and D_i^U represent the lower and upper level of demand for product $i \in N$, respectively. Then, the material balance that governs the operation of the petrochemical network can be expressed as shown in constraints (1) and (2):

$$F_i + \sum_{j=1}^{M} a_{ij} X_j \geq D_i^L \qquad i = 1, 2, \ldots, N \tag{1}$$

$$F_i + \sum_{j=1}^{M} a_{ij} X_j \leq D_i^U \qquad i = 1, 2, \ldots, N \tag{2}$$

For a given subset of chemicals where $i \in N$, these constraints control the production of different processes based on final products upper and lower demands of the petrochemical market. In constraint (3), defining the binary variables Y_j for each process $j \in M$ is required for the process selection requirement as Y_j will equal 1 only if process j is selected or zero otherwise. Furthermore, if only process j is selected, its production level must be at least equal to the process minimum economic capacity B_j. This can be written for each process j as follows:

$$B_j Y_j \leq X_j \leq K Y_j \qquad j = 1, 2, \ldots, M \tag{3}$$

where K is a valid upper bound. In the case where it is preferred or to choose only one process technology to produce a single chemical, constraints (4) and (5) can be included for each intermediate and product chemical type, respectively:

$$\sum_{i \in I_1} Y_j \leq 1 \qquad j \in J \text{ where } I_1 \text{ is a subset of intermediate chemicals} \tag{4}$$

$$\sum_{i \in I_2} Y_j \leq 1 \qquad j \in J \text{ where } I_2 \text{ is a subset of final product chemicals} \tag{5}$$

Finally, we can specify limitations on the supply of feedstock S_i for each chemical type *i* though constraint (6) as follow:

$$F_i \leq S_i \qquad i \in I_3 \text{ where } I_3 \text{ is a subset of chemicals with feed limitations} \tag{6}$$

The economical objective in the model can either be represented as operating cost minimization or added-value maximization. In the case of added-value maximization, products prices are subtracted from the cost of feedstocks for each process. If Pr_i is the price of chemical *i*, the added-value objective function can be represented as:

$$Maximize_{x_j} \quad \sum_{i=1}^{N} \sum_{j=1}^{M} a_{ij} Pr_i X_j \tag{7}$$

2.2 Two-Stage Stochastic Model

In the previous section, all parameters of the model were assumed to be known with certainty. However, the current situation of fluctuating high petroleum crude oil and petrochemical product prices and demands is an indication of the high market and industry volatility. Acknowledging the shortcomings of deterministic models, parameter uncertainty is considered in the process yield a_{ij}, raw material and product prices Pr_i, and upper and lower product demand D_i^L and D_i^U, respectively. The problem is formulated as a two-stage stochastic programming model. The uncertainty is considered through discrete distribution of the random parameters with a finite number S of possible outcomes (scenarios) $\xi_k = (a_{ijk}, Pr_{ik}, D_{ik}^L, D_{ik}^U)$ corresponding to a probability p_k. The formulation of the stochastic model is as follows:

$$Max_{x_j, y_{ik}^+, y_{ik}^-} \quad \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{S} a_{ijk}\, Pr_{ik}\, X_j - \sum_{i=1}^{N} \sum_{k=1}^{S} p_k\, q_i^+\, y_{ik}^+ - \sum_{i=1}^{N} \sum_{k=1}^{S} p_k\, q_i^-\, y_{ik}^- \tag{8}$$

Subject to

$$F_i + \sum_{j=1}^{M} a_{ijk} X_j + y_{ik}^+ - y_{ik}^- = D_{ik}^L \qquad i = 1,2,\ldots,I \quad k = 1,2,\ldots,S \tag{9}$$

$$F_i + \sum_{j=1}^{M} a_{ijk} X_j + y_{ik}^{+} - y_{ik}^{-} = D_{ik}^{U} \qquad \begin{array}{l} i = 1,2,...,I \\ k = 1,2,...,S \end{array} \tag{10}$$

$$B_j Y_j \le X_j \le K Y_j \qquad j = 1,2,...,M \tag{11}$$

$$\sum_{i \in I_1} Y_j \le 1 \qquad j \in J \text{ where } I_1 \text{ is a subset of intermediate chemicals} \tag{12}$$

$$\sum_{i \in I_2} Y_j \le 1 \qquad j \in J \text{ where } I_2 \text{ is a subset of final product chemicals} \tag{13}$$

$$F_i \le S_i \qquad i \in I_3 \text{ where } I_3 \text{ is a subset of chemicals with feed limitations} \tag{14}$$

The above formulation is a two-stage mixed-integer linear programming (MILP) model. The recourse variables y_{ik}^{+} and y_{ik}^{-} represent the shortfall and surplus for each random realization $k \in S$, respectively. These will compensate for the violations in constraints (9) and (10) and will be penalized in the objective function using the appropriate shortfall and surplus costs q_i^{+} and q_i^{-}, respectively. Uncertain parameters are assumed to follow a normal distribution for each outcome of the random realization ξ_k. The scenarios for all random parameters are generated simultaneously. In this way, the recourse variables will compensate for the violations in the constraints for a specific scenario and not for a particular random parameter. The recourse variables y_{ik}^{+} and y_{ik}^{-} in this formulation will compensate for deviations from the mean of both lower and upper market demands D_i^L and D_i^U, respectively and process yield a_{ij}.

2.3 Two-Stage Stochastic Model with Risk Consideration

The stochastic model with recourse in the previous section takes a decision merely based on first-stage and expected second-stage costs leading to an assumption that the decision-maker is risk-neutral (Sahinidis, 2004). In order to capture the concept of risk in stochastic programming, Mulvey et al. (1995) proposed the following amendment to the objective function:

$$Min_{x,y} \;\; c^T x + \mathrm{E}[Q(x, \xi(\omega))] + \lambda f(\omega, y)$$

where $\mathrm{E}[Q(x, \xi(\omega))]$ is the fixed recourse, f is a measure of variability (i.e. second moment) of the second-stage costs, and λ is a non-negative scalar representing risk tolerance. The representation through risk management using variance as a risk measure is often referred to as robust stochastic programming (Mulvey et al., 1995). This is also a typical risk measure following the Markowitz mean–variance (MV) model (Markowitz, 1952). The robustness is incorporated through the consideration of higher moments (variance) of the random parameter distribution ξ_k in the objective function and hence measuring the tradeoffs between mean value and variability.

In this study, operational risk was accounted for in terms of variance in both projected benefits, represented by first stage variables, and forecasted demand, represented by the recourse variables. The variability in the projected benefit represents the solution robustness where the model solution will remain close to optimal for all scenarios. On the other hand, variability of the recourse term represents the model robustness where the model solution will almost be feasible for all scenarios. This approach gives rise to a multiobjective analysis in which scaling factors are used to evaluate the sensitivity due to variations in each term. The projected benefits variation was scaled by θ_1 and deviation from forecasted demand was scaled by θ_2 where different values of θ_1 and θ_2 were used in order to observe the sensitivity of each term on the final petrochemical complex. The objective function with risk consideration can be written as follows:

$$\begin{aligned} Max_{x_j, y_{ik}^+, y_{ik}^-} \quad & \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{S} a_{ijk}\, Pr_{ik}\, X_j - \sum_{i=1}^{N}\sum_{k=1}^{S} p_k\, q_i^+\, y_{ik}^+ - \sum_{i=1}^{N}\sum_{k=1}^{S} p_k\, q_i^-\, y_{ik}^- \\ & - \theta_1 \sqrt{V(\text{Profit uncertainty})} - \theta_2 \sqrt{V(\text{Recourse uncertainty})} \end{aligned} \quad (15)$$

Since the randomness in the profit uncertainty term is a multiplication of two random parameters, process yield a_{ijk} and chemical prices Pr_{ik}, its variance can be written based on the variance of a product of two variables x and y (Johnson and Tetley, 1955), i.e.:

$$V_{xy} = V_x V_y + V_x \mu_y + V_y \mu_x$$

Where $V(x)$ and $\mu(x)$ represent the variance and mean value of a random number x; respectively. Hence, the objective function can be expressed as:

$$\begin{aligned} Max_{x_j, y_{ik}^+, y_{ik}^-} \quad & \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{S} a_{ijk}\, Pr_{ik}\, X_j - \sum_{i=1}^{N}\sum_{k=1}^{S} p_k\, q_i^+\, y_{ik}^+ - \sum_{i=1}^{N}\sum_{k=1}^{S} p_k\, q_i^-\, y_{ik}^- \\ & - \theta_1 \sqrt{\begin{aligned} & \sum_{i=1}^{N}\sum_{j=1}^{M} X_j^2 V(a_{ijk}) V(Pr_{ik}) + \sum_{i=1}^{N}\sum_{j=1}^{M} X_j^2 V(a_{ijk})\, \mu(Pr_{ik}) \\ & + \sum_{i=1}^{N}\sum_{j=1}^{M} X_j^2\, \mu(a_{ijk})\, \text{var}(Pr_{ik}) \end{aligned}} \\ & - \theta_2 \sqrt{\sum_{i=1}^{N} \left[q_i^+\right]^2 V(y_{ik}^+) + \sum_{i=1}^{N} \left[q_i^-\right]^2 V(y_{ik}^-)} \end{aligned} \quad (16)$$

By expanding the mean and variance terms of a_{ijk} , Pr_{ik} , y_{ik}^{+} y_{ik}^{-} , the objective function can be recast as:

$$
\begin{aligned}
Max_{x_j, y_{ik}^{+}, y_{ik}^{-}} \quad & \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{S} a_{ijk}\, Pr_{ik}\, X_j - \sum_{i=1}^{N}\sum_{k=1}^{S} p_k\, q_i^{+}\, y_{ik}^{+} - \sum_{i=1}^{N}\sum_{k=1}^{S} p_k\, q_i^{-}\, y_{ik}^{-} \\
& - \theta_1 \sqrt{\begin{aligned} & \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{S} X_j^2\, p_k \left[a_{ijk} - \sum_{k=1}^{S} p_k\, a_{ijk}\right]^2 \left[Pr_{ik} - \sum_{k=1}^{S} p_k\, Pr_{ik}\right]^2 \\ & + \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{S} X_j^2\, p_k \left[a_{ijk} - \sum_{k=1}^{S} p_k\, a_{ijk}\right]^2 \left(\sum_{k=1}^{S} p_k\, Pr_{ik}\right) \\ & + \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{S} X_j^2\, p_k \left[Pr_{ik} - \sum_{k=1}^{S} p_k Pr_{ik}\right]^2 \left(\sum_{k=1}^{S} p_k\, a_{ijk}\right) \end{aligned}} \\
& - \theta_2 \sqrt{\sum_{i=1}^{N}\left[q_i^{+}\right]^2 \sum_{k=1}^{S} p_k \left[y_{ik}^{+} - \sum_{k=1}^{S} p_k\, y_{ik}^{+}\right]^2 + \sum_{i=1}^{N}\left[q_i^{-}\right]^2 \sum_{k=1}^{S} p_k \left[y_{ik}^{-} - \sum_{k=1}^{S} p_k\, y_{ik}^{-}\right]^2}
\end{aligned}
\qquad (17)
$$

In order to understand the effect of each term on the overall objective function of the petrochemical network, different values of θ_1 and θ_2 should be evaluated as will be shown in the illustrative case study.

3. Value of Information and Stochastic Solution

Since stochastic programming adds computational burden on practical problems, it is desirable to quantify the benefits of considering uncertainty. In order to address this point, there are generally two values of interest. One is *expected value of perfect information* (EVPI) which measures the maximum amount the decision maker is welling to pay in order to get accurate information on the future. The second is *value of stochastic solution* (VSS) which is the difference in the objective function between the solutions of mean value problem (replacing random events with their means) and the stochastic solution (SS). (Birge, 1982)

A solution based on perfect information would yield optimal first stage decisions for each realization of the random parameters ξ. Then the expected value of these decisions, known as "wait-and-see" (WS) can be written as (Madansky, 1960):

$$WS = E_{\xi}[Min\ z(x,\xi)]$$

However, since our objective is profit maximization, the expected value of perfect information (EVPI) can be calculated as:

$$EVPI = WS - SS \qquad (18)$$

The other quantity of interest is the value of stochastic solution (VSS). In order to quantify it, we first need to solve the mean value problem, also referred to as the expected value problem (EV). This can be defined as $Min\ z(x, E[\xi])$ where $E[\xi] = \bar{\xi}$ (Birge, 1982). The solution of the EV problem provides the first stage decisions variables evaluated at expectation of the random realizations. The expectation of the EV problem, evaluated at different realization of the random parameters, is then defined as (Birge, 1982):

$$EEV = E_{\xi}[z(\bar{x}(\bar{\xi}), \xi)]$$

Where $\bar{x}(\bar{\xi})$ is evaluated from the EV model, allowing the optimization problem to choose second stage variables with respect to ξ. Similarly since our objective is profit maximization, the value of stochastic solution can be expressed as:

$$VSS = SS - EEV \tag{19}$$

The value of stochastic solution can also be evaluated as the cost of ignoring uncertainty in the problem. These concepts will be evaluated in our case study.

4. Illustrative Case Study

A number of case studies were developed to demonstrate the performance of the optimization models and illustrate the effect of process yield, raw material and product prices, and upper and lower product market demand variations. The case study presented in this paper is based on Al-Sharrah et al. (2006). The petrochemical network included 81 processes connecting the production and consumption of 65 chemicals. The uncertainty is considered through discrete distribution with a total number of 200 scenarios for each random parameter. A simplified network of processes and chemicals included in the petrochemical network are given in Figure 1 and Table 1; respectively. The chemicals are classified according to their function as follows:

a) Primary raw material (*PR*)

b) Secondary raw material (*SR*)

c) Intermediate (*I*)

d) Primary final product (*PF*)

e) Secondary final product (*SF*)

PR chemicals are derived from petroleum and natural gas and other basic feedstock, whereas the *SR* chemicals are those needed as additives or in small quantities. The chemicals classified as *I* those produced and consumed in the petrochemical network. Finally, the *PF* and *SF* chemicals are the selected final products by selected processes and the associated byproducts in the network; respectively.

Table 1: A list of chemicals included in the model*

Chemical	Function	Chemical	Function
acetaldehyde	SF+I	hydrogen cyanide	I
acetic acid	I+PF	hydrogen peroxide	I
acetone	PF	isopropyl alcohol	I
acetylene	I	methane	PR+SF
acrylic fibers	PF	methanol	I
acrylonitrile	I	methyl acrylate	SR
acrylonitrile–butadiene	PF	methyl methacrylate	SR
styrene		naphtha	PR
ammonia	PR	*n*-butane	PR
benzene	SF+I	*n*-butylenes (1- and 2-)	PR
butadiene	I	pentane	SR
butenes (mixed *n*-, iso-,	SF+PR	phenol	PF
-dienes, etc.)		polybutadiene rubber	SR
C-4 fraction (mixed butanes,	SF+PR	polystyrene (crystal grade)	I+PF
-enes, etc.)		polystyrene (expandable beads)	PF
carbon dioxide	SR	polystyrene (impact grade)	PF
carbon monoxide	I	poly(vinyl acetate)	I
chlorine	PR	poly(vinyl alcohol)	SR
chlorobenzene	I	poly(vinyl chloride)	PF
coke	PR	propane	SF+PR
cumene	I+PF	propylene (chemical grade)	SF+I
ethane	PR	propylene (refinery grade)	PR
ethanol	I	propylene oxide	SF
ethyl benzene	I	sodium carbonate	SR
ethylene	SF+I	sodium hydroxide	SR
ethylene dichloride	I	styrene	I
formic acid	SF	sulfuric acid	I
fuel gas	SF	sulfur	PR
fuel oil	SF+PR	synthesis gas 3:1	I
gas oil	PR	synthesis gas 2:1	SF
gasoline	SF	toluene	PR+SF
hydrochloric acid	SR	vinyl acetate	I+PF
hydrogen	SR+SF	vinyl chloride	I
hydrogen chloride	SR+SF	xylene (mixed)	SR+SF

* Also indicated the potential function of each chemical; PR= primary raw material, SR= secondary raw material, I= intermediate, PF= primary final product, SF= secondary final product.

The modeling system GAMS (Brooke et al., 1996) is used for setting up the optimization models. The computational tests were carried out on a Pentium M processor 2.13 GHz. The models were solved with DICOPT (Viswanathan & Grossmann, 1990). The NLP subproblems were solved with CONOPT2 (Drud, 1994), while the MILP master problems were solved with CPLEX (CPLEX Optimization Inc, 1993).

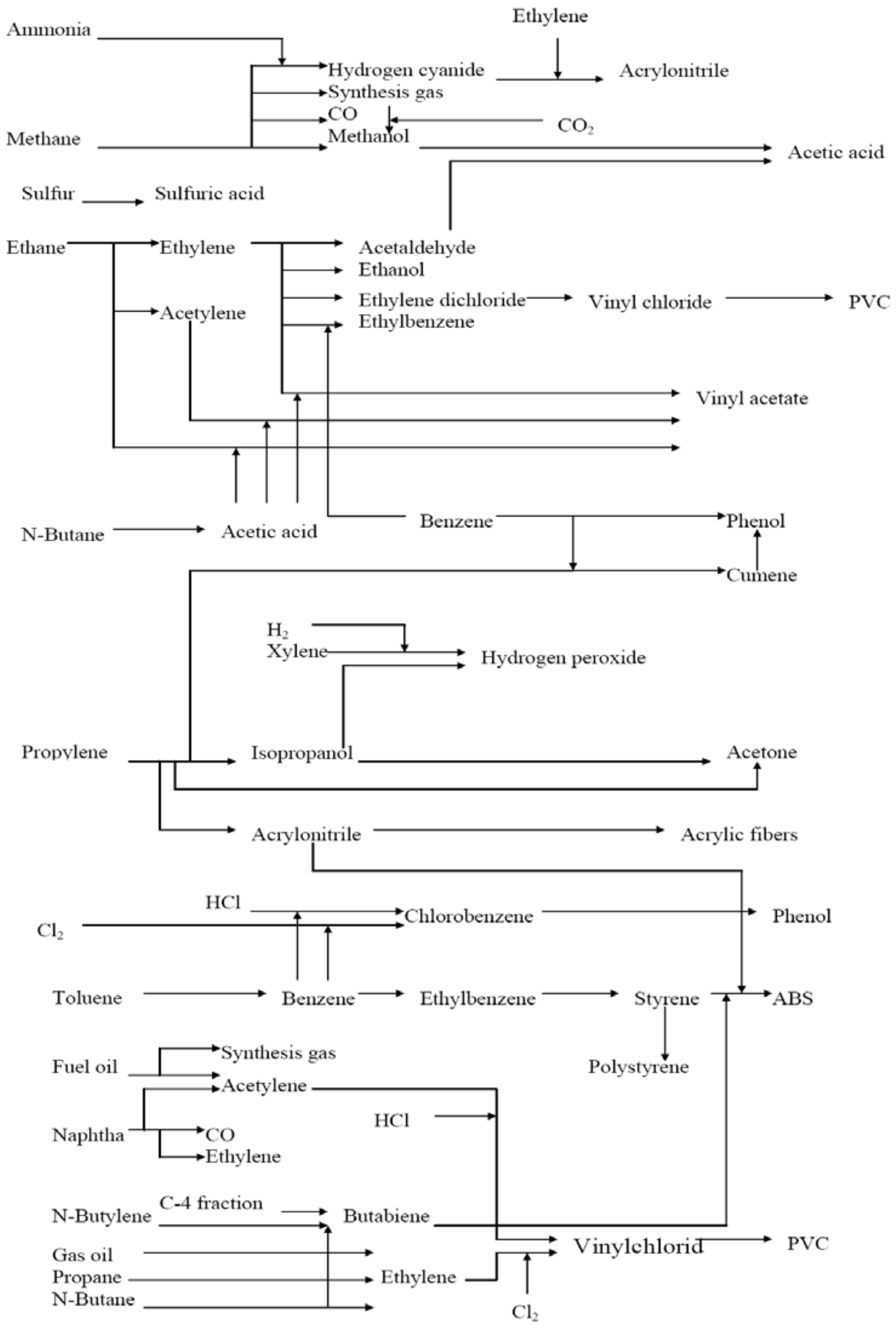

Figure 1: A simplified network of processes in the model

4.1 Solution of the deterministic model

The model in this form is moderate in size and the solution indicated the selection of 22 processes out of the 81 processes proposed. The selected processes and their respective capacities are shown in Table 2. This case study represents an ideal situation were all parameters are know with certainty.

The final petrochemical network suggests the use of lighter petroleum refining feedstocks. The petrochemical network mainly used ethane, propane, C-4 fractions (mixed butanes, -enes, etc.), pentane, and refinery grade propylene. In the case of lower lighter petroleum product availability, the network will suggest the use of steam cracking of naphtha or gas oil. This will be required in order to obtain the main petrochemical building blocks for the downstream processes that include ethylene and chemical grade propylene. The annual production benefit of the petrochemical network was found to be $ 2,202,268.

Table 2: Deterministic model solution

Process selected	Production Capacity (10^3 tons/yr)
acetaldehyde by the one-step oxidation from ethylene	1015.5
acetic acid by air oxidation of acetaldehyde	404.6
acetone by oxidation of propylene	169.8
acetylene by submerged flame process	179.8
acrylic fibers by batch suspension polymerization	246
acrylonitrile by cyanation/oxidation of ethylene	294.9
ABS by suspension/emulsion polymerization	386.9
benzene by hydrodealkylation of toluene	432.3
butadiene by extractive distillation	96.7
chlorobenzene by oxychlorination of benzene	73.0
cumene by the reaction of benzene and propylene	72.0
Ethylbenzene by the alkylation of benzene	458.8
ethylene by steam cracking of ethane-propane (50-50 wt%)	1068.3
hydrogen cyanide by the ammoxidation of methane	177.0
Phenol by dehydrochlorination of chlorobenzene	61.4
polystyrene (crystal grade) by bulk polymerization	66.8
polystyrene (expandable beads) by suspension polymerization	51.5
polystyrene (impact grade) by suspension polymerization	77.1
poly(vinyl chloride) by bulk polymerization	408.0
styrene from dehydrogenation of ethylbenzene	400.0
vinyl acetate from reaction of ethane and acetic acid	113.9
vinyl chloride by the hydrochlorination of acetylene	418.2

4.2 Solution of the stochastic model

The two-stage mixed-integer stochastic program with recourse that includes a total number of 200 scenarios for each random parameter is considered in this section. All random parameters were assumed to follow a normal distribution and the scenarios for all random parameters were generated simultaneously. Therefore, the recourse variables account for the deviation from a given scenario as apposed to the deviation from a particular random number realization.

The solution indicated the selection of 22 processes with a slightly different configuration and production capacities from the deterministic case. For example, acetic acid was produced by direct oxidation of *n*-butylenes instead of the air oxidation of acetaldehyde. Furthermore, ethylene was produced by pyrolysis of ethane instead of steam cracking of ethane-propane (50-50 wt%). These changes as well as the different production capacities obtained illustrate the effect of the uncertainty in process yield, raw material and product prices, and upper and lower product demands. In fact, ignoring uncertainty of key parameters in decision problems can yield non-optimal and infeasible decisions (Birge, 1995). The annual profit of the petrochemical network studied under uncertainty was found to be $ 2,698,552. However, in order to properly evaluate the added-value of including uncertainty of the problem parameters, we will investigate both the expected value of perfect information (EVPI) and the value of stochastic solution (VSS).

In order to evaluate the value of stochastic solution (VSS) we first solved the deterministic problem, as illustrated in the previous section, and fixed the petrochemical network and the production rate of the processes. We then solved the EEV problem by allowing the optimization problem to choose second stage variables with respect to the realization of the uncertain parameters ξ. From (19), the VSS is:

$$VSS = 2{,}698{,}552 - EEV$$
$$EEV = 2{,}184{,}930$$
$$VSS = 513{,}622$$

This indicates that the benefit of incorporating uncertainty in the different model parameters for the petrochemical network investment is $ 513,622. On the other hand, the expected value of perfect information (EVPI) can be evaluated by first finding the "wait-and-see" (WS) solution. The latter can be obtained by taking the expectation for the optimal first stage decisions evaluated at each realization ξ. From (18), the EVPI is:

$$EVPI = WS - 2{,}698{,}552$$
$$WS = 2{,}724{,}040$$
$$EVPI = 25{,}488$$

This implies that if it were possible to know the future realization of the demand, prices and yield perfectly, the profit would have been $2,724,040 instead of $2,698,552, yielding savings of $25,488. However, since acquiring perfect information is not viable, we will merely consider the value of stochastic solution (SS) as the best result. These results show that the stochastic model provided an excellent solution as the objective function value was not too far from the result obtained by the WS solution.

Table 3: Stochastic model solution

Process selected	Production Capacity (10^3 tons/yr)
acetaldehyde by the one-step oxidation from ethylene	991.0
acetic acid by direct oxidation of *n*-butylenes	397.6
acetone by oxidation of propylene	169.6
acetylene by submerged flame process	179.7
acrylic fibers by batch suspension polymerization	245.8
acrylonitrile by cyanation/oxidation of ethylene	300.9
ABS by suspension/emulsion polymerization	419.6
benzene by hydrodealkylation of toluene	767.4
butadiene by extractive distillation	104.9
chlorobenzene by oxychlorination of benzene	146.0
cumene by the reaction of benzene and propylene	144.3
Ethylbenzene by the alkylation of benzene	692.8
ethylene by pyrolysis of ethane	1051.8
hydrogen cyanide by the ammoxidation of methane	180.6
Phenol by dehydrochlorination of chlorobenzene	122.7
polystyrene (crystal grade) by bulk polymerization	133.4
polystyrene (expandable beads) by suspension polymerization	102.8
polystyrene (impact grade) by suspension polymerization	154.1
poly(vinyl chloride) by bulk polymerization	407.6
styrene from ethylbenzene by hydroperoxide process	607.7
vinyl acetate from reaction of ethylene and acetic acid	113.8
vinyl chloride by the hydrochlorination of acetylene	417.8

However, as mentioned in the previous section, the stochastic model takes a decision based on first-stage and expected second-stage costs and hence does not account for a decision-maker risk behavior (risk-averse or risk taker). For this reason, a more realistic approach would consider higher moments where the tradeoff between the mean value and the variations of different scenarios is appropriately reflected.

4.3 Solution of stochastic model with risk consideration

Considering risk in terms of variations in both projected benefits and recourse variables provided a more robust analysis of the problem. As explained earlier, the problem will have a more robust solution as the results will remain close to optimal of all given scenarios through minimizing the variations of the projected benefit. On the other hand, the model will be more robust as minimizing the variations in the recourse variables leads to a model that is almost feasible for all the scenarios considered. In order to investigate the effect of each term on the original problem, the spectrum of results generated by varying the scaling factors must be explored. For this reason, the model was repeatedly solved for different values of θ_1 (profit variations) and θ_2 (recourse variables variations) in order to construct the efficient frontier plot of expected profit versus risk measured by standard deviation. Figures 2 and 3 illustrate the change in expected profit with risk in terms of standard deviation at different θ_1 and θ_2 values, respectively. The graphs show the decline in expected profit as we penalize the variations in process yield, profit and demand by increasing the values of θ_1 and θ_2. These values will depend on the policy adopted by the investor whether being risk-averse or risk taker and can be read directly from the efficient frontier plots.

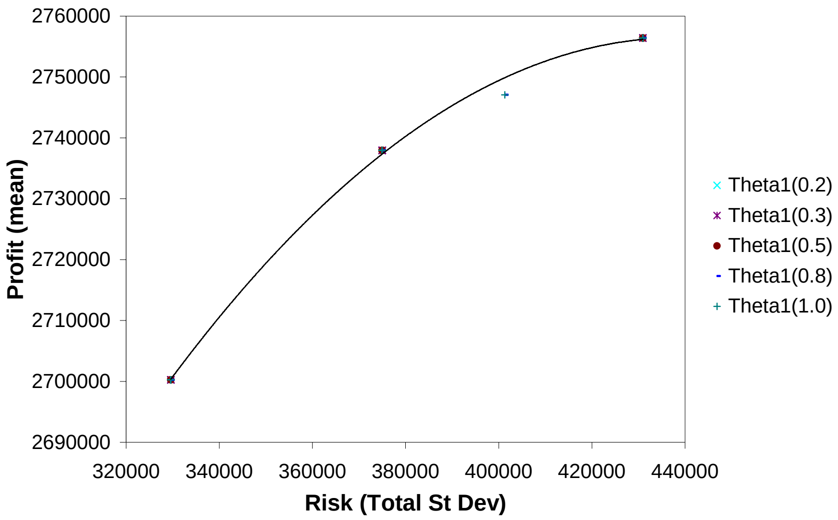

Figure 2: Risk vs. projected benefits at different θ_1

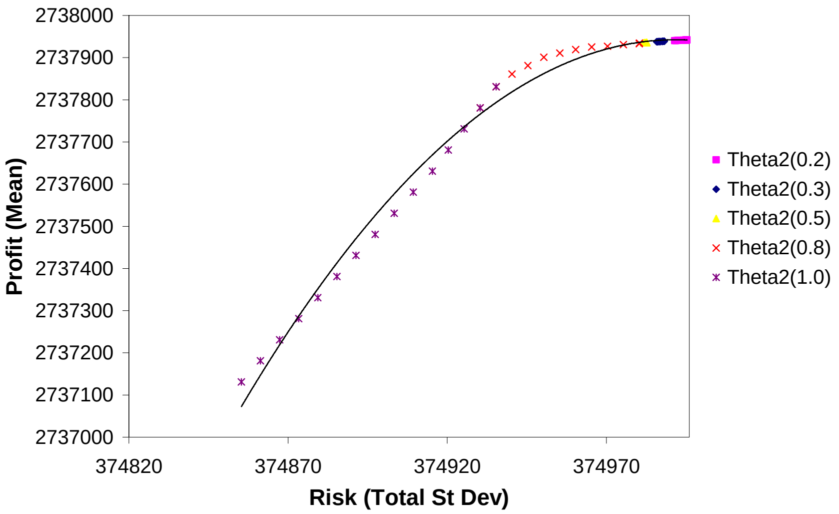

Figure 3: Risk vs. projected benefits at different θ_2

Furthermore, it was found that the problem bears more sensitivity to variations in product demand for values of θ_1 and θ_2 that maintain the final petrochemical structure. However, as the values of θ_1 and θ_2 increase some processes became too risky to include in the petrochemical network and instead, importing some final chemicals became a more attractive alternative. This type of analysis requires accurate pricing structure of the local market under study as compared to global market. In this study, however, we restricted the range of the variations of scaling parameters θ_1 and θ_2 to values that will maintain all processes obtained from the stochastic model. This approach was adopted as the objective of the study was to include all required processes that will meet a given demand.

5. Conclusion

A robust mixed-integer nonlinear programming model for maximizing profit in the design of petrochemical networks was presented. Uncertainty in process yield, raw material and product prices, and upper and lower product market demand were considered. In addition, operational risk was accounted for in terms of variance in projected benefits, process yield and forecasted demand. Including these different sources of uncertainty in the problem as well as modeling risk provided a more robust analysis for this type of highly strategic planning applications in the chemical industry. The proposed approach increased solution robustness and model robustness by incorporating penalty terms for both deviation from both projected benefits and recourse variables; respectively.

The results of the model studied under uncertainty and with risk consideration, as one can intuitively anticipate, yielded different petrochemical network configurations and plant capacities when compared to the deterministic model results. The concepts of Expected Value of Perfect Information (EVPI) and Value of the Stochastic Solution (VSS) were introduced and numerically illustrated. The results obtained from the stochastic model provided good results as the objective function value was not too far from the results obtained using the wait-and-see approach. Furthermore, the study showed that the final petrochemical network bears more sensitivity to variation in product demand when the values of θ_1 and θ_2 were selected to maintain the final petrochemical structure.

Acknowledgment

This work was supported in part by Saudi Aramco and an NSERC discovery grant.

References

Ahmed, S., & Sahinidis, N. V. (1998). Robust process planning under uncertainty. *Industrial & Engineering Chemistry Research*, 37, 1883.

Ahmed, S., Sahinidis, N. V., & Pistikopoulos, E. N. (2000). An improved decomposition algorithm for optimization under uncertainty. *Computers & Chemical Engineering*, 23, 1589.

Al-Amir, A. M. J.; Al-Fares, H.; & Rahman, F. (1998). Towards Modeling the Development of the Petrochemical Industry in the Kingdom of Saudi Arabia. *Arabian Journal of Science &. Engineering*, 23, 113.

Al-Fares, H. K.; & Al-Amir, A. M. (2002). An Optimization Model for Guiding the Petrochemical Industry Development in Saudi Arabia. *Engineering Optimization*, 34, 671.

Al-Sharrah, G. K., Hankinson G., & Elkamel A. (2006). Decision-making for petrochemical planning using multiobjective and strategic tools. *Chemical Engineering Research and Design*, 84(A11), 1019.

Al-Sharrah, G. K.; Alatiqi, I.; & Elkamel, A. (2002). Planning an Integrated Petrochemical Business Portfolio for Long-Range Financial Stability. *Industrial & Engineering Chemistry Research*, 41, 2798.

Al-Sharrah, G. K.; Alatiqi, I.; & Elkamel, A. (2003). Modeling and Identification of Economic Disturbances in the Planning of the Petrochemical *Industry. Industrial & Engineering Chemistry Research*, 42, 4678.

Al-Sharrah, G. K.; Alatiqi, I.; Elkamel, A.; & Alper, E. (2001). Planning an Integrated Petrochemical Industry with an Environmental Objective. *Industrial & Engineering Chemistry Research*, 40, 2103.

Barbaro, A., & Bagajewicz, M. J. (2004). Managing financial risk in planning under uncertainty. *AIChE Journal*, 5, 963.

Bell, J. T. (1990). Modeling of the Global Petrochemical Industry. Ph.D. Thesis. University of Wisconsin-Madison.

Birge, J. R. (1995). Models and model value in stochastic programming. *Annals of Operations Research*, 59, 1.

Birge, J. R. (1982). Stochastic linear programs with fixed recourse. *Mathematical Programming*, 24, 314.

Bok, J., Lee, H., & Park, S. (1998). Robust investment model for long-range capacity expansion of chemical processing networks under uncertain demand forecast scenarios. *Computers & Chemical Engineering*, 22, 1037.

Brooke, A., Kendrick, D., & Meeraus, A., Raman, R. (1996). *GAMS—A User's Guide*. Washington DC: GAMS Development Corporation.

Clay, R. L., & Grossmann, I. E. (1997). A disaggregation algorithm for the optimization of stochastic planning models. *Computers & Chemical Engineering*, 21, 751.

CPLEX Optimization, Inc. (1993). *Using the CPLEX Callable Library and CPLEX Mixed Integer Library*; CPLEX Optimization, Inc.: Incline Village, NV.

Drud, A. S. (1994). CONOPT: a large scale GRG code. *ORSA Journal of Computing*, 6, 207.

Energy information administration (EIA). (2006). *International Energy Outlook*. http://www.eia.doe.gov/oiaf/ieo/index.html, accessed on October 20, 2006.

Fathi-Afshar, S.; & Yang, J. (1985). Designing the Optimal Structure of the Petrochemical Industry for Minimum Cost and Least Gross Toxicity of Chemical Production. *Chemical Engineering Science*, 40, 781.

Ierapetritou, M. G.; & Pistikopoulos, E. N. (1994). Novel Optimization Approach of Stochastic Planning Models. *Industrial & Engineering Chemistry Research*, 33, 1930.

Jimenez, A.; & Rudd, D. F. (1987). Use of a Recursive Mixed-Integer Programming Model to Detect an Optimal Integration Sequence for the Mexican Petrochemical Industry. *Computers & Chemical Engineering*, 11, 291.

Jimenez, A.; Rudd, D. F.; & Meyer, R. R. (1982). Study of the Development of Mexican Petrochemical Industry using Mixed- Integer Programming. *Computers & Chemical Engineering*, 6, 219.

Johnson, N. L., & Tetley, H. (1955). *Statistics*, vol. I. Cambridge University Press.

Liu, M. L.; & Sahinidis, N. V. (1995). Computational Trends and Effects of Approximations in an MILP Model for Process Planning. *Industrial & Engineering Chemistry Research*, 34, 1662.

Liu, M. L.; & Sahinidis, N. V. (1996). Optimization in Process Planning under Uncertainty. *Industrial & Engineering Chemistry Research*, 35, 4154.

Liu, M. L.; & Sahinidis, N. V. (1997). Process Planning in a Fuzzy Environment. *European Journal of Operational Research*, 100, 142.

Madansky, A. (1960). Inequalities for stochastic linear programming problems. *Management science*, 6,197.

Malcolm, S. A., & Zenios, S. A. (1994). Robust optimization of power systems capacity expansion under uncertainty. *Journal of the Operational Research Society*, 45, 1040.

Markowitz, H. M. (1952). Portfolio selection. *Journal of Finance*, 7, 77.

Mulvey, J. M., Vanderbei, R. J., & Zenios, S. A. (1995). Robust optimization of large-scale systems. *Operations Research*, 43, 264.

Neiro, S. M. S., & Pinto, J. M. (2005). Multiperiod optimization for production planning of petroleum refineries. *Chemical Engineering Communications*, 192,62.

Shah, N. (1998). Single- and multisite planning and scheduling: current status and future challenges. AIChE Symposium Series: Proceedings of the Third International Conference of the Foundations of Computer-Aided Process Operations, Snowbird, Utah, USA, July 5–10, 94, 75.

Sokic, M.; & Stevancevic, D. (1983). The Optimal Structure of the Petrochemical Industry. *Chemical Engineering Science*, 38, 265.

Sophos, A.; Rotstein, E.; & Stephanopoulos, G. (1980). Multiobjective Analysis in Modeling the Petrochemical Industry. *Chemical Engineering Science*, 38, 2415.

Stadtherr, M. A.; & Rudd, D. F. (1976). Systems study of the Petrochemical Industry. *Chemical Engineering Science*, 31, 1019.

Stadtherr, M. A.; & Rudd, D. F. (1978). Resource Use by the Petrochemical Industry. *Chemical Engineering Science*, 33, 923.

Subrahmanyam, S., Pekny, J., & Reklaitis, G.V. (1994). Design of batch chemical plants under market uncertainty. *Industrial & Engineering Chemistry Research*, 33, 2688.