NOVEL COST ALLOCATION FRAMEWORK FOR NATURAL GAS PROCESSES: METHODOLOGY AND APPLICATION TO PLAN ECONOMIC OPTIMIZATION

A Dissertation

by

WON-HYOUK JANG

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2004

Major Subject: Chemical Engineering

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Approved as to style and content by:

_____	_____
Kenneth R. Hall	David M. Ford
(Co-Chair of Committee)	(Member)
_____	_____
Juergen Hahn	Alexander G. Parlos
(Co-Chair of Committee)	(Member)
_____	_____
Mahmoud El-Halwagi	Kenneth R. Hall
(Member)	(Head of Department)

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ABSTRACT

Novel Cost Allocation Framework for Natural Gas Processes: Methodology and Application to Plan Economic Optimization. (May 2004)

Won-Hyouk Jang, B.S., Hanyang University;

M.S., Texas A&M University

Co-Chairs of Advisory Committee: Dr. Kenneth R. Hall
Dr. Juergen Hahn

Natural gas plants can have multiple owners for raw natural gas streams and processing facilities as well as for multiple products. Therefore, a proper cost allocation method is necessary for taxation of the profits from natural gas and crude oil as well as for cost sharing among gas producers. However, cost allocation methods most often used in accounting, such as the sales value method and the physical units method, may produce unacceptable or even illogical results when applied to natural gas processes.

Wright and Hall (1998) proposed a new approach called the design benefit method (DBM), based upon engineering principles, and Wright *et al.* (2001) illustrated the potential of the DBM for reliable cost allocation for natural gas processes by applying it to a natural gas process.

In the present research, a rigorous modeling technique for the DBM has been developed based upon a Taylor series approximation. Also, we have investigated a cost allocation framework that determines the virtual flows, models the equipment, and

evaluates cost allocation for applying the design benefit method to other scenarios, particularly those found in the petroleum and gas industries. By implementing these individual procedures on a computer, the proposed framework easily can be developed as a software package, and its application can be extended to large-scale processes.

To implement the proposed cost allocation framework, we have investigated an optimization methodology specifically geared toward economic optimization problems encountered in natural gas plants. Optimization framework can provide co-producers who share raw natural gas streams and processing plants not only with optimal operating conditions but also with valuable information that can help evaluate their contracts. This information can be a reasonable source for deciding new contracts for co-producers.

For the optimization framework, we have developed a genetic-quadratic search algorithm (GQSA) consisting of a general genetic algorithm and a quadratic search that is a suitable technique for solving optimization problems including process flowsheet optimization. The GQSA inherits the advantages of both genetic algorithms and quadratic search techniques, and it can find the global optimum with high probability for discontinuous as well as non-convex optimization problems much faster than general genetic algorithms.

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1. INTRODUCTION

Natural gas has been used as a raw material for many chemical products and as a major energy source since its discovery (Busby, 1999). Compared to petroleum, natural gas has only been commercial relatively recently. Natural gas was not considered a valuable product before the rise of the natural gas industry and it was vented or flared (Smith & Brock, 1959). Currently, natural gas is recognized as a crucial energy resource accounting for 24% of the USA total energy need (in 1996) and whose production and consumption should increase rapidly considering its reserves and technical improvements in exploration and production (Busby, 1999).

Unlike most industrial plants, which usually are owned by a single company, natural gas plants often have multiple owners for raw natural gas streams and processing facilities (Bullin, 1999). Natural gas usually is transported and processed through shared pipelines and processing facilities to reduce net costs. When multiple gas producers share transportation or production facilities, the costs as well as the profits also must be shared under a contract (Duewall, 1999).

Because natural gas processes inherently yield multiple products, the co-producers require a methodology for allocating costs associated with each product. This activity becomes even more important when plants can operate under multiple conditions, which can also produce different amounts of each product. The eventual cost assigned to co-

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producers should be proportional to their contribution of the products. Additionally, some countries impose different tax rates on profits derived from each product, which requires cost allocations. For these situations, the United Nations Center on Transnational Corporations (UNCTC) recommends a specific accounting guideline regarding the preparation of a procedure for the cost allocation between gas and liquid products. This guideline must be followed to compute profits properly (UNCTC, 1987).

While the most common methods for cost allocation in accounting are the sales value method and the physical units method, they may produce unacceptable or even illogical results when applied to natural gas processes. Lacking a relationship between product price and processing cost, multiple split-off points, and a logical and common physical attribute, the traditional methods are inappropriate for natural gas processes (Wright & Hall, 1998). Under current economic conditions, a demand exists for a new approach to replace the traditional methods.

Wright and Hall (1998) have proposed a new approach based upon engineering principles called the “design benefit method” (DBM). The basic idea of this new technique is to utilize a process simulator within a framework for cost allocation. The cost can be allocated causally from the mathematical information that takes into account the unit size of process equipment. Wright *et al.* (2001) applied this idea to a natural gas process and illustrated that the design benefit method can be a reliable cost allocation technique for natural gas processes.

In the present research, we have investigated a new modeling technique for the design benefit method, which is more mathematically reasonable and more easily implemented on a computer.

In order to illustrate the potential application of the proposed cost-allocation framework, we have further investigated an optimization framework that is appropriate to find the optimal operating condition for gas plant economic optimization that includes cost allocation results. For the optimization framework, a new genetic algorithm, named the “genetic quadratic search algorithm” (GQSA), has been developed. The GQSA consists of a general genetic algorithm, which can be any existing algorithm, and a quadratic search, which improves the convergence speed of the algorithm. The optimization framework would provide co-producers sharing raw natural gas streams and a processing plant not only with the optimal operating condition but also with valuable information that can help to evaluate their contracts, which are complicated by contract terms such as: quality of raw streams, process efficiency, product prices, *etc.* (Bullin, 1999). This information could be a reasonable source for deciding new contracts for co-producers.

2. BACKGROUND

2.1. Products and cost allocation for natural gas processes

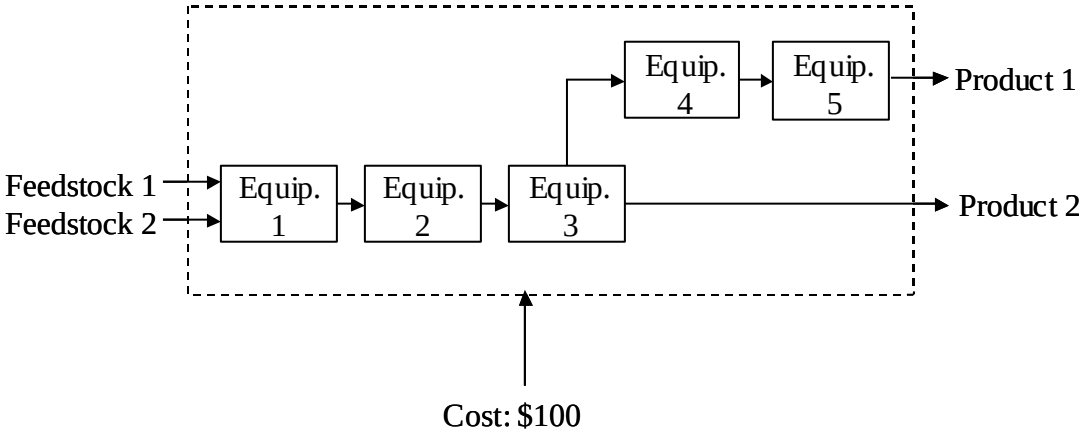
The major components of natural gas are methane, ethane, propane, butanes, pentanes, and small amounts of hexanes, heptanes, octanes, *etc*. Also, natural gas generally contains many impurities, such as carbon dioxide (acid gas), hydrogen sulfide (sour gas), water, nitrogen, helium, *etc.* (Ikoku, 1984; Busby, 1999).

In natural gas processing plants, raw natural gas is separated into a gas product and liquid products referred to as natural gas liquids (NGL). Methane is by far the most abundant component in pipeline natural gas and it is supplied to homes, businesses, and industries. The NGL is sold as a Y-Grade product or, with more processing, fractured to products having higher market value as fuel or feedstock to chemical plants (Ikoku, 1984; Bullin, 1999). The impurities should be removed from natural gas to protect facilities from toxic and corrosive components, such as hydrogen sulfide, as well as to obtain products satisfying required quality. Some impurities can be sold as a by-product: carbon dioxide and nitrogen are injected into depleted oil fields to enhance production and helium is used in electronic manufacturing and for inflating blimps and balloons (Busby, 1999).

The unique characteristic of natural gas processes is the different ownership with respect to raw natural gas streams and processing facilities, which causes very complicated natural gas plant economics that need to be combined with joint products, such as gas and liquid products. These characteristics essentially require appropriate

methodologies to return fairly costs as well as profits to co-producers who own raw natural gas stream(s) or the processing facility. The co-producers can share joint products directly generally based upon heating values, the amount of molecules, and component prices (Bullin, 1999). Costs are allocated to the gas and liquid products first, and then eventually assigned to co-producers based upon the proportion of shared products. However, how to determine the capital and operating costs allocated to the joint products is a very difficult problem because of the lack of a reasonable basis.

Joint cost allocation in traditional methods often is determined based upon revenues and physical measures, such as heating values and flow rates, of products. The sale value method (or the net revenue method) determines joint cost allocation using the



Equip. 1 Cost	Equip. 2 Cost	Equip. 3 Cost	Equip. 4 Cost	Equip. 5 Cost	Total Cost
$20	$20	$20	$20	$20	$100

Fig. 1. Example process having two joint products.

market value of the final products (Taher, 1966). Figure 1 is an example of a simple process having two joint products. Feedstock 1 and Feedstock 2 are converted to joint products, Product1 and Product 2, with $100 of cost.

Table 1 shows joint cost allocation determined by the sales value method. Based upon simply the proportion of the market value of joint products, $80 and $20 of costs are allocated to Product 1 and Product 2, respectively.

The basic assumption of the sales value method is that the more revenue, the higher the cost. In the gas and petroleum industries, the joint product having the largest portion of revenueoften does not incur the most processing cost (Duewall, 1999). Another problem with the sales value method applied to natural gas processes is the existence of big difference in the price trends of gas and oil products. While oil sales prices are influenced by world market prices and tend to fluctuate with the variation of international supply and demand, gas sales prices result from local and long-term contracts and are relatively stable (Porter, 1965). Therefore, when the sales price of one product severely fluctuates but that of the other product is stable, this method results in inconsistent joint cost allocation.

Table 1. Joint cost allocation determined by the sales value method

	Market Value	Allocated Cost
Product 1	$400	$\$80 = \$100\frac{\$400}{\$500}$
Product 2	$100	$\$20 = \$100\frac{\$100}{\$500}$
Total	$500	$100

Table 2. Joint cost allocation determined by the physical unit method

	Mass	Allocated Cost
Product 1	30lb	$\$30 = \$100\frac{30\text{lb}}{100\text{lb}}$
Product 2	70lb	$\$70 = \$100\frac{70\text{lb}}{100\text{lb}}$
Total	100lb	$100

The physical unit method provides joint cost allocation based upon prorating of a physical measure for many processes in an objective manner (Barfield et al, 1994). This method needs a common and measurable physical characteristic of the joint products. Basis units commonly used for many industries are pounds, gallons, bales, and board feet (Blocker, 1940). Table 2 shows resulting joint cost allocation when applying the physical unit method using mass as a basis unit to the example process in Fig. 1. Being prorated to mass, $100 of total costs is allocated to Product 1 for $30 and Product 2 for $70, respectively.

Polimeni *et al.* (1991) stated the assumption of the physical unit method: “It is assumed that the products are homogeneous and one product does not require more or less effort (cost) than any other product in the group.” The physical unit method is useful for processes with joint products whose sales price is very unstable. According to the above assumption, it is, however, not an adequate method for application to natural gas processes whose joint products are mostly multiple phases, such as gas and oil. Another potential problem is that there are many possible bases, such as volume, mass, energy,

etc., in natural gas processes. Therefore, the selection of an appropriate allocation basis can be another issue because each chosen basis should result in different cost allocation.

The DBM provides joint cost allocation using unit-by-unit analysis based upon engineering principles related to equipment design and construction. Wright *et al*. (2001) descried the relationship between engineering principles and costs: “Part of the design process involves developing a cost analysis based upon the principle that capital and operating costs are a function of equipment size. Engineers posit that equipment design is causal in the sense that the physical existence of the equipment (*i.e*., causes) the costs”. Therefore, if each equipment size is determined, then the combined capital cost for the entire processes is the sum of the parts. Similarly, operating cost can be obtained from the utility consumption, such as steam, coolant, electric power, *etc*.

In the DBM, the joint costs allocated to eventual products represent eventual products in each unit and is proportional to the contribution of eventual products to the unit size/utility consumption of each unit: eventual products are called “virtual product flows” in this dissertation. Table 3 shows joint cost allocation determined by the DBM applied to the example process in Fig. 1. Because the cost of each unit is known or can be estimated, each unit cost allocated among the joint products can be determined based upon the contribution of joint products to equipment sizes in natural gas processes. The resulting joint costs allocated to Product 1 and Product 2 are $65 and $35, respectively. Also, the costs of Equipment 4 and Equipment 5 are allocated solely to Product 1 because both units process no components of Product 2, and the contribution of Product 2 to their unit size becomes zero. This observation is reasonable in terms of engineering

sense and can reflect an aspect of advantages acquired when the DBM is used for cost allocation.

In the previous research, Wright *et al.* (2001) determined the contribution of joint products to equipment sizes using mathematical information provided with a partial derivative. Wright and Hall (1998) described the partial derivative as: "… a partial derivative which is the change in a dependent variable (size) caused by changing one of the independent variables (throughput of an eventual product) while holding all other independent variables (throughput of all other eventual products) constant." The partial derivatives were evaluated using a set of data, which was generated by a process simulator, of equipment size *versus* throughput over a range from zero flow to actual flow: the throughput of a product flow varies over the range while holding that of all other product flows constant (*e.g.*. actual flow). After collecting data, the partial derivatives can be determined by regression techniques.

Table 3. Joint cost allocation determined by the design benefit method

	Equip. 1 Cost	Equip. 2 Cost	Equip. 3 Cost	Equip. 4 Cost	Equip. 5 Cost	Allocated Cost
Product 1	$5	$5	$15	$20	$20	$65
Product 2	$15	$15	$5	$0	$0	$35
Total	$20	$20	$20	$20	$20	$100

However, this approach to evaluate the partial derivatives is useful when the change of equipment size with respect to joint products is linear. If the relationship between equipment size and joint products is nonlinear, then the evaluated partial derivatives could be far from their correct values. This unfavorable case would be unavoidable in many units employed by natural gas plants. Furthermore, for the same range of the variation domain of eventual product flows, process simulation with specific units (*e.g.*, distillation column) may not be successful because of an infeasible simulation condition. Therefore, more rigorous modeling techniques that can deal with the flexible variation domain of eventual product flows as well as with higher order models are necessary to achieve adequate accuracy for any type of equipment.

2.2. Optimization of natural gas plant economics by genetic algorithms

Because the cost-allocation framework gives us cost allocation results using a process simulator that already has a process flowsheet consisting of a rigorous process model, no additional task exists for developing a process model to solve the optimization problem for natural gas plant economics. Natural gas plant economic problems need process flowsheet optimization characterized by discontinuity and non-convexity in order to collect process information required to compute their objective functions. Each evaluation of the objective function requires convergence of the process flowsheet, which has discontinuous characteristics such that the cost function shows discontinuous behavior as well. Also, because elements of the process flowsheet show nonlinear characteristics according to their operating range, the optimization problem may have

multiple local optima. Despite their high computational efficiency, typical gradient-based optimization techniques may not work properly in this application because of the discontinuity and non-convexity of the optimization problem (Rao, 1996). For solving this type of optimization problems, different approaches based upon stochastic search algorithms, such as genetic algorithms (Wang *et al.*, 2000), evolutionary algorithms (Gross & Roosen, 1998), and simulated annealing (Li *et al*., 2000), have been applied.

Genetic algorithms are among the most widely used stochastic search algorithms and are recognized as promising alternatives to the gradient-based optimization techniques that need specific numerical implementation to be applied to optimization problems characterized by mixed continuous-discrete variables, and discontinuous and/or non-convex system spaces. However, the drawback of genetic algorithms is the excessive and uncontrollable number of runs for obtaining a solution having acceptable quality caused by to their stochastic nature (Wang *et al*., 2000; Wang *et al*., 2004). When genetic algorithms are applied to optimization problems coupled with a process simulator, the number of objective function evaluations can be crucial because each solution set requires the completion of flowsheet convergence whose computation time dominates the time required for other components in each genetic algorithm loop. Therefore, it is extremely important to develop an efficient search algorithm that requires a smaller number of objective function evaluations.

Although genetic algorithms were originally developed by Holland (1975), many useful variants of the genetic algorithm have been applied to solve various optimization problems by Goldberg (1989) and Davis (1991) (Ahuja *et al*., 2000; Cong & Li, 1994).

The most common approach is “hybridization” that combines a special algorithm and a basic genetic algorithm to improve search performance.

Lü *et al*. (2003) and Yan *et al*. (2003) introduce chaos to avoid premature convergence by maintaining suitable diversity in each population. Premature convergence means that the solution sticks to a local optimum and does not improve. Hanagandi and Nikolaou (1998) propose a genetic algorithm incorporating Törn’s (1977) clustering technique to generate populations with diverse individuals by measuring the density of clusters consisting of a group of individuals. More examples of hybrid genetic algorithms are in a variety of textbooks, such as: Chambers (1995), Davis (1991), Gen and Cheng (1997), Goldberg (1989), Man *et al.* (1999), and Martin and Spears (2001).

The hybrid genetic algorithm incorporating an additional algorithm to search for local optima is among the most popular. Gen and Cheng (1997) describe the characteristics and advantages of such an approach : “… local optimization is applied to each newly generated offspring to move it to a local optimum before injecting it into the population. Genetic algorithms are used to perform global exploration among a population, while heuristic methods are used to perform local exploitation around chromosomes. Because of complementary properties of genetic algorithms and conventional heuristics, the hybrid approach often outperforms either method operating alone.” The GQSA is also a hybrid genetic algorithm of this category. In the GQSA, a typical genetic algorithm is coupled with a sub-optimal algorithm based upon a quadratic search using individuals around the temporal optimum. The elitist strategy in genetic

algorithms inherently results in a cluster around the global optimum or promising local optima: according to De Jong(1975), this property causes the premature convergence in simple genetic algorithms. The GQSA utilizes the cluster to determine a quadratic model and to conduct sub-optimization based upon an explicit mathematical expression. The basic assumption of this technique is that the cluster is likely located in the convex region that includes the global optimum and that the smaller the radius of the cluster surrounding the global optimum, the closer the solution of the quadratic model determined by individuals in the cluster. Because of these properties of a cluster in genetic algorithms, the GQSA can significantly reduce the required number of objective function evaluations for obtaining a solution having acceptable quality.

3. OBJECTIVE

The objective of the present research is to develop a rigorous cost allocation framework based upon the DBM for natural gas processes. Additionally, this research aims at extending the application of the proposed framework to problems arising in the natural gas industry.

A reasonable and physically explainable modeling technique for the DBM has been developed based upon a Taylor series approximation. This modeling technique not only employs a generalized modeling procedure applicable to a wide variety of equipment, but it is also more easily convertible to digital coding and implementation on a computer system.

A cost allocation framework based upon the DBM has been investigated for extending the application of the design benefit method to other scenarios, particularly those found in the petroleum and gas industries. Also, computer programming code sets of the proposed framework and software interface between the programming code sets and the process simulator have been developed to ensure that the proposed framework applies to large-scale processes through automated computation.

Finally, an optimization framework for natural gas economics resulting from product-sharing contracts has been proposed based upon a new hybrid genetic algorithm, which is suitable for solving optimization problems including process flowsheet optimization.

4. DESIGN BENEFIT METHOD

Unit size is a dominant factor in equipment cost, and there are many ways to estimate the capital cost of a process using individual equipment costs. In other words, the capital cost can be evaluated by determining the unit size of the individual equipment. Similarly, operating cost can be obtained from utility consumption, such as steam, coolant, electrical power, etc. The design benefit method computes cost allocation using numerical information derived from the equipment model for the unit size/utility consumption of process equipment because components of the equipment model can reflect the effect of products on changes in the unit size/utility consumption.

We use the equipment models within a Taylor series approximation with respect to "virtual flows" (defined in this dissertation). The composition of the virtual flows are determined based upon that of eventual gas and liquid products. A set of data for modeling is composed of a series of unit size/utility consumption and a series of the corresponding virtual product flow rates. The data set is generated by evaluating the unit size/utility consumption at the new steady-states corresponding to the perturbed virtual product flow rates.

For the remainder of this dissertation, we base all equations and descriptions upon a natural gas process that produces only gas and liquid products.

4.1. Virtual flows

Two main tasks reside within the design benefit method: determination of virtual flows and modeling of process equipment. The inlet stream of a processing plant contains three virtual flows: a “virtual product gas flow”, a “virtual product liquid flow”, and a “virtual surplus flow”. We establish the virtual flows by assigning components of the inlet stream to them based upon the component analysis of the eventual products.

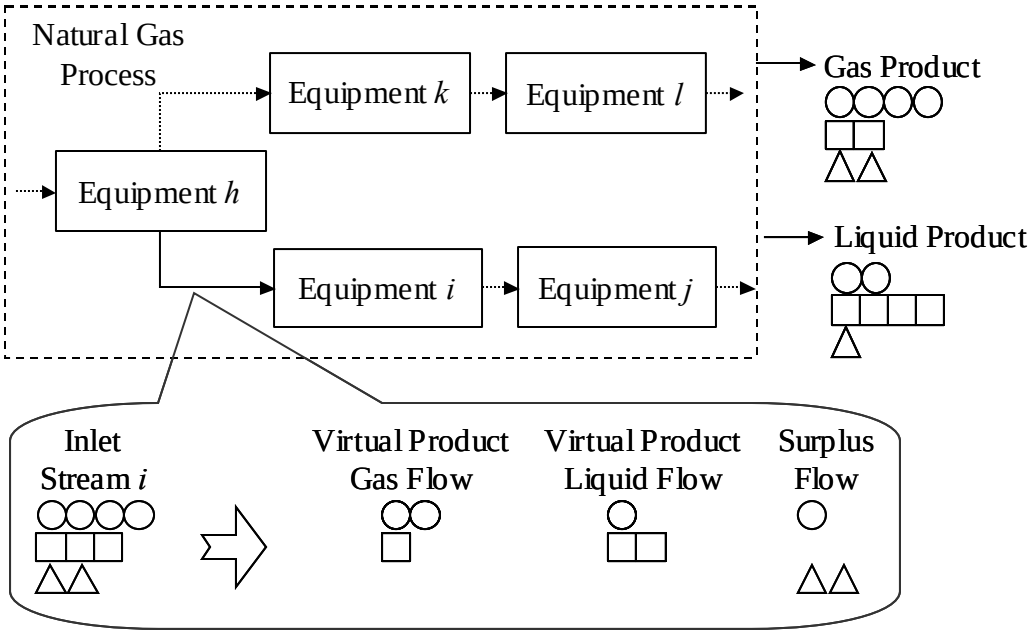


Fig. 2. Equipment block diagram of a natural gas process with two products.

Fig. 2 shows a simple block diagram that illustrates how to determine the virtual flows. In the block diagram, the inlet stream, *i*, splits into virtual flows. Circles and rectangles represent valuable components of the inlet stream. These components are assigned to the virtual product gas flow and the virtual product liquid flow on the basis of the composition of the eventual products. Thus, the compositions of the virtual gas product and the virtual liquid product flows are identical to those of the corresponding eventual gas and liquid products.

The role of the virtual surplus flow is to account for additional valuable components that cannot appear in either the virtual product gas flow or the virtual product liquid flow (denoted by a "circle" in Fig. 2) under the constraint of composition, as well as for valueless components (denoted by a "triangle" in Fig. 2). While the virtual surplus flow cannot be attributed directly to either of the products, it nevertheless is an important concept for determining equipment size. Additionally, natural gas processes commonly transport valueless components together with valuable components in a single product stream. This selection would distort the cost allocation using the traditional methods. However, performing cost allocation based upon virtual flows instead of the real flows eliminates this problem.

For determining virtual flows, it is advantageous to split the inlet and product streams into component flows belonging to different groups: the "monopoly-group" or the "shared-group." Components within the monopoly-group belong exclusively to one of the virtual flows while components within the shared-group distribute among two or more virtual flows. Components present in only negligible amounts as well as valueless

components, such as nitrogen, carbon dioxide, *etc.*, fall in the monopoly-group and are assigned to the virtual surplus flow. We note that the component classification needs an exception because streams in natural gas processes generally consist of many components, whose relegation to gas and liquid products has a wide variety of values. Assume that a heavier hydrocarbon is transported to both gas and liquid products. In general, most of it passes to the liquid product while small amount comes out with the gas product. In this case, if the component is placed into the shared-group, then the amount in the determined virtual product gas flow will be a trivial value to make the composition of the determined virtual product gas flow the same as that of the gas product with respect to components within the shared-group. Therefore, when a component is dominantly transported into an eventual product, the component should be classified into the monopoly-group, and the virtual product flow corresponding to the eventual product has the monopoly on the component.

Components of an inlet stream belonging to the shared-group can be allocated among the virtual flows by solving a minimization problem. The objective function corresponds to the virtual surplus flow rate:

$$\text{Minimize: } \sum_{j=1}^{n_{sc}} f_{C_j,ins} - \alpha \sum_{j=1}^{n_{sc}} f_{C_j,gas}^{prod} - \beta \sum_{j=1}^{n_{sc}} f_{C_j,liq}^{prod} \tag{1}$$

$$\begin{aligned} \text{Subject to: } & f_{C_j,ins} - \alpha f_{C_j,gas}^{prod} - \beta f_{C_j,liq}^{prod} \geq 0,\ j = 1,\ldots,n_{sc} \\ & 0 \leq \alpha \leq 1 \\ & 0 \leq \beta \leq 1 \end{aligned} \tag{2}$$

where n_{sc} = number of components belonging to the shared-group

$f_{C_j,ins}$, $f_{C_j,gas}^{prod}$ and $f_{C_j,liq}^{prod}$ = j^{th} component flow rates of the inlet stream,

the eventual gas product, and the eventual liquid product

α = proportion of the eventual gas product assigned to the product gas flow

β = proportion of the eventual liquid product assigned to the product liquid flow

In Eq. (1), the second and third terms are the virtual product gas and the virtual product liquid flow rates, respectively. The goal of this minimization problem is to determine α and β which minimize the virtual surplus flow rate and simultaneously satisfy the constraints for the virtual gas product and the virtual liquid product flows, *i.e*. their compositions equal those corresponding to the eventual gas and liquid products. This optimization allows an optimal cost allocation. Because α and β are the only parameters to be determined, a conventional linear programming (LP) technique is sufficient for the problem. The LP technique can be found in may textbooks, such as Edgar *et al.* (2001), Fletcher (2000), Rao (1996), and Venkataraman (2001).

After obtaining optimal values for α and β, the virtual flows of the inlet stream can be determined by the following components distribution functions:

- When the i$^{\text{th}}$ component belongs to the shared-group,

$$f_{C_i,gas} = \alpha f_{C_i,gas}^{prod} \tag{3}$$

$$f_{C_i,liq} = \beta f_{C_i,liq}^{prod} \tag{4}$$

$$f_{C_i,sur} = f_{C_i,ins} - \alpha f_{C_i,gas}^{prod} - \beta f_{C_i,liq}^{prod} \tag{5}$$

- When the i$^{\text{th}}$ component belongs to the monopoly-group,

$$f_{C_i,gas} = \begin{cases} f_{C_i,ins}, \text{ if the product gas flow has monopoly on the i}^{\text{th}} \text{ component} \\ 0, \text{ otherwise} \end{cases} \quad (6)$$

$$f_{C_i,liq} = \begin{cases} f_{C_i,ins}, \text{ if the product liquid flow has monopoly on the i}^{\text{th}} \text{ component} \\ 0, \text{ otherwise} \end{cases} \quad (7)$$

$$f_{C_i,sur} = \begin{cases} f_{C_i,ins}, \text{ if the surplus flow has monopoly on the i}^{\text{th}} \text{ component} \\ 0, \text{ otherwise} \end{cases} \quad (8)$$

where $i = 1,...,n_{tc}$

n_{tc} = number of total components

$f_{C_i,gas}$, $f_{C_i,liq}$, and $f_{C_i,sur}$ = i^{th} component flow rates of the virtual product gas flow, the virtual product liquid flow, and the virtual surplus flow

4.2. Equipment modeling and individual equipment cost allocation

Models describing the relationship between cost and equipment sizing/utility consumption and the corresponding virtual product flows can determine the cost associated with a stream. The procedure is to generate data using detailed, first principles-based models from a simulator and building a model for cost allocation based upon these data. Specifically, this data set results from perturbing the virtual product flow rates for a piece of equipment and determining the unit size/utility consumption based upon this perturbation. The equipment model is a function of the virtual flows:

$$D = D(f_g, f_l, f_s) \quad (9)$$

where D = unit size/utility consumption of a piece of equipment

f_g, f_l, and f_s = virtual product gas flow rate, virtual product liquid flow, and virtual surplus flow rates

We set the virtual surplus flow to its nominal value which is fixed at steady-state because costs are only allocated to the product flows. Therefore, Eq. (9) simplifies to:

$$D = D(f_g, f_l) \tag{10}$$

A Taylor series approximation can describe the equipment model with respect to the virtual flows. The parameters of the equipment model come from the generated data set. We set the order of the equipment model *a priori*, but we must check the validity of the chosen model structure *a posteriori* by computing a statistical coefficient (Filed, 2000; Milton & Arnold, 1995; Montgomery, 1997):

$$R^2 = 1 - \frac{\sum_{i=1}^{n_d} (\tilde{D}_i - \hat{D}_i)^2}{\sum_{i=1}^{n_d} (\tilde{D}_i - \bar{D})^2} \tag{11}$$

where n_d = number of modeling data points

$$\bar{D} = \frac{1}{n_d} \sum_{i=1}^{n_d} \tilde{D}_i$$

$\tilde{D}_i$ and $\hat{D}_i$ = simulation result and estimation result

A suggested condition for the quality of the model is $R^2 \geq 0.9$. If this model validity is not satisfied with a lower model structure, then the model order should be increased. In general, first or second order models can satisfy the model validity for natural gas processes.

If the model returns feasible and realistic results over an interval, we assume the model is valid. The perturbation of the virtual product flows for generating the modeling data set results in variations of the compositions as well as the flow rates. However, the operating conditions and the principal design specifications, *e.g.* the number of trays in a distillation column, of the equipment do not change. Under these circumstances, a model can sometimes be infeasible for a given set of perturbed virtual product flows. For example, in as distillation column, when the component composition and the flow rate of a perturbed inlet stream are too far from their nominal values, the simulator returns an error message and suggests changing some of the design specifications. In this case, we must reduce the model interval to the region in which the model is feasible. We must also ensure that the model identified from the data set describes the original model with a sufficient degree of accuracy over the specified operating region. The model interval is:

$$\begin{aligned} f_g &\in [f_{g,L}, f_{g,0}] \\ f_l &\in [f_{l,L}, f_{l,0}] \end{aligned} \tag{12}$$

where $f_{g,0}$ and $f_{l,0}$ = virtual product gas and liquid flow rates at the nominal point

$$f_{g,L} = (1-\delta) f_{g,0}$$

$$f_{l,L} = (1-\delta) f_{l,0}$$

$$0 < \delta \leq 1$$

$f_{g,L}$ and $f_{l,L}$ are the smallest perturbed virtual product gas and liquid flow rates, respectively, over the feasible model interval. When the model is feasible over the entire model interval, the interval constant, δ is unity. In the case that the model feasibility

cannot be satisfied over the whole model space, δ needs to be decreased until the feasibility is satisfied over the resulting reduced model space. The equipment unit size/utility consumption evaluated from the equipment model over the model interval belongs to the following interval:

$$D \in [D(\underline{f}_L), D(\underline{f}_0)] \tag{13}$$

where $\underline{f}_L = \left(f_{g,L}, f_{l,L}\right)$

$\underline{f}_0 = \left(f_{g,0}, f_{l,0}\right)$

When the variation of the unit size/utility consumption of the equipment exhibits linear behavior with respect to the virtual product flows over the model interval, a first order Taylor series approximation can represent the equipment model (Henson & Seborg, 1997; Kreyszig, 1983; Luyben, 1990; Seborg *et al.*, 1989):

$$D(\underline{f}) \cong D(\underline{f}_0) + \left.\frac{\partial D}{\partial f_g}\right|_{\underline{f}_0} (f_g - f_{g,0}) + \left.\frac{\partial D}{\partial f_l}\right|_{\underline{f}_0} (f_l - f_{l,0}) \tag{14}$$

where $\underline{f} = \left(f_g, f_l\right)$

Eq. (14) can be simplified by the following representation:

$$D(\underline{f}) \cong b_0 + b_1(f_g - f_{g,0}) + b_2(f_l - f_{l,0})_l \tag{15}$$

where $b_0 = D(\underline{f}_0)$, $b_1 = \left.\frac{\partial D}{\partial f_g}\right|_{\underline{f}_0}$, and $b_2 = \left.\frac{\partial D}{\partial f_l}\right|_{\underline{f}_0}$

After estimating the equipment model parameters using a linear regression method with data resulting from equipment simulations, the unit size/utility consumption of the equipment can be represented by the following expression:

$$\hat{D}(\underline{f}) = \hat{b}_0 + \hat{b}_1(f_g - f_{g,0}) + \hat{b}_2(f_l - f_{l,0}) \tag{16}$$

where $\hat{b}_0 = \hat{D}(\underline{f}_0)$, $\hat{b}_1 = \left.\frac{\partial \hat{D}}{\partial f_g}\right|_{\underline{f}_0}$, and $\hat{b}_2 = \left.\frac{\partial \hat{D}}{\partial f_l}\right|_{\underline{f}_0}$

Eq. (16) can be rewritten replace $\hat{b}_0$ by $\hat{D}(\underline{f}_0)$:

$$\hat{D}(\underline{f}) = \hat{D}(\underline{f}_0) + \hat{b}_1(f_g - f_{g,0}) + \hat{b}_2(f_l - f_{l,0}) \tag{17}$$

The unit size/utility consumption of the equipment at the nominal point can be obtained substituting $\underline{f}_L$ into $\underline{f}$ in Eq. (17) and rearranging the resulting representation:

$$\hat{D}(\underline{f}_0) = \hat{D}(\underline{f}_L) + \hat{b}_1(f_{g,0} - f_{g,L}) + \hat{b}_2(f_{l,0} - f_{l,L}) \tag{18}$$

The relationship between the unit size/utility consumption of the equipment and the virtual product flows come from Eq. (18) because the equipment design is based upon the stream flow rates at the nominal point. We note that the gradient terms, $\hat{b}_1$ and $\hat{b}_2$, in the above expression play an important role together with the flow rate of the virtual product flows in the design benefit method. The gradient terms indicate the effect of the gas and liquid products on the unit size/utility consumption of the process equipment. For example, if the influence of the gas product on the pipe diameter is greater than that of the liquid product, then the gradient with respect to the product gas flow is larger than the gradient with respect to the product liquid flow.

We suggest basing the cost allocation for equipment upon variations of the unit size/utility consumption caused by flow rate changes of the virtual products. It is obvious that $\hat{b}_1(f_{g,0} - f_{g,L})$ and $\hat{b}_2(f_{l,0} - f_{l,L})$ in Eq. (18) are exclusively part of the “gas

product contribution" and the "liquid product contribution" (the contributions correspond to the influence of products on the unit size/utility consumption of the process equipment). However, no immediately apparent way exists to assign $\hat{D}(\underline{f}_L)$ from Eq. (18) to the gas product contribution and the liquid product contribution because it is independent of the virtual product flows but highly dependent upon the virtual surplus flow. Considering that the virtual surplus flow can contain some valuable components not assigned to the virtual product gas flow or the virtual product liquid flow and that all valueless components of the inlet streams are lumped into the virtual surplus flow, the gas product contribution and the liquid product contribution should share this common term. To determine the assigned proportion of the virtual surplus flow for the gas product contribution and the liquid product contribution, we introduce a proportional constant, γ. The proportional constant can be chosen in a variety of different ways, one of which is:

$$\gamma = \frac{f_{g,0}}{f_{g,0} + f_{l,0}} \tag{19}$$

The gas product contribution and the liquid product contribution are then:

$$\mathcal{D}_g = \hat{b}_1(f_{g,0} - f_{g,L}) + \gamma \hat{D}(\underline{f}_L) \tag{20}$$

$$\mathcal{D}_l = \hat{b}_2(f_{l,0} - f_{l,L}) + (1-\gamma)\hat{D}(\underline{f}_L) \tag{21}$$

If a first order model does not result in a process description with sufficient accuracy over the investigated operating region, a higher order model is necessary.

When a second order Taylor series approximation is required, the equipment model can be represented by the following expression:

$$\begin{aligned} D(\underline{f}) \cong D(\underline{f}_0) &+ \left.\frac{\partial D}{\partial f_g}\right|_{\underline{f}_0} (f_g - f_{g,0}) + \left.\frac{1}{2!}\frac{\partial^2 D}{\partial f_g^{\,2}}\right|_{\underline{f}_0} (f_g - f_{g,0})^2 + \left.\frac{\partial D}{\partial f_l}\right|_{\underline{f}_0} (f_l - f_{l,0}) \\ &+ \left.\frac{1}{2!}\frac{\partial^2 D}{\partial f_l^2}\right|_{\underline{f}_0} (f_l - f_{l,0})^2 + \left.\frac{2}{2!}\frac{\partial^2 D}{\partial f_g \partial f_l}\right|_{\underline{f}_0} (f_g - f_{g,0})(f_l - f_{l,0}) \end{aligned} \tag{22}$$

Eq. (14) can be simplified by the following representation:

$$\begin{aligned} D(\underline{f}) \cong\ & b_0 + b_1(f_g - f_{g,0}) + b_2(f_g - f_{g,0})^2 + b_3(f_l - f_{l,0}) + b_4(f_l - f_{l,0})^2 \\ & + b_5(f_g - f_{g,0})(f_l - f_{l,0}) \end{aligned} \tag{23}$$

where $b_0 = D(\underline{f}_0)$, $b_1 = \left.\frac{\partial D}{\partial f_g}\right|_{\underline{f}_0}$, $b_2 = \left.\frac{1}{2!}\frac{\partial^2 D}{\partial f_g^{\,2}}\right|_{\underline{f}_0}$, $b_3 = \left.\frac{\partial D}{\partial f_l}\right|_{\underline{f}_0}$, $b_4 = \left.\frac{1}{2!}\frac{\partial^2 D}{\partial f_l^2}\right|_{\underline{f}_0}$,

and $b_5 = \left.\frac{2}{2!}\frac{\partial^2 D}{\partial f_g \partial f_l}\right|_{\underline{f}_0}$

The parameters of this second order model can be also estimated using a linear regression method with data resulting from equipment simulations. Then, the estimated equipment model can be represented by the following expression:

$$\begin{aligned} \hat{D}(\underline{f}) = \hat{b}_0 &+ \hat{b}_1(f_g - f_{g,0}) + \hat{b}_2(f_g - f_{g,0})^2 + \hat{b}_3(f_l - f_{l,0}) + \hat{b}_4(f_l - f_{l,0})^2 \\ &+ \hat{b}_5(f_g - f_{g,0})(f_l - f_{l,0}) \end{aligned} \tag{24}$$

where $\hat{b}_0 = \hat{D}(\underline{f}_0)$, $\hat{b}_1 = \left.\frac{\partial \hat{D}}{\partial f_g}\right|_{\underline{f}_0}$, $\hat{b}_2 = \left.\frac{1}{2}\frac{\partial^2 \hat{D}}{\partial f_g^{\,2}}\right|_{\underline{f}_0}$, $\hat{b}_3 = \left.\frac{\partial \hat{D}}{\partial f_l}\right|_{\underline{f}_0}$, $\hat{b}_4 = \left.\frac{1}{2}\frac{\partial^2 \hat{D}}{\partial f_l^2}\right|_{\underline{f}_0}$,

and $\hat{b}_5 = \left.\frac{\partial^2 \hat{D}}{\partial f_g \partial f_l}\right|_{\underline{f}_0}$

Replace $\hat{b}_0$ with $\hat{D}(\underline{f}_0)$ in Eq. (24),

$$\begin{aligned}\hat{D}(\underline{f}) = \hat{D}(\underline{f}_0) + \hat{b}_1(f_g - f_{g,0}) + \hat{b}_2(f_g - f_{g,0})^2 + \hat{b}_3(f_l - f_{l,0}) + \hat{b}_4(f_l - f_{l,0})^2 \\ + \hat{b}_5(f_g - f_{g,0})(f_l - f_{l,0})\end{aligned} \tag{25}$$

The unit size/utility consumption of the equipment at the nominal point corresponding to the second order model can be obtained substituting $\underline{f}_L$ into $\underline{f}$ in Eq. (26) and rearranging the resulting representation:

$$\begin{aligned}\hat{D}(\underline{f}_0) = \hat{D}(\underline{f}_L) + \hat{b}_1(f_{g,0} - f_{g,L}) - \hat{b}_2(f_{g,0} - f_{g,L})^2 + \hat{b}_3(f_{l,0} - f_{l,L}) - \hat{b}_4(f_{l,0} - f_{l,L})^2 \\ - \hat{b}_5(f_{g,0} - f_{g,L})(f_{l,0} - f_{l,L})\end{aligned} \tag{27}$$

Similarly, the gas product contribution and the liquid product contribution for a second order Taylor series approximation can be obtained from the unit size/utility consumption of the equipment at the nominal point in Eq. (27):

$$\mathcal{D}_g = \hat{b}_1(f_{g,0} - f_{g,L}) - \hat{b}_2(f_{g,0} - f_{g,L})^2 - \frac{1}{2}\hat{b}_5(f_{g,0} - f_{g,L})(f_{l,0} - f_{l,L}) + \gamma\hat{D}(\underline{f}_L) \tag{28}$$

$$\mathcal{D}_l = \hat{b}_3(f_{l,0} - f_{l,L}) - \hat{b}_4(f_{l,0} - f_{l,L})^2 - \frac{1}{2}\hat{b}_5(f_{g,0} - f_{g,L})(f_{l,0} - f_{l,L}) + (1-\gamma)\hat{D}(\underline{f}_L) \tag{29}$$

Unlike the first approximation model, the second order model has a cross term with respect to the virtual product gas flow and the virtual product liquid flow, and the cross term is evenly shared by the gas and liquid products because the last term in the right hand side of Eq. (27) has the following relationship:

$$\begin{aligned}\hat{b}_5(f_{g,0} - f_{g,L})(f_{l,0} - f_{l,L}) = \frac{1}{2}\left.\frac{\partial^2\hat{D}}{\partial f_g \partial f_l}\right|_{\underline{f}_0}(f_{g,0} - f_{g,L})(f_{l,0} - f_{l,L}) \\ + \frac{1}{2}\left.\frac{\partial^2\hat{D}}{\partial f_l \partial f_g}\right|_{\underline{f}_0}(f_{l,0} - f_{l,L})(f_{g,0} - f_{g,L})\end{aligned} \tag{30}$$

When complex expressions represent the unit size/utility consumption of process equipment, it is also possible to use higher order models. In general, however, first or second order models appear to contain sufficient accuracy for the processes under study. This accuracy results from determining if $R^2 \geq 0.9$ can be satisfied.

4.3. Overall cost allocation

We base the cost of the gas and the liquid products upon the gas and liquid product contributions (how much the contribute to or benefit from the design):

$$\mathcal{D}^k = \mathcal{D}_g^k + \mathcal{D}_l^k \tag{31}$$

where $\mathcal{D}_g^k$ = gas product contribution of the k^{th} equipment

$\mathcal{D}_l^k$ = liquid product contribution of the k^{th} equipment

Then, the individual equipment cost allocation to the gas product and the liquid product becomes:

$$\mathcal{A}_g^k = \frac{\mathcal{D}_g^k}{\mathcal{D}_g^k + \mathcal{D}_l^k} \tag{32}$$

$$\mathcal{A}_l^k = \frac{\mathcal{D}_l^k}{\mathcal{D}_g^k + \mathcal{D}_l^k} \tag{33}$$

where $\mathcal{A}_g^k$ = cost allocation of the k^{th} equipment to the gas product

$\mathcal{A}_l^k$ = cost allocation of the k^{th} equipment to the liquid product

From the individual cost allocation results obtained for each individual piece of equipment, the overall cost allocation to the gas product and the liquid product are:

$$\mathcal{A}_g^{tot} = \frac{\sum_{k=1}^{n_s} \mathcal{A}_g^k C^k}{\sum_{k=1}^{n_s} C^k} \tag{34}$$

$$\mathcal{A}_l^{tot} = \frac{\sum_{k=1}^{n_s} \mathcal{A}_l^k C^k}{\sum_{k=1}^{n_s} C^k} \tag{35}$$

where n_s = number of cost allocation segments of the capital/operating cost

C^k = capital/operating cost of the k^{th} equipment

$\mathcal{A}_g^{tot}$ = overall cost allocation to the gas product for the capital/operating cost

$\mathcal{A}_l^{tot}$ = overall cost allocation to the liquid product for the capital/operating cost

Because we allocate the cost on an unit-by-unit basis, it is possible to split the computation of the cost into several smaller subsets. Additionally, the design benefit method can allocate the capital and the operating costs independently to the gas and the liquid products, which is impossible using the traditional cost allocation methods. Also, for processes in which one product has exclusive use of a unit (*e.g*. a compressor for the gas product), the other product(s) would usually share costs associated with this equipment when using traditional cost allocation methods. However, the design benefit method provides a more appropriate allocation of the cost to the individual products.

5. GENETIC-QUADRATIC SEARCH ALGORITHM

The GQSA can solve optimization problems that are coupled with flowsheet simulations. This class of programs requires extensive function evaluations as well as discontinuity and non-convexity. The quadratic search of the GQSA reduces the required number of objective function evaluations when applied to optimization problems whose objective function evaluations require long computation time. A major advantage of the quadratic search is that it can reach a desired optimum for a quadratic objective function in one iteration, resulting in a significant reduction in computation time. Fig. 3 shows the pseudo-code of the GQSA. Because the GQSA has a very simple structure consisting of a general genetic algorithm and a quadratic search, any genetic algorithm can incorporate the quadratic search without loosing its characteristic behavior.

Another unique feature of the GQSA is employment of the 'hyper-cube' initialization, which produces a uniformly distributed initial population with a sufficient level of population diversity to improve the performance of the GQSA.

5.1. Genetic algorithm-based search

The genetic algorithm-based search of the GQSA mainly follows the general structure of genetic algorithms described by Gen and Cheng (1997). However, some variations are applied to a general genetic algorithm to maintain population diversity for each generation.

```
START
generate initial population;
k=0;
repeat
    k=k+1;
    i=0;
    repeat
        i=i+1;
        choose genetic operator at random;
        if (mutation selected); perform mutation;
        if (crossover selected); perform crossover; i=i+1;
        if (random selected); perform random;
        if (i = population size-1); perform mutation;
    until (i < population size)
    quadratic search
    update the optimal point;
    select individuals for the next population;
until (k < desired number of generations)
print the optimal point;
END
```

Fig. 3. Pseudo-code of the GQSA.

The hyper-cube initialization method generates an initial population . The application of genetic algorithms to constrained optimization problems requires a constraint handling technique. Recently developed techniques are: rejecting, repairing, modifying genetic operators, and penalizing strategies (Gen & Cheng, 1997). Basically, the GQSA can employ any strategy, its selection depends upon the type of constraints, such as linear, non-linear, discontinuous, *etc*., and the choice of a sub-optimization technique, such as quadratic programming (QP) and successive quadratic programming (SQP).

Then, offspring are created by genetic operators, mutation, crossover (a variation), and a "random" factor introduced to improve population diversity by incorporating a variation of a typical individual selection method for the next generation. The majority of offspring come from a crossover operator while others are generated by either mutation or a random operator. The created offspring are stored in a temporary population pool with their parents. In addition to offspring generation by the genetic operators, the quadratic search creates one more offspring and adds it to the temporary population pool as long as the quadratic search is successful.

Most individuals of the next generation are selected from the pool by the roulette wheel method. Hanagandi and Nikolaou (1998) have provided a very good description and pseudo-code for this method. Using the roulette wheel method, more fit individuals are more likely retained in the next generation and are more likely to pass on their genes to the next generation of offspring. In addition to this random element, the algorithm uses the best individual and also passes it on to the next generation. Also, another

variation, that randomly selects a few individuals to survive the next generation without taking fitness into account, is applied to the selection procedure to maintain population diversity. Although their role is important for the creation of diverse individuals, offspring created by random elements likely have lower fitness and probably cannot be selected as a member for the next generation because of elitism. Individuals having lower fitness may have a greater possibility to be selected for the next generation when using this random selecting method rather than the roulette wheel method.

After completing a specific number of generations, the optimal point of the last generation is the solution of the problem.

5.1.1. Representation of the individuals

A string of binary numbers called a chromosome represent the individuals . The chromosome consists of genes that are a piece of the string. Each gene corresponds to each system variable so that the chromosome can denote the system vector. Because a set of discrete values represents the system variables, the representation accuracy depends upon the string size of the genes.

5.1.2. Genetic operators

The most commonly used genetic operators are crossover and mutation (Reeves, 1994). While crossover improves the average quality of the population, mutation diversifies a population and ensures coverage of a large area of the variable space (Peña

& Larrañaga, 1999). In addition to the common operators, a random operator also can maintain diversity in each generation. The genetic operator is chosen randomly on the basis of offspring creation probabilities assigned to crossover, mutation, and random during each execution of the loop for generating offspring.

Crossover and mutation require selection of parent/parents to create offspring while random can generate offspring without a parent. Parent/parents for crossover and mutation are selected by the roulette wheel method using its/their fitness corresponding to fitness function values. Individuals having higher fitness are more likely to be chosen than those with lower objective function values. The crossover used in this research is a variation of typical ones, because parents are sometimes randomly selected with a very small possibility of maintaining population diversity by mating parents whose solution vectors are not similar to each other.

Through crossover, two parents are selected, and then two offspring are produced by swapping a randomly selected string block of both parents. Mutation creates an offspring by changing each binary bit within a randomly selected string block of the parent chosen by the roulette wheel method.

When an offspring is created by a genetic operation that is identical to an individual of its parent population, the product is discarded, and the operation is repeated until the offspring is different from any member in the parent population. This technique is used within the tabu search and has been adopted for this algorithm because it produces more diverse offspring. Because the implemented algorithm allows passing on

some individuals from one generation to another, it is not necessary to generate even more individuals with the same genes.

5.1.3. Calculation of fitness

A variety of different techniques for calculating the fitness of individuals exists. The choice of a technique affects the selection of the parent(s) for a genetic operator. Gen and Cheng (1997) review several fitness calculation methods.

In this research, we introduce a hybrid method composed of the normalization and the ranking methods. The fitness results from mixing the fitness of two methods described below using a proportional constant. The fitness of an individual in the normalization method is:

$$\overline{f}_k^n = \frac{f_{\max} - f_k}{f_{\max} - f_{\min}} \tag{36}$$

where $\overline{f}_k^n \in [0,1]$

$f_{\max}$ and $f_{\min}$ = the maximum and the minimum function values, respectively

The above fitness equation is different from a general one in order to be suitable for minimization problems. The fitness of an individual using the rank method is:

$$\overline{f}_k^r = \frac{r_k}{n_p} \tag{37}$$

where $\overline{f}_k^r \in (0,1]$

r_k = rank in descending order of the individuals

n_p = population size

The ultimate fitness is:

$$\bar{f}_k = \alpha \bar{f}_k^n + (1-\alpha)\bar{f}_k^r \tag{38}$$

where $\alpha \in (0,1)$, resulting in a $\bar{f}_k$ which also belongs to (0,1]

5.2. Quadratic search

The quadratic search can boost the convergence speed of general genetic algorithms. As a loop (generation) for solution search is repeated, the solution of genetic algorithms converge to an optimum, and a cluster around the solution or, sometimes, multiple clusters around other best individuals form. The quadratic search determines a quadratic model using individuals belonging to the cluster around the solution and produces a solution by a sub-optimization based upon the quadratic model.

Fig. 4 shows two clusters formed around the global optimum and a local optimum. In the case of the cluster formed around the global optimum, the quadratic search likely produces a solution that is close to the global optimum. According to the basic assumption of the quadratic search technique, when the size of the cluster is small enough, the space corresponding to the cluster can be estimated by a quadratic model and the solution obtained by the quadratic search should be very close to the optimum of the space.

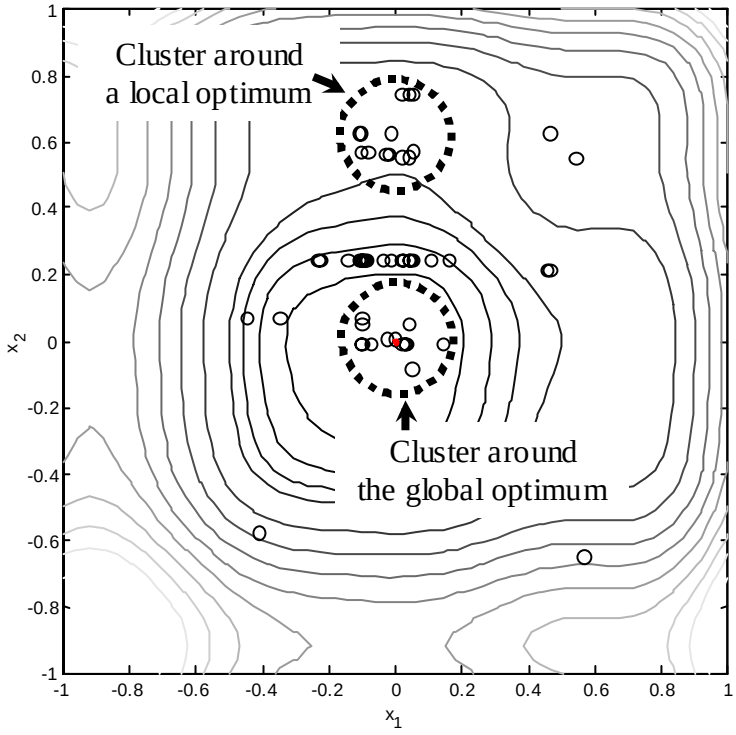


Fig. 4. Example of clusters formed around global and local optima.

The quadratic model can be determined by individuals in either single or multiple past generation(s). When the quadratic model results from individuals from a parent generation, a large population size would be required for high dimensional optimization problems in order to make sure that the number of individuals forming the cluster is large enough to determine the quadratic model. Therefore, in this case, the GQSA would have a larger population size than typical genetic algorithms. On the other hand, when the quadratic model is determined by individuals from a collection of past generations, this option can have advantages in terms of convergence speed as well as population

size. Because individuals created in multiple past generations can be used for determining the quadratic model, the GQSA may not require a large population size. Furthermore, as the cluster is more rapidly formed, faster convergence speed is likely.

The flowchart of the quadratic search is Fig. 5. As shown in the flowchart, the creation of a new individual, which requires a objective function evaluation, is not performed before all criteria are satisfied. Criteria required for the successful quadratic search appear later.

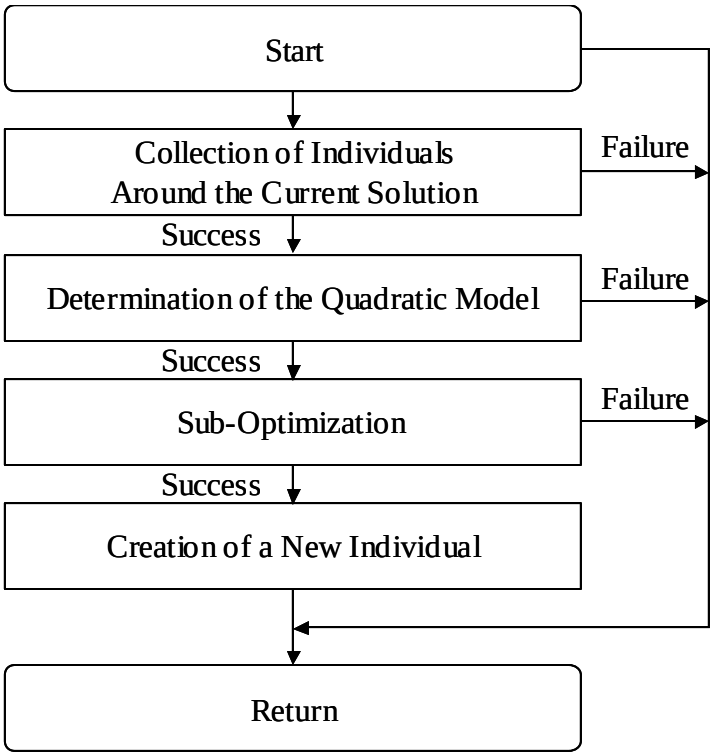


Fig. 5. Flowchart of the quadratic search.

Data required to determine the quadratic model come from the collection of individuals in past generations based upon the distance between the current optimal solution and each individual. The individuals having the shortest distance from the current solution are selected first as data.

The number of data is determined in order to satisfy the "over-determined estimation" for the quadratic model, which means that the required number of data should be more than the number of quadratic model parameters for any dimensional system. The required number of data can be determined by the following relationship:

$$m = \min\left\{ g \in N \middle| g \geq \omega \frac{(n+1)(n+2)}{2} \right\} \tag{39}$$

where m = required number of data

n = dimension of the system

ω = real number that is greater than or equal to unity

After obtaining the required data set, the quadratic model can be represented by the following matrix and vector form:

$$F = XB \tag{40}$$

where $F = \begin{bmatrix} f_1 \\ \vdots \\ f_m \end{bmatrix}$

$$X = \begin{bmatrix} 1 & x_{1,1} & \cdots & x_{n,1} & x_{1,1}x_{2,1} & \cdots & x_{n-1,1}x_{n,1} & x_{1,1}^2 & \cdots & x_{n,1}^2 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 1 & x_{1,m} & \cdots & x_{n,m} & x_{1,m}x_{2,m} & \cdots & x_{n-1,m}x_{n,m} & x_{1,m}^2 & \cdots & x_{n,m}^2 \end{bmatrix}$$

$$B = \begin{bmatrix} b_1 \\ \vdots \\ b_{\frac{(n+1)(n+2)}{2}} \end{bmatrix}$$

The quadratic model can be estimated by the least square method only when $X^T X$ is strictly positive definite and invertible. The condition for the successful estimation is identical with that for the rank of X being equal to n (Lewis & Syrmos, 1995; Ljung, 1999). After estimating the parameter vector, B, the sub-optimization problem can be obtained by the flowing representation:

$$\begin{aligned} &\text{Minimize: } q = \frac{1}{2} x^T H x + f^T x + c \\ &\text{Subject to: } g_i(x) \le 0 \quad i = 1, \ldots, k \\ &\qquad\qquad\quad h_j(x) = 0 \quad j = 1, \ldots, l \end{aligned} \tag{41}$$

where H = symmetric Hessian matrix

f = gradient vector

c = constant

k = number of inequality constraints

l = number of equality constraints

In order to solve the sub-optimization problem, either the QP or the SQP can be chosen based upon the type of optimization problems. The quadratic search can utilize the QP for the application of optimization problems that have only a linear constraint(s) or whose constraints, other than the linear constraints, can be transformed into penalty functions (Rao, 1996). Otherwise, the SQP or another optimization techniques can be

utilized (Edgar *et al.*, 2001; Fletcher, 2000; Nocedal & Wright 1999; Rao, 1996; Venkataraman, 2001).

5.3. Hyper-cube initialization

Many different techniques exist for generating the initial population (Chen, 1995; Nawaz *et al.*, 1983). The random method is the most common one used for genetic algorithms (Reeves, 1994). It involves the creation of random individuals throughout the variable space. The hyper-cube method derives from a tabu search algorithm proposed by Chelouah and Siarry (2001). They use this concept to generate uniformly dispersed initial solutions over the search space for a tabu search algorithm.

The random method randomly assigns 0 or 1 to each digit in the chromosome string. An example of an initial population resulting from the random method appears as Fig. 6. When the population size is very large compared to the dimensionality of the variable space, individuals most likely are well distributed. In the case of a relatively small population size, some parts of the space may be crowded while other parts of the state space contain few or no individuals. However, the populations generated by a random method tend to be very diverse.

For the hyper-cube method, a vector corresponding to each individual has a specific territory in the variable space in the shape of a hyper-cube in the normalized space. During the generation of the initial population, only individuals whose territory does not overlap with that of previously generated individuals are accepted as new members.

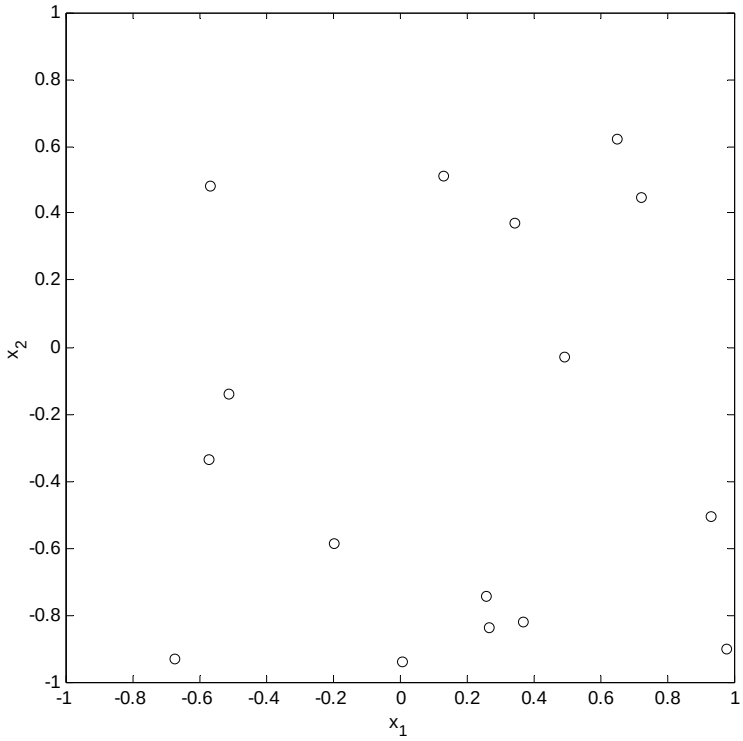


Fig. 6. Initial population resulting from the random method for 16 individuals.

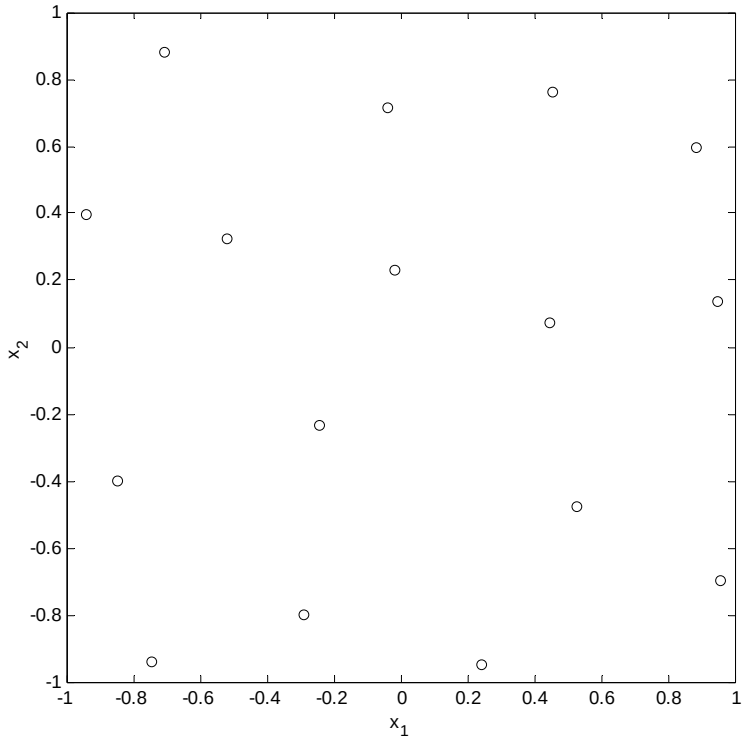


Fig. 7. Initial population resulting from the hyper-cube method for 16 individuals.

The desired side lengths of the hyper-cubes can be obtained using the desired length, d_x, defined in the following relationship:

$$n_p(d_x)^p = \tau_f \tau_c (x_{ub} - x_{lb})^p \tag{42}$$

where d_x = desired length between grid points

p = number of variables

n_p = population size

x_{ub} = upper bound of the normalization

x_{lb} = lower bound of the normalization

τ_f = ratio of the feasible space to the entire variable space

τ_c = "space coverage" by individuals.

In Eq. (42), the left hand side corresponds to the summation of the space occupied by individuals in the initial population and the right hand side corresponds to the space occupied by individuals within the total feasible space. Although the space coverage can theoretically approach a value of unity, high values are not recommended in order to prevent deadlocking of the generation loop. Generally, the higher the dimensionality of the optimization problem, the smaller the space coverage must be to keep the population size at a reasonable level. In the hyper-cube method, the space coverage is a useful tool for controlling the distribution of the initial population.

An example of an initial population resulting from the hyper-cube method is Fig. 7. The hyper-cube method can generate a well-distributed initial population by adjusting the space coverage. At the same time, the hyper-cube method creates the initial population in the same manner as the random method, which can result in as diverse

initial populations as those created by the random method. Therefore, using the hyper-cube method can result in an initial population that is well distributed over the variable space as well as being composed of diverse individuals.

6. APPLICATION

The proposed cost allocation and optimization frameworks are applied to a turbo-expander plant. The turbo-expander plant was developed for the separation of NGL from raw natural gas streams at cryogenic temperatures in order to improve NGL recoveries in 1964. However, its use has evolved over time and the turbo-expander plant is most generally applied to recover NGL due to its efficiency in extracting ethane and propane from natural gas streams (Bullin, 1999).

The turbo-expander process under investigation is Fig. 8. There are two feed streams (S1 and S2) from different suppliers. The feed stream S1 is a lean gas having a higher methane composition (91.5 mol% methane, 7.0 mol% ethane and propane, and 1.5 mol% others), while the feed stream S2 is a rich gas having much higher heavier hydrocarbon compositions (32.0 mol% methane, 64.0 mol% ethane and propane, and 4.0 mol% others). Both streams are first fed to a mixer (MIX1) and the mixed stream (S3) split into two streams (S4 and S5). S4 is bypassed to a mixer (MIX2), whereas S5 is cooled in heat exchanger (B2) by a residue gas stream (S11) from a demethanizer (B6). S4 and S5 are mixed again by the mixer MIX2, and the mixed stream (S7) is chilled to about -13^{o}F by a propane chiller (B4). S7 expands through a turbo-expander (B5) reducing its temperature and pressure to about -105^{o}F and 450psi, respectively, while it is performing shaft work, which is used for residue recompression. Gas and liquid products are separated through a demethanizer (B6) composed of 19 stages and a reboiler. The operating condition of the demethanizer is determined by setting the exit pressure to 290psi and the methane recovery to 99.0 mol%. Its bottom product is sold as

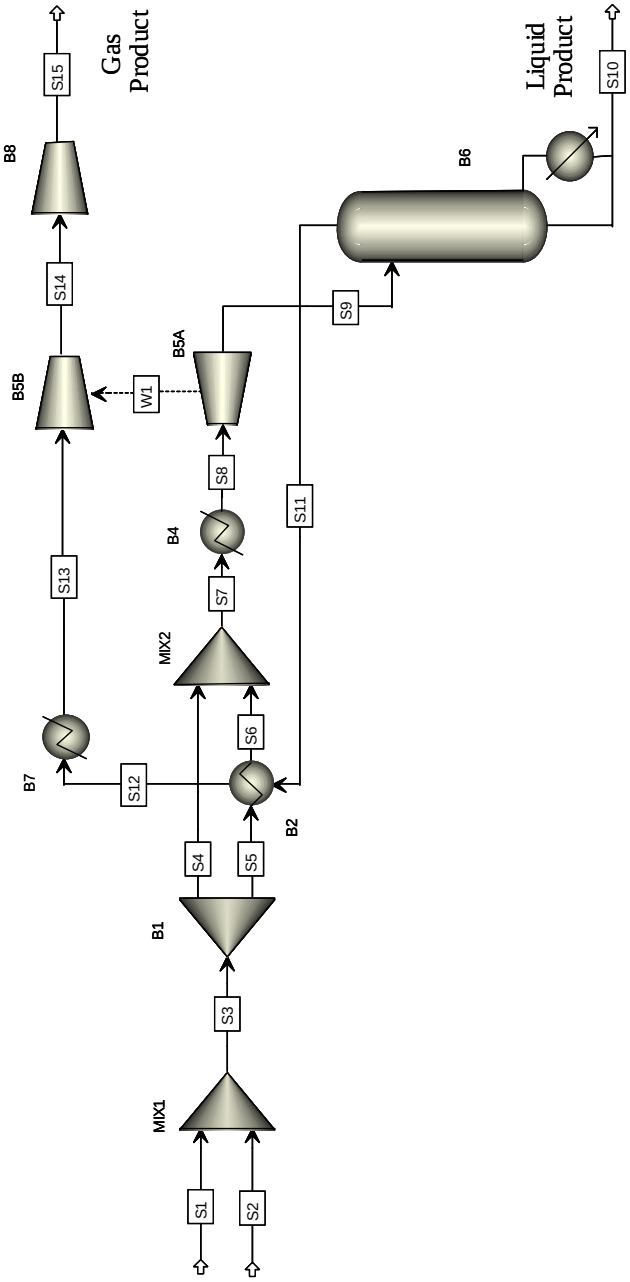


Fig. 8. Turbo-expander plant.

Table 4. Product sharing contract

	Gas Product Allocation	Liquid Product Allocation
Plant	25%	25%
Supplier 1	75%	35%
Supplier 2	0%	40%

a liquid product (NGL) without further processing, while its top product is further processed through a series of heat exchangers, B2 and B7, and compressors, B5 and B8, before becoming the final gas product.

The revenues and costs of this turbo-expander plant are shared under a product sharing contract by three co-producers: a plant owner (Plant), the supplier of the feed stream S1 (Supplier 1), and the supplier of the feed stream S2 (Supplier 2). Table 4 shows the product sharing contract describing the portion of gas and liquid product assigned to each co-producer. According to the sharing contract, capital and operating costs are allocated to the joint products as well as revenues are assigned to these co-producers based upon their proportion of gas and liquid products. An unique characteristics of this contract is that the suppliers not only pay operating costs but also capital costs in form of the depreciation of the plant, which is defined by the following equation:

$$\text{Depreciation}=\frac{\text{Capital Cost}}{\text{Life Span}}(1+\text{Interest Rate})^{\text{Life Span}} \tag{43}$$

This equation is specially introduced in order to evaluate depreciation in a simple manner. For more detail, one can be referred to several text books: El-Halwagi (1997),

Garrett (1989), and Peters and Timmerhaus (1991). In this application, the expected life span is 10 years and the interest rate is 3.3%/year. The Plant's portion of gas and liquid products in Table 4 is the suppliers' payment as natural gas processing fee. Plant invests the entire capital required to build the plant and expects to recover its investment by co-producing natural gas products with the suppliers.

6.1. Cost allocation based upon the DBM

As the DBM requires a lot of computations and flowsheet simulations, its automation becomes a crucial task for the development of the cost allocation framework. Aspen Plus™ and several subroutines for the cost allocation framework written in Matlab™ have been developed to automate the simulation of the process as well as the individual pieces of equipment. Interaction between the software is provided *via* ActiveX™, which is the standard interface for software running on a Microsoft Windows™ platform.

The flowchart and the software configuration of the developed framework are shown in Fig. 9 and Fig. 10, respectively. Virtual flows can be obtained by solving an LP and by using the component distribution function from the previous chapter using the component flow information of all the streams in the plant, which result from the process simulation. Equipment modeling requires simulations of the individual pieces of equipment for the determination of the interval and order of the model for each equipment. The required information of inlet streams to an individual equipment for individual equipment simulations is set by the perturbed virtual flow rates and the

simulation results of the turbo-expander plant under its normal operating condition are x_1 = 0.15, x_2 = 450psi, x_3 = 290psi, and x_4 = -4^{o}F. Costs allocated to gas and liquid products can be evaluated using mathematical information obtained from equipment models.

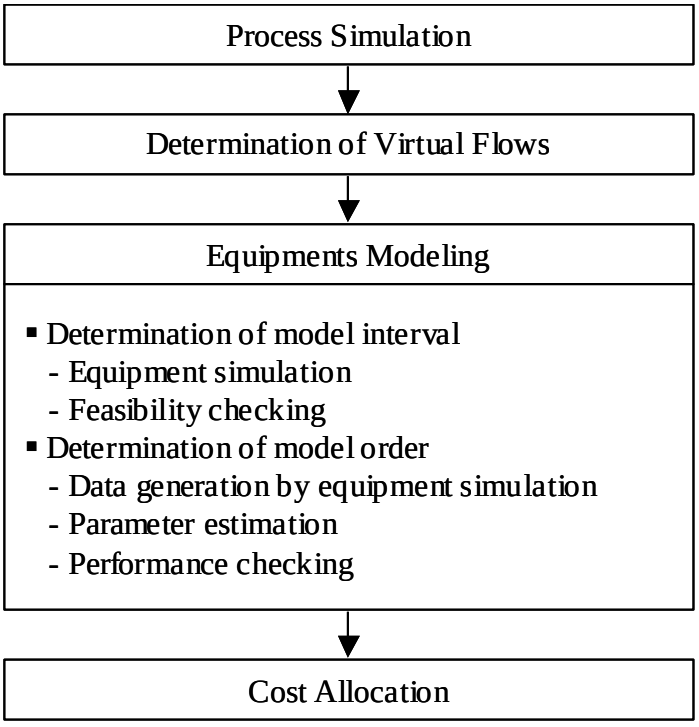


Fig. 9. Flowchart of the cost allocation framework.

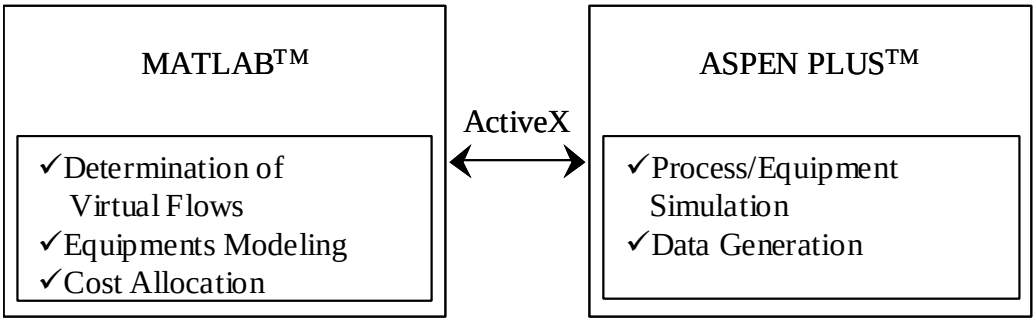


Fig. 10. Software configuration of the cost allocation framework.

6.1.1. Determination of virtual flows

The proposed cost allocation framework requires a lot of physical and chemical information about each equipment, which can be provided by a process simulator. Component flows of each stream are necessary for the determination of virtual flows. Table 5 shows the component flows of each stream and their group classification. Hydrocarbons, such as methane, ethane, and propane belong to the shared-group, whereas valueless components, such as nitrogen and carbon dioxide are in the monopoly-group, and the virtual surplus flow contains all the non-hydrocarbon components. Table 6 shows the optimal values for α and β of each stream. Note that either α or β equals unity for S10 and S11, which are eventually separated product streams. Both α and β are identical for the streams from S3 to S9 because the streams are the mixture of both products. The α and β of S4, S5, and S6 of the streams are also identical but are lower than unity because they are segregated from the mixture of gas and liquid products.

Table 5. Components of the streams

Components	Stream S1 (lbmol/h)	Stream S2 (lbmol/h)	Stream S3 (lbmol/h)	Stream S4 (lbmol/h)	Stream S5 (lbmol/h)	Group Classification
METHANE	6405.00	320.00	6725.00	1008.75	5716.25	Shared
ETHANE	350.00	420.00	770.00	115.50	654.50	Shared
PROPANE	140.00	220.00	360.00	54.00	306.00	Shared
NITROGEN	35.00	20.00	55.00	8.25	46.75	Monopoly
CO2	70.00	20.00	90.00	13.50	76.50	Monopoly
Total	7000.00	1000.00	8000.00	1200.00	6800.00	

Components	Stream S6 (lbmol/h)	Stream S7 (lbmol/h)	Stream S8 (lbmol/h)	Stream S9 (lbmol/h)	Stream S10 (lbmol/h)	Group Classification
METHANE	5716.25	6725.00	6725.00	6725.00	67.25	Shared
ETHANE	654.50	770.00	770.00	770.00	449.59	Shared
PROPANE	306.00	360.00	360.00	360.00	312.55	Shared
NITROGEN	46.75	55.00	55.00	55.00	0.00	Monopoly
CO2	76.50	90.00	90.00	90.00	26.59	Monopoly
Total	6800.00	8000.00	8000.00	8000.00	855.99	

Components	Stream S11 (lbmol/h)	Stream S12 (lbmol/h)	Stream S13 (lbmol/h)	Stream S14 (lbmol/h)	Stream S15 (lbmol/h)	Group Classification
METHANE	6657.75	6657.75	6657.75	6657.75	6657.75	Shared
ETHANE	320.41	320.41	320.41	320.41	320.41	Shared
PROPANE	47.45	47.45	47.45	47.45	47.45	Shared
NITROGEN	55.00	55.00	55.00	55.00	55.00	Monopoly
CO2	63.41	63.41	63.41	63.41	63.41	Monopoly
Total	7144.01	7144.01	7144.01	7144.01	7144.01	

Table 6. Optimal α and β of the streams

Streams	α	β	Classification
S1	0.9611	0.0935	Feed Stream
S2	0.0410	0.6977	Feed Stream
S3	1.0000	1.0000	Mixed Stream
S4	0.1500	0.1500	Mixed Stream
S5	0.8500	0.8500	Mixed Stream
S6	0.8500	0.8500	Mixed Stream
S7	1.0000	1.0000	Mixed Stream
S8	1.0000	1.0000	Mixed Stream
S9	1.0000	1.0000	Mixed Stream
S10	0.0000	1.0000	Liquid Stream
S11	1.0000	0.0000	Gas Stream
S12	1.0000	0.0000	Gas Stream
S13	1.0000	0.0000	Gas Stream
S14	1.0000	0.0000	Gas Stream
S15	1.0000	0.0000	Gas Stream

The determined virtual flows for the streams are shown in from Table 7 to Table 15. While the virtual product flows share hydrocarbon components within the shared-group, the virtual surplus flow consists of only non-profitable components within the monopoly-group. The virtual flows for the streams from S1 to S9 are not determined since no need exists for cost allocation involving the streams from S10 and S15 because they are exclusively utilized by either gas or liquid product.

Table 7. Virtual flows of the stream S1

Components	Stream S1 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	6405.00	6398.70	6.29	0.00	Shared
ETHANE	350.00	307.94	42.06	0.00	Shared
PROPANE	140.00	45.60	29.24	65.16	Shared
NITROGEN	35.00	0.00	0.00	35.00	Monopoly
CO2	70.00	0.00	0.00	70.00	Monopoly
Total	7000.00	6752.24	77.59	170.16	

Table 8. Virtual flows of the stream S2

Components	Stream S2 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	320.00	273.08	46.92	0.00	Shared
ETHANE	420.00	13.14	313.66	93.20	Shared
PROPANE	220.00	1.95	218.05	0.00	Shared
NITROGEN	20.00	0.00	0.00	20.00	Monopoly
CO2	20.00	0.00	0.00	20.00	Monopoly
Total	1000.00	288.17	578.63	133.20	

Table 9. Virtual flows of the stream S3

Components	Stream S3 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	6725.00	6657.80	67.25	0.00	Shared
ETHANE	770.00	320.41	449.59	0.00	Shared
PROPANE	360.00	47.45	312.55	0.00	Shared
NITROGEN	55.00	0.00	0.00	55.00	Monopoly
CO2	90.00	0.00	0.00	90.00	Monopoly
Total	8000.00	7025.66	829.39	145.00	

Table 10. Virtual flows of the stream S4

Components	Stream S4 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	1008.80	998.66	10.09	0.00	Shared
ETHANE	115.50	48.06	67.44	0.00	Shared
PROPANE	54.00	7.12	46.88	0.00	Shared
NITROGEN	8.25	0.00	0.00	8.25	Monopoly
CO2	13.50	0.00	0.00	13.50	Monopoly
Total	1200.05	1053.84	124.41	21.75	

Table 11. Virtual flows of the stream S5

Components	Stream S5 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	5716.30	5659.10	57.16	0.00	Shared
ETHANE	654.50	272.35	382.15	0.00	Shared
PROPANE	306.00	40.33	265.67	0.00	Shared
NITROGEN	46.75	0.00	0.00	46.75	Monopoly
CO2	76.50	0.00	0.00	76.50	Monopoly
Total	6800.05	5971.78	704.98	123.25	

Table 12. Virtual flows of the stream S6

Components	Stream S6 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	5716.30	5659.10	57.16	0.00	Shared
ETHANE	654.50	272.35	382.15	0.00	Shared
PROPANE	306.00	40.33	265.67	0.00	Shared
NITROGEN	46.75	0.00	0.00	46.75	Monopoly
CO2	76.50	0.00	0.00	76.50	Monopoly
Total	6800.05	5971.78	704.98	123.25	

Table 13. Virtual flows of the stream S7

Components	Stream S7 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	6725.00	6657.80	67.25	0.00	Shared
ETHANE	770.00	320.41	449.59	0.00	Shared
PROPANE	360.00	47.45	312.55	0.00	Shared
NITROGEN	55.00	0.00	0.00	55.00	Monopoly
CO2	90.00	0.00	0.00	90.00	Monopoly
Total	8000.00	7025.66	829.39	145.00	

Table 14. Virtual flows of the stream S8

Components	Stream S8 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	6725.00	6657.80	67.25	0.00	Shared
ETHANE	770.00	320.41	449.59	0.00	Shared
PROPANE	360.00	47.45	312.55	0.00	Shared
NITROGEN	55.00	0.00	0.00	55.00	Monopoly
CO2	90.00	0.00	0.00	90.00	Monopoly
Total	8000.00	7025.66	829.39	145.00	

Table 15. Virtual flows of the stream S9

Components	Stream S9 (lbmol/h)	Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Group Classification
METHANE	6725.00	6657.80	67.25	0.00	Shared
ETHANE	770.00	320.41	449.59	0.00	Shared
PROPANE	360.00	47.45	312.55	0.00	Shared
NITROGEN	55.00	0.00	0.00	55.00	Monopoly
CO2	90.00	0.00	0.00	90.00	Monopoly
Total	8000.00	7025.66	829.39	145.00	

6.1.2. Determination of equipment models

Data for modeling are obtained from the simulation of individual equipments using the process simulator, Aspen Plus™. The simulation of individual equipments is performed in the flowsheet composed of several segments of the turbo expander plant: pipelines, heat exchanger, chiller, expander, and demethanizer.

Fig. 11 shows a segment for the simulation of pipelines. The segment is simulated setting perturbed virtual flow rates to its inlet streams: SL1 is a node for the virtual product gas flow, SL2 is a node for the virtual product liquid flow, and SL3 is a node for the surplus flow. The operating condition of the segment, such as pressure and temperature, is set by that of the corresponding pipeline.

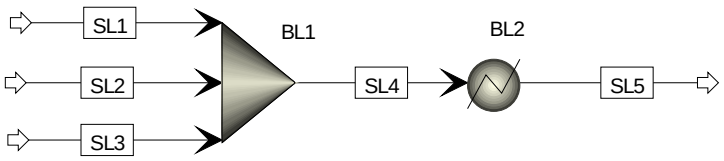


Fig. 11. Segment for the simulation of pipelines.

Table 16. Data used to determine the model of the pipeline S1 and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Pipe ID (in)	Estimated Pipe ID (in)
0.00	0.00	170.16	0.84	0.89
0.00	25.86	170.16	0.86	0.91
0.00	51.72	170.16	0.89	0.93
0.00	77.59	170.16	0.91	0.96
2,250.80	0.00	170.16	3.11	2.96
2,250.80	25.86	170.16	3.12	2.98
2,250.80	51.72	170.16	3.14	3.00
2,250.80	77.59	170.16	3.15	3.01
4,501.50	0.00	170.16	4.17	4.31
4,501.50	25.86	170.16	4.18	4.32
4,501.50	51.72	170.16	4.18	4.33
4,501.50	77.59	170.16	4.19	4.34
6,752.30	0.00	170.16	4.97	4.92
6,752.30	25.86	170.16	4.97	4.93
6,752.30	51.72	170.16	4.98	4.93
6,752.30	77.59	170.16	4.99	4.94

After the segment simulation is completed, physical properties required to evaluate the diameter of a pipeline are provided by the process simulator. The diameter of pipelines is calculated using the equation for the optimum economic pipe diameter provided by Peters and Timmerhaus (1991). When calculating the diameter of pipelines, we assume that their lengths are all 100 ft. Table 16 shows data used to determine the model of the pipeline S1 and its estimates. The model information as well as performance index can be found in Table 23.

It is important to note that to perform cost allocation it is required that the equipment model for the unit sizing/utility consumption depend upon changes in throughput since the unit size/utility consumption of equipments is a key parameter to estimate its unit/utility cost. For the pipelines, the diameter is the key parameter to estimate their unit cost.

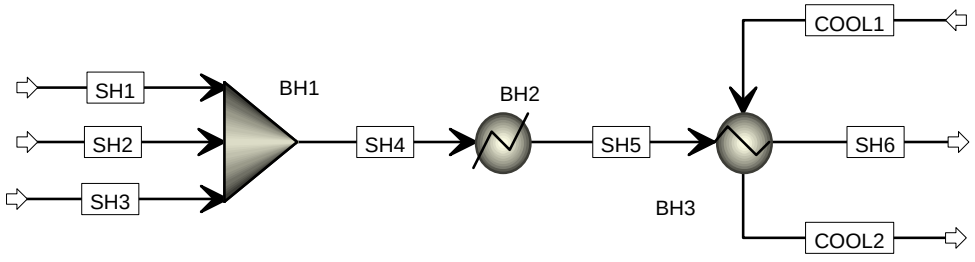


Fig. 12. Segment for the simulation of a heat exchanger.

Table 17. Data used to determine the model of the heat exchanger B2 and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Exc. Area (ft2)	Estimated Exc. Area (ft2)
0.00	0.00	123.25	0.00	38.02
0.00	234.99	123.25	0.00	-18.94
0.00	469.99	123.25	0.00	-32.83
0.00	704.98	123.25	0.00	-3.65
1,990.60	0.00	123.25	712.89	694.58
1,990.60	234.99	123.25	560.54	579.87
1,990.60	469.99	123.25	488.84	508.23
1,990.60	704.98	123.25	447.86	479.66
3,981.20	0.00	123.25	1,472.80	1,431.90
3,981.20	234.99	123.25	1,264.00	1,259.40
3,981.20	469.99	123.25	1,134.40	1,130.00
3,981.20	704.98	123.25	1,046.10	1,043.70
5,971.80	0.00	123.25	2,234.50	2,249.90
5,971.80	234.99	123.25	1,998.20	2,019.70
5,971.80	469.99	123.25	1,832.10	1,832.60
5,971.80	704.98	123.25	1,708.50	1,688.50

A segment for the simulation of a heat exchanger is shown in Fig. 12. The inlet streams and the operating condition of this segment can be set in the same manner as the segment for the pipelines. However, this segment needs an additional setting for its coolant stream. Since it is a residue gas stream from the demethanizer, the component compositions, temperature, and pressure of the coolant COOL1 can be set by those of the residue gas stream S11. The temperature approach between the cold outlet stream COOL2 and the hot inlet stream SH5 is used as a required design specification and is set to a value of 10^{o}F. Its exchange area corresponding to the perturbed virtual flow rates is automatically evaluated following a simple design method implemented on the simulator. The exchange area is the key parameter to estimate the unit cost of a heat exchanger. Table 17 shows data used to determine the model of the heat exchanger B2 and its estimates.

Fig. 13 shows a segment for the simulation of a chiller. Its chilling source is propane at a temperature of -35^{o}F and a pressure of 300psi. The design specification of the chiller is the increase of the chilling source temperature through the chiller, which is set by a value of 5^{o}F. The role of the chiller is to reduce the temperature of its hot stream to -4^{o}F under the normal operating condition. This segment can be used for both unit size and utility consumption modeling. Its exchange area and required chilling duties correspond to perturbed virtual flow rates and are also automatically obtained from the simulator. The exchange area and the chilling duty are key parameters to its unit and utility costs, respectively. Data used to determine the model of the heat exchanger B2 and its chilling duty appear in Table 18 and Table 19, respectively.

Fig. 14 shows a segment for the simulation of a turbo-expander. The turbo-expander generates shaft work and reduces the temperature of the stream by expanding it to a pressure of 450psi. The key parameter estimating the unit cost of a turbo-expander is its shaft work. Table 20 shows data used to determine the model of the expander B5 and its estimates.

A segment for the simulation of a demethanizer appears in Fig. 15. The design specification and the operating condition of this segment are the same as those of the demethanizer in Fig. 8. This segment can be also used for both unit size and utility consumption modeling. Its column diameters and reboiler duties correspond to perturbed virtual flow rates and are automatically obtained from the simulator. The column diameter and reboiler duty are key parameters to their unit and utility costs, respectively. Data used to determine the model of the demethanizer B6 and its reboiler duty appear in Table 21 and Table 22, respectively.

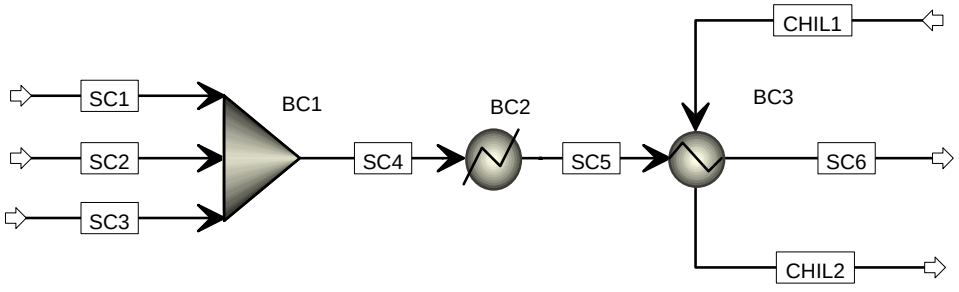


Fig. 13. Segment for the simulation of a chiller.

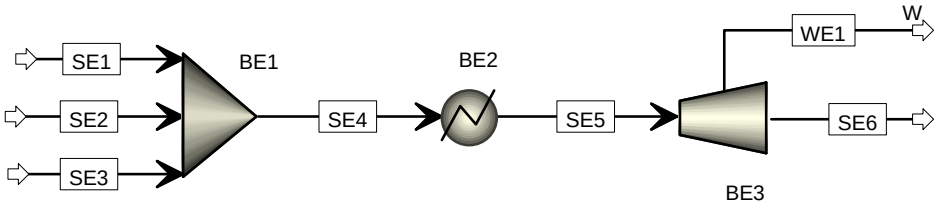


Fig. 14. Segment for the simulation of a turbo-expander.

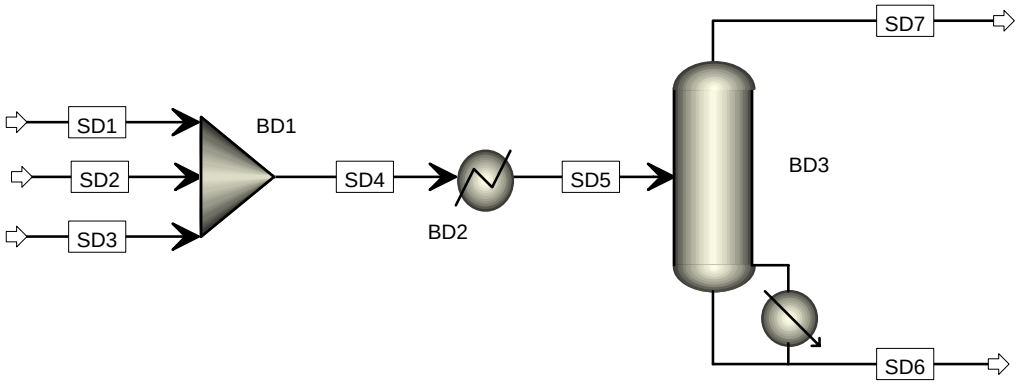


Fig. 15. Segment for the simulation of a demethanizer.

Table 18. Data used to determine the model of the chiller B4 and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Exc. Area (ft2)	Estimated Exc. Area (ft2)
0.00	0.00	145.00	5.09	-2.28
0.00	276.46	145.00	9.21	6.82
0.00	552.93	145.00	14.83	18.47
0.00	829.39	145.00	20.59	32.67
2,341.90	0.00	145.00	37.95	46.17
2,341.90	276.46	145.00	57.44	59.41
2,341.90	552.93	145.00	89.26	75.19
2,341.90	829.39	145.00	107.50	93.51
4,683.70	0.00	145.00	73.36	80.21
4,683.70	276.46	145.00	90.09	97.57
4,683.70	552.93	145.00	112.28	117.48
4,683.70	829.39	145.00	141.60	139.93
7,025.60	0.00	145.00	108.77	99.82
7,025.60	276.46	145.00	124.62	121.31
7,025.60	552.93	145.00	143.88	145.35
7,025.60	829.39	145.00	167.10	171.93

Table 19. Data used to determine the model of the chiller (B4) duty and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Chiller Duty (MMBtu)	Estimated Chiller Duty (MMBtu)
0.00	0.00	145.00	0.02	-0.01
0.00	276.46	145.00	0.04	0.03
0.00	552.93	145.00	0.06	0.07
0.00	829.39	145.00	0.08	0.13
2,341.90	0.00	145.00	0.15	0.18
2,341.90	276.46	145.00	0.23	0.24
2,341.90	552.93	145.00	0.36	0.30
2,341.90	829.39	145.00	0.43	0.37
4,683.70	0.00	145.00	0.29	0.32
4,683.70	276.46	145.00	0.36	0.39
4,683.70	552.93	145.00	0.45	0.47
4,683.70	829.39	145.00	0.56	0.56
7,025.60	0.00	145.00	0.43	0.40
7,025.60	276.46	145.00	0.50	0.48
7,025.60	552.93	145.00	0.57	0.58
7,025.60	829.39	145.00	0.67	0.68

Table 20. Data used to determine the model of the expander B5 and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Brake hp (hp)	Estimated Brake hp (hp)
0.00	0.00	145.00	16.72	19.44
0.00	276.46	145.00	22.26	26.91
0.00	552.93	145.00	30.39	29.79
0.00	829.39	145.00	39.96	28.06
2,341.90	0.00	145.00	353.89	350.75
2,341.90	276.46	145.00	364.86	360.04
2,341.90	552.93	145.00	362.10	364.73
2,341.90	829.39	145.00	344.12	364.83
4,683.70	0.00	145.00	688.34	685.92
4,683.70	276.46	145.00	699.53	697.03
4,683.70	552.93	145.00	709.01	703.55
4,683.70	829.39	145.00	710.45	705.46
7,025.60	0.00	145.00	1,022.80	1,025.00
7,025.60	276.46	145.00	1,033.20	1,037.90
7,025.60	552.93	145.00	1,044.80	1,046.20
7,025.60	829.39	145.00	1,053.10	1,050.00

Table 21. Data used to determine the model of the demethanizer B6 and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Column ID (ft)	Estimated Column ID (ft)
2,107.70	248.82	145.00	3.48	3.53
2,107.70	442.34	145.00	5.09	5.05
2,107.70	635.87	145.00	6.65	6.62
2,107.70	829.39	145.00	8.19	8.22
3,747.00	248.82	145.00	3.48	3.49
3,747.00	442.34	145.00	4.91	4.88
3,747.00	635.87	145.00	6.33	6.31
3,747.00	829.39	145.00	7.76	7.77
5,386.30	248.82	145.00	3.64	3.57
5,386.30	442.34	145.00	4.69	4.82
5,386.30	635.87	145.00	6.13	6.11
5,386.30	829.39	145.00	7.43	7.43
7,025.60	248.82	145.00	3.78	3.76
7,025.60	442.34	145.00	4.82	4.87
7,025.60	635.87	145.00	6.06	6.03
7,025.60	829.39	145.00	7.22	7.21

Table 22. Data used to determine the model of the reboiler (B6) duty and its estimates

Virtual Product Gas Flow (lbmol/h)	Virtual Product Liquid Flow (lbmol/h)	Surplus Flow (lbmol/h)	Observed Reboiler Duty (MMBtu)	Estimated Reboiler Duty (MMBtu)
2,107.70	248.82	145.00	1.29	1.28
2,107.70	442.34	145.00	2.21	2.22
2,107.70	635.87	145.00	3.12	3.14
2,107.70	829.39	145.00	4.02	4.03
3,747.00	248.82	145.00	1.19	1.22
3,747.00	442.34	145.00	2.27	2.21
3,747.00	635.87	145.00	3.17	3.17
3,747.00	829.39	145.00	4.13	4.11
5,386.30	248.82	145.00	1.17	1.16
5,386.30	442.34	145.00	2.11	2.20
5,386.30	635.87	145.00	3.26	3.20
5,386.30	829.39	145.00	4.16	4.19
7,025.60	248.82	145.00	1.16	1.11
7,025.60	442.34	145.00	2.08	2.19
7,025.60	635.87	145.00	3.34	3.24
7,025.60	829.39	145.00	4.23	4.26

Table 23. Model information and performance indices for equipment

Equipments	Model Order	δ	R^2
Pipeline S1	Second	1.00	0.9953
Pipeline S2	Second	1.00	0.9838
Pipeline S3	Second	1.00	0.9960
Pipeline S4	Second	1.00	0.9960
Pipeline S5	Second	1.00	0.9960
Pipeline S6	Second	1.00	0.9935
Pipeline S7	Second	1.00	0.9940
Pipeline S8	Second	1.00	0.9936
Pipeline S9	Second	1.00	0.9960
Pipeline S10	-	-	-
Pipeline S11	-	-	-
Pipeline S12	-	-	-
Pipeline S13	-	-	-
Pipeline S14	-	-	-
Pipeline S15	-	-	-
Heat Exc. B2	Second	1.00	0.9991
Chiller B4	Second	1.00	0.9772
Expander B5	Second	1.00	0.9997
Column B6	Second	0.70	0.9991
Heat Exc. B7	-	-	-
Compressor B8	-	-	-

Table 24. Model information and performance indices for utilities

Utilities	Model Order	δ	R^2
Chiller (B4) Duty	Second	1.00	0.9774
Reboiler (B6) Duty	Second	0.70	0.9978
Heater (B7) Duty	-	-	-
Brake (B8) hp	-	-	-

Information about the equipments and utilities model, such as the interval over which the model is valid, the order of the model, and the accuracy of the model for the individual pieces of equipment and utilities, is shown in Table 23 and Table 24, respectively. It needs to be noted that equipments and utilities exclusively utilized by either gas or liquid product do not need cost allocation and their models are not required. We find that a second order model results in a good representation of the system behavior for the process under investigation. The model intervals for the demethanizer and reboiler are finite because both the column and reboiler models become infeasible for the region where δ is greater than 0.7. The model performance indices shown in Table 23 and Table 24 indicate that each model is sufficiently accurate.

6.1.3. Evaluation of cost allocations

Gas product and liquid product contributions to the unit sizes and utility consumptions of equipment is represented in Table 25 and Table 26, respectively. Cost

Table 25. Contribution of gas and liquid products to unit sizes

Equipments	Units	Size	Gas Product Contribution	Liquid Product Contribution
Pipeline S1	in	4.99	4.94	0.05
Pipeline S2	in	1.74	0.72	1.02
Pipeline S3	in	5.15	4.69	0.46
Pipeline S4	in	2.20	2.00	0.20
Pipeline S5	in	4.79	4.36	0.43
Pipeline S6	in	4.24	3.96	0.28
Pipeline S7	in	4.66	4.33	0.32
Pipeline S8	in	4.60	4.30	0.31
Pipeline S9	in	6.18	5.85	0.33
Pipeline S10	in	1.54	0.00	1.54
Pipeline S11	in	7.35	7.35	0.00
Pipeline S12	in	8.10	8.10	0.00
Pipeline S13	in	8.32	8.32	0.00
Pipeline S14	in	7.95	7.95	0.00
Pipeline S15	in	7.09	7.09	0.00
Heat Exc. B2	ft2	1,708.52	1,708.52	0.00
Chiller B4	ft2	167.10	115.32	51.79
Expander B5	hp	1,053.11	1,034.15	18.96
Column B6	ft	7.22	2.77	4.45
Heat Exc. B7	ft2	89.84	89.84	0.00
Compressor B8	hp	2,945.96	2,945.96	0.00

Table 26. Contribution of gas and liquid products to utility consumption

Utilities	Units	Consumption	Gas Product Contribution	Liquid Product Contribution
Chiller (B4) Duty	MMBtu/h	0.67	0.46	0.21
Reboiler (B6) Duty	MMBtu/h	4.23	1.16	3.06
Heater (B7) Duty	MMBtu/h	2.31	2.31	0.00
Brake (B8) hp	hp	2,945.96	2,945.96	0.00

allocation results for the total capital and operating costs as well as for the individual equipment costs are shown in Table 27 and Table 28, respectively. The total capital and operating cost allocation result from individual equipment and utility cost allocations to the gas and liquid products, respectively. The equipment and utility costs shown in Table 27 and Table 28 are estimated from the equipment and utility cost information found in Peters and Timmerhaus (1991). The resulting total capital cost allocation to the gas and liquid products are 93.28% and 6.72%, respectively. Also, the resulting operating cost allocated to the gas and liquid products are 93.80% and 6.20%, respectively.

This cost allocation result indicates that both the capital and operating costs are dominated by the gas product. That is because only the gas product is further processed through the heat exchanger B7 and the compressor B8, which is the most expensive equipment and whose utility cost is the majority of the total operating cost. Furthermore, the cost of the turbo-expander B5, which is the second most expensive equipment, is also mostly allocated to the gas product. The combined cost of the compressor and the

Table 27. Cost allocation results for the capital cost

Equipments	Equipment Costs ($)	Cost Alloc. to Gas Prod.	Cost Alloc. to Liquid Prod.	Alloc. Costs to Gas Prod. ($)	Alloc. Costs to Liquid Prod. ($)
Pipeline S1	205	0.9899	0.0101	203	2
Pipeline S2	90	0.4120	0.5880	37	53
Pipeline S3	211	0.9101	0.0899	192	19
Pipeline S4	106	0.9103	0.0897	97	10
Pipeline S5	198	0.9101	0.0899	180	18
Pipeline S6	179	0.9343	0.0657	167	12
Pipeline S7	193	0.9304	0.0696	180	13
Pipeline S8	192	0.9332	0.0668	179	13
Pipeline S9	248	0.9460	0.0540	234	13
Pipeline S10	83	0.0000	1.0000	0	83
Pipeline S11	289	1.0000	0.0000	289	0
Pipeline S12	316	1.0000	0.0000	316	0
Pipeline S13	324	1.0000	0.0000	324	0
Pipeline S14	310	1.0000	0.0000	310	0
Pipeline S15	280	1.0000	0.0000	280	0
Heat Exc. B2	17,085	1.0000	0.0000	17,085	0
Chiller B4	1,671	0.6901	0.3099	1,153	518
Expander B5	382,901	0.9820	0.0180	376,008	6,892
Column B6	150,523	0.3838	0.6162	57,771	92,752
Heat Exc. B7	898	1.0000	0.0000	898	0
Compressor B8	938,492	1.0000	0.0000	938,492	0
Total	1,494,793	0.9328	0.0672	1,394,396	100,397

Table 28. Cost allocation results for the operating cost

Utilities	Utility Costs ($/h)	Cost Alloc. to Gas Prod.	Cost Alloc. to Liquid Prod.	Alloc. Costs to Gas Prod. ($/h)	Alloc. Costs to Liquid Prod. ($/h)
Chiller (B4) Duty	4.66	0.6903	0.3097	3.21	1.44
Reboiler (B6) Duty	4.23	0.2754	0.7246	1.16	3.06
Heater (B7) Duty	2.31	1.0000	0.0000	2.31	0.00
Brake (B8) hp	61.45	1.0000	0.0000	61.45	0.00
Total	72.64	0.9380	0.0620	68.14	4.51

Table 29. Cost allocation results for the capital cost of common processes

Equipments	Equipment Costs ($)	Cost Alloc. to Gas Prod.	Cost Alloc. to Liquid Prod.	Alloc. Costs to Gas Prod. ($)	Alloc. Costs to Liquid Prod. ($)
Pipeline S1	205	0.9899	0.0101	203	2
Pipeline S2	90	0.4120	0.5880	37	53
Pipeline S3	211	0.9101	0.0899	192	19
Pipeline S4	106	0.9103	0.0897	97	10
Pipeline S5	198	0.9101	0.0899	180	18
Pipeline S6	179	0.9343	0.0657	167	12
Pipeline S7	193	0.9304	0.0696	180	13
Pipeline S8	192	0.9332	0.0668	179	13
Pipeline S9	248	0.9460	0.0540	234	13
Heat Exc. B2	17,085	1.0000	0.0000	17,085	0
Chiller B4	1,671	0.6901	0.3099	1,153	518
Expander B5	382,901	0.9820	0.0180	376,008	6,892
Column B6	150,523	0.3838	0.6162	57,771	92,752
Total	553,802	0.8189	0.1811	453,487	100,315

Table 30. Cost allocation results for the operating cost of common processes

Utilities	Utility Costs ($/h)	Cost Alloc. to Gas Prod.	Cost Alloc. to Liquid Prod.	Alloc. Costs to Gas Prod. ($/h)	Alloc. Costs to Liquid Prod. ($/h)
Chiller (B4) Duty	4.66	0.6903	0.3097	3.21	1.44
Reboiler (B6) Duty	4.23	0.2754	0.7246	1.16	3.06
Total	8.88	0.4928	0.5072	4.38	4.51

heat exchanger is over 90% of the total capital cost. This economic situation might make the capital and operating cost allocations determined by the DBM appear unreasonable.

However, considering that expanders and compressors are mainly applied to process gas streams, the above cost allocations is reasonable. Capital and operating costs allocation to gas and liquid products are reevaluated by taking into account only shared equipments, such as pipelines from S1 to S9, the heat exchanger B2, the chiller B4, the turbo-expander B5, and the demethanizer B6. The revised cost allocation results for the total capital and operating costs as well as for the individual equipment costs appear in Table 29 and Table 30, respectively. The reevaluated total capital cost allocation to the gas and liquid products are 81.89% and 18.11%, respectively. Also, The reevaluated operating cost allocated to the gas and liquid products are 49.28% and 50.72%, respectively. In addition to these results, when removing B5 from Table 29, the new total capital cost allocation to the gas and liquid products are 45.35% and 54.66%, respectively. For both the total capital and operating costs, costs allocated to the liquid product become greater than those allocated to the gas product, which is contradictory to the prior cost allocation results. These changes of cost allocation resulting from the different process configurations demonstrates the potential of the DBM to produce flexible and reasonable cost allocation results by the direct use of causality in the unit size/utility consumption and the contribution of the gas and liquid products.

Table 31 compares cost allocation results from the design benefit method and traditional methods, such as the sales value method and the physical unit method. Unlike the traditional methods, the design benefit method can distinguish between costs such as

capital costs or operating costs because of its unit-by-unit evaluation. Total cost allocation for the gas and liquid products from the sales value method are 34.83% and 65.17%, respectively, while those from the physical unit method are 89.30% and 10.70%. The comparison indicates that the two traditional methods produce contradicting results. In general, the sales value method is more widely used than the physical unit method in the gas industry. However, when applying the sales value method, a significant problem exists in that the price of gas products is determined by local and long-term contracts while the liquid product value is determined by the world spot market. A question about the validity of the results arises if stable gas prices and fluctuating liquid prices are the bases for the evaluation, as is the case for the sales value methods. The design benefit method on the other hand directly relates the unit size and utility consumption to the cost associated with each of the products. Therefore, it offers the potential to be widely acceptable for causal cost allocation.

Table 31. Comparison of cost allocation results between the design benefit method and traditional methods

	Design Benefit Method		†Sales Value Method	‡Physical Units Method
	Capital Cost	Operating Cost	Capital/Operating Cost	Capital/Operating Cost
Gas Product	0.9328	0.9380	0.3483	0.8930
Liquid Product	0.0672	0.0620	0.6517	0.1070

† gas price = $1.2/MMBtu and liquid price = $0.07/gal
‡ flow rate base

6.2. Natural gas plant economics based upon the optimization framework

When there are changes on product prices, utility costs, *etc.*, the plant will be adapted to the new economic condition by changing to a new optimal operating point. Determining the optimal operating condition can result in questions with regard to the objectives of the optimization problem. In general, the objective should be to maximize the plant-wide net profit. However, co-producers, e.g. Plant, Supplier 1, and Supplier 2 probably want to maximize only their profit under the contract with other co-producers. That may result in more profit for one of co-producer but may sacrifice some of the plant-wide net profit as well as the share of the profit of other co-producers. The relationship between the plant-wide net profit, the individual profit of co-producers, and optimal operating conditions can be represented by the following logical expressions:

$$J^{Plant}(x^{*,Plant}) \geq J^{Plant}(x^{*,Ind}) \tag{44}$$

$$J^{Ind}(x^{*,Ind}) \geq J^{Ind}(x^{*,Plant}) \tag{45}$$

where J^{Plant} = plant-wide net profit

J^{Ind} = individual profit of co-producers

$x^{*,Plant}$ = vector of the optimal operating condition to maximize the plant-wide net profit

$x^{*,Ind}$ = vector of the optimal operating condition to maximize the individual profit of co-producers

From this relationship, it can be concluded that in reality, when a plant is optimized for a co-producer/plant owner, the plant-wide net profit very unlikely reaches its true optimal

value and other co-producers would have to give up a part of their expected profits. Therefore, the determination of the operating condition can be a disputable issue among the co-producers.

The evaluation of all co-producers' profits and the plant-wide net profit can provide useful information to the co-producers. The profit evaluation results corresponding to new operating conditions can be a measure for evaluating plant operations. Whether the plant is properly operated or not can be revealed by checking the conditions in Eq. (44) and (45). In addition to the monitoring purpose, the careful analysis of the co-producers' profit status can provide the co-producers with important information for renewing and reevaluating the contractual agreement.

6.2.1. Description of the plant economic optimization problem

The turbo-expander plant processing raw natural gas streams to produce gas and liquid products has four principal operating variables:

- x_1 : bypass ratio of the feed mixture S3 to MIX2, which is the flow rate of S4 divided by the flow rate of S3, 0.1 ~ 0.3 [.]
- x_2 : discharge pressure of the expander B5, 400 ~ 500 [psi]
- x_3 : top pressure of the demethanizer B6, 270 ~ 310 [psi]
- x_4 : temperature change through the chiller B4, -8 ~ 0 [^{o}F]

Either the plant-wide net profit or the individual profit of one of the co-producers can be maximized by adjusting these operating variables. An optimization problem whose

objective is to maximize the plant-wide net profit is defined as the following representation:

$$\begin{aligned} &\text{Maximize: } J^{Plant}(x) = R_{Gas}(x) + R_{Liq}(x) - C_{Cap} - C_{Opr}(x) \\ &\text{Subject to: } 0.1 \le x_1 \le 0.3 \\ &\qquad\qquad 400 \le x_2 \le 500 \\ &\qquad\qquad 270 \le x_3 \le 310 \\ &\qquad\qquad -8 \le x_4 \le 0 \end{aligned} \tag{46}$$

where x = vector of operating conditions

$R_{Gas}(x)$ = annualized revenue of the gas product

$R_{Liq}(x)$ = annualized revenue of the liquid product

C_{Cap} = annualized capital cost

$C_{Opr}(x)$ = annualized operating cost

In this application, a measure of the individual profit of the co-producers requires cost allocation results because capital and operating costs assign to the co-producers are determined based upon the cost allocation results. Therefore, optimization problems for the maximization of the profit of one of the co-producers can be defined by the following representation:

$$\begin{aligned} &\text{Maximize: } J^{Ind}(x) = P_{Gas}^{Ind}\left[R_{Gas}(x) - A_{Cap}^{Gas}C_{Cap} - A_{Opr}^{Gas}C_{Opr}(x)\right] \\ &\qquad\qquad + P_{Liq}^{Ind}\left[R_{Liq}(x) - A_{Cap}^{Liq}C_{Cap} - A_{Opr}^{Liq}C_{Opr}(x)\right] \\ &\text{Subject to: } 0.1 \le x_1 \le 0.3 \\ &\qquad\qquad 400 \le x_2 \le 500 \\ &\qquad\qquad 270 \le x_3 \le 310 \\ &\qquad\qquad -8 \le x_4 \le 0 \end{aligned} \tag{47}$$

where x = vector of operating conditions

Table 32. Information for the plant economic optimization

- Annual operating hours = 8500hours/year
- Total capital investment = [†] $4.8 \times 1,494,793 = \$7,175,006$
- [‡] Annualized capital cost = $\frac{7,175,006}{10}(1+0.033)^{10} = \$992,717/\text{year}$
- Price of the gas product = \$1.2/MMBtu
- Price of the liquid product = \$0.05/gal
- Price of heating source = \$1.0/MMBtu
- Price of chilling source = \$7.0/MMBtu
- Electric price = \$0.028/kWh

[†] Lang multiplication factor for the estimation of capital investment for fluid-processing plants (Peters & Timmerhaus,1991)

[‡] following the definition of depreciation in Eq. (43)

$R_{Gas}(x)$ = annualized revenue of the gas product

$R_{Liq}(x)$ = annualized revenue of the liquid product

C_{Cap} = annualized capital cost

$C_{Opr}(x)$ = annualized operating cost

P_{Gas}^{Ind} = gas product allocation to a co-producer

P_{Liq}^{Ind} = liquid product allocation to a co-producer

A_{Cap}^{Gas} = capital cost allocation to the gas product

A_{Opr}^{Gas} = operating allocation to the gas product

A_{Cap}^{Liq} = capital cost allocation to the liquid product

A_{Opr}^{Liq} = operating allocation to the liquid product

To solve these optimization problems requires a lot of information regarding plant economics, such as product sharing contract, cost allocation results, utilities costs, financial data, *etc*. The product allocation to each co-producer and the cost allocation to gas and liquid products can be found in Table 4 and Table 31, respectively. Other required information to evaluate the objective function is given in Table 32.

6.2.2. Application of the GQSA to the plant economic optimization

Natural gas plant economic optimization problems incorporating process flowsheet are characterized by discontinuity and non-convexity. Despite their high computational

efficiency, typical gradient-based optimization techniques may not be applied to these optimization problems because of their discontinuity and non-convexity. The result of sensitivity tests for the plant-wide net profit and the individual profit of co-producers with respect to operating variables appears in from Fig. 16 to Fig. 19. The change of all the profits with respect to x_1 and x_2 shows linear characteristic while that with respect to x_3 and x_4 shows nonlinear characteristic. The result analysis of the sensitivity tests indicate that the objective function of each optimization problem may be a non-convex system over the given operating range. Fig. 20 shows the convergence error of the flowsheet, which results from 40 Monte Carlo simulations at the normal operating condition. In each simulation, the flowsheet is simulated at the normal operating condition after a simulation at randomly chosen operating condition. The errors in the flowsheet convergence cause the typical gradient-based optimization techniques to fail since evaluation of the gradient is required for determining a search direction. This randomness in flowsheet convergence and the non-convexity of the profit optimization problems justify the application of the GQSA to the natural gas plant economic optimization.

The GQSA algorithm used in this research is coded in MATLAB™ Version 6.0 and implemented on a Dell™ OptiPlex GX240 running Windows™ 2000. The GQSA and the flowsheet are also interfaced by ActiveX®, like the cost allocation framework. The parameters for the GQSA are given in Table 33. In this application, the sub-optimization problem based upon a determined quadratic model can be defined by the flowing representation:

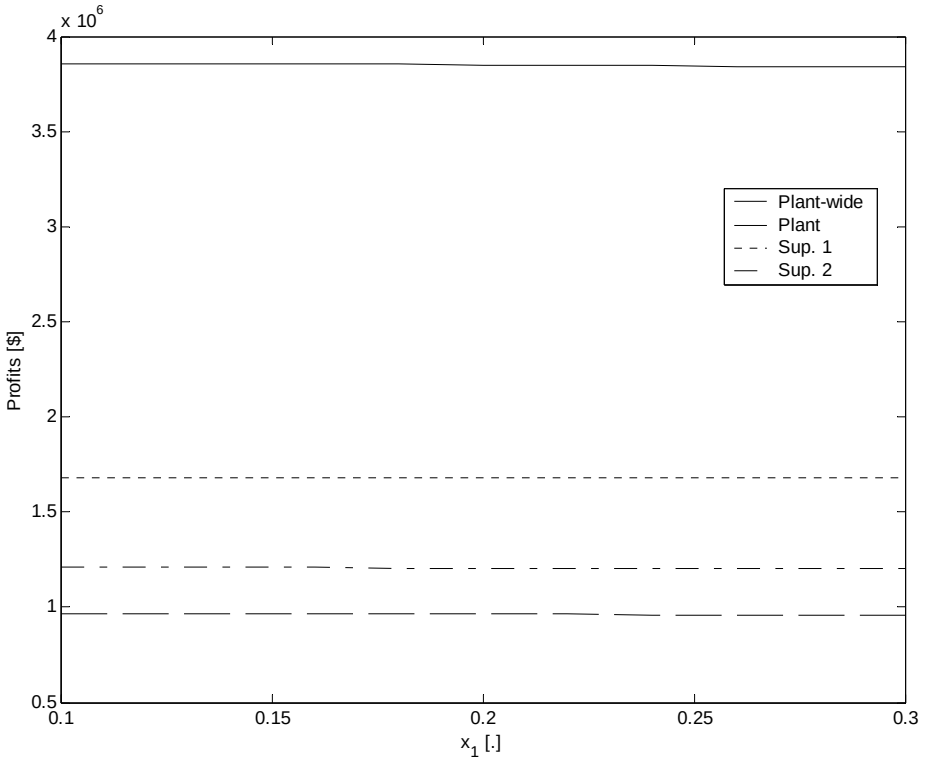


Fig. 16. Change of profits with respect to x_1 at x_2 = 450psi, x_3 = 290psi, and x_4 = -4°F.

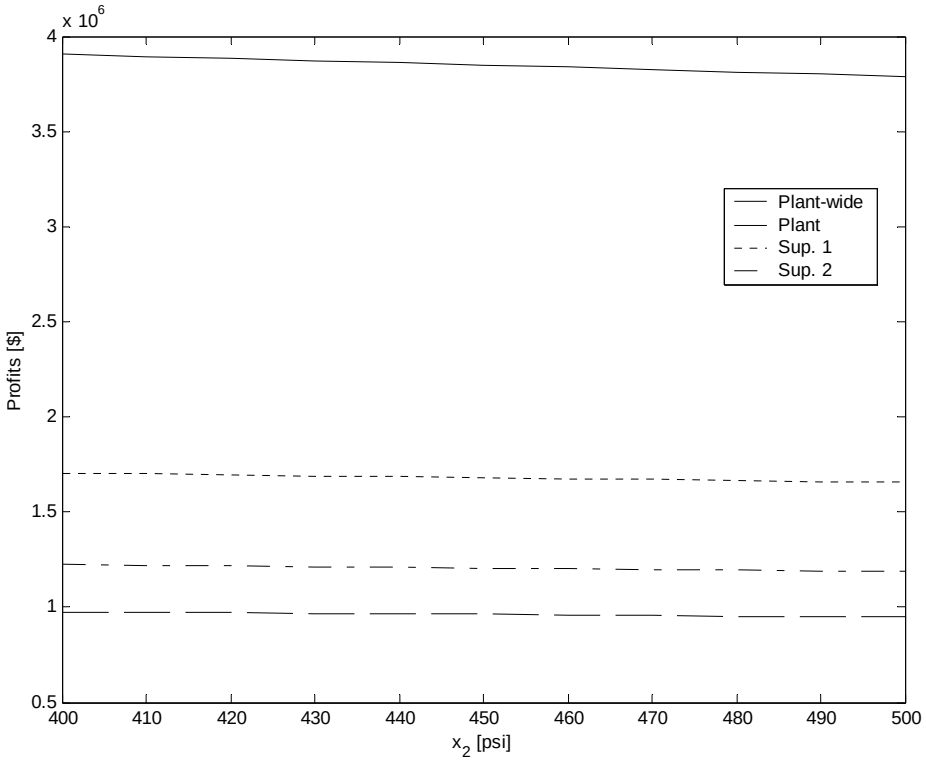


Fig. 17. Change of profits with respect to x_2 at x_1 = 0.15, x_3 = 290psi, and x_4 = - 4°F.

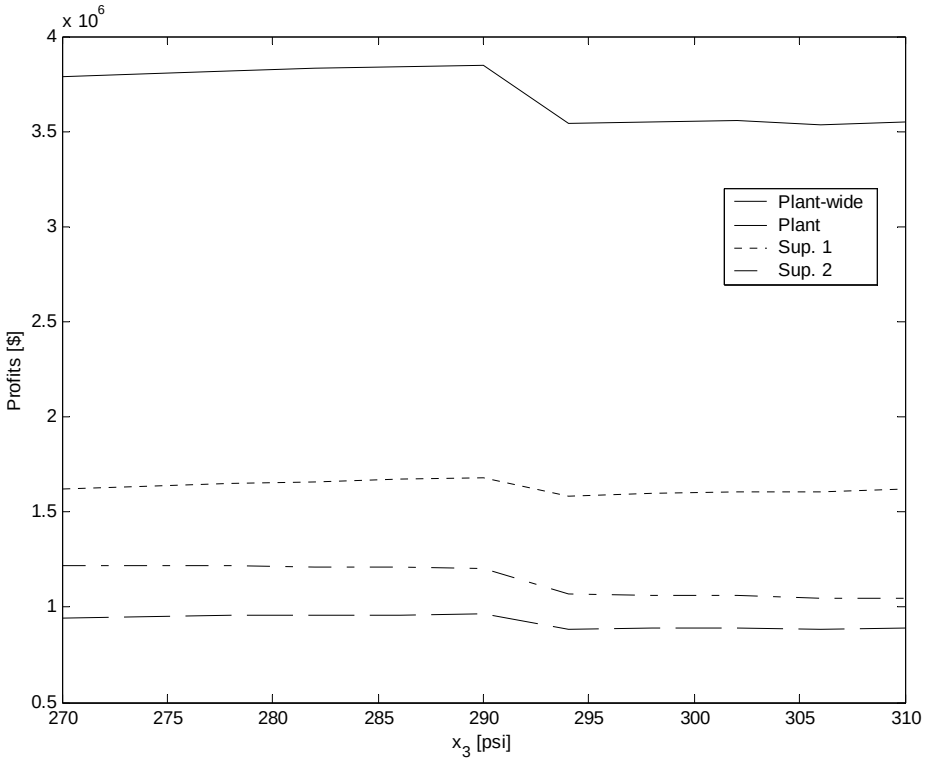


Fig. 18. Change of profits with respect to x_3 at $x_1 = 0.15$, $x_2 = 450$psi, and $x_4 = -4^{\circ}\mathrm{F}$.

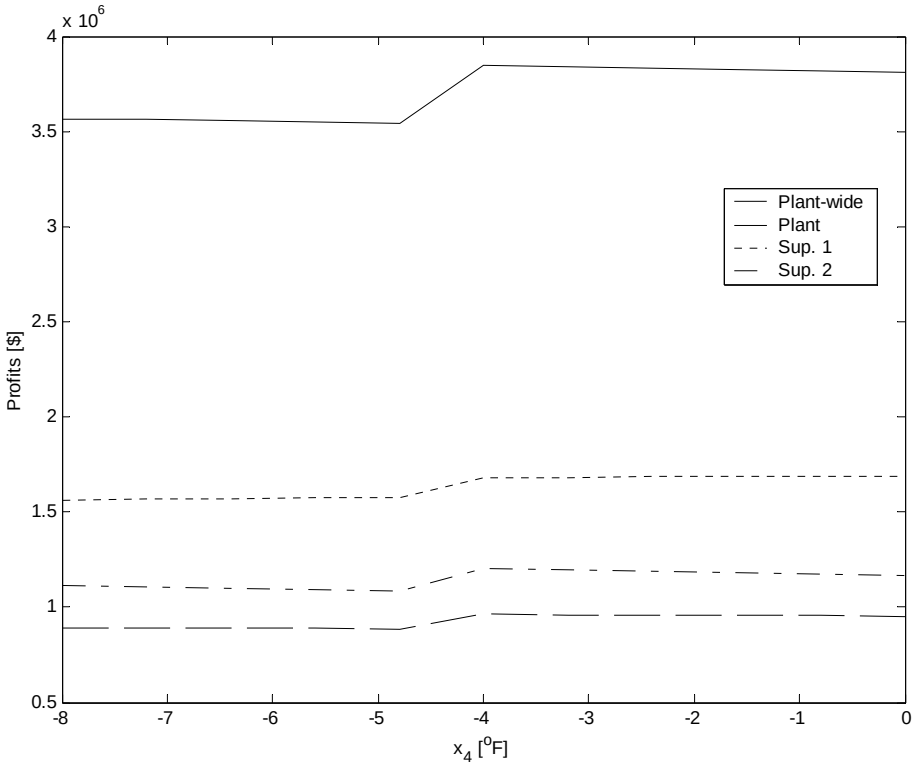


Fig. 19. Change of profits with respect to x_4 at x_1 = 0.15, x_2 = 450psi, and x_3 = 290psi.

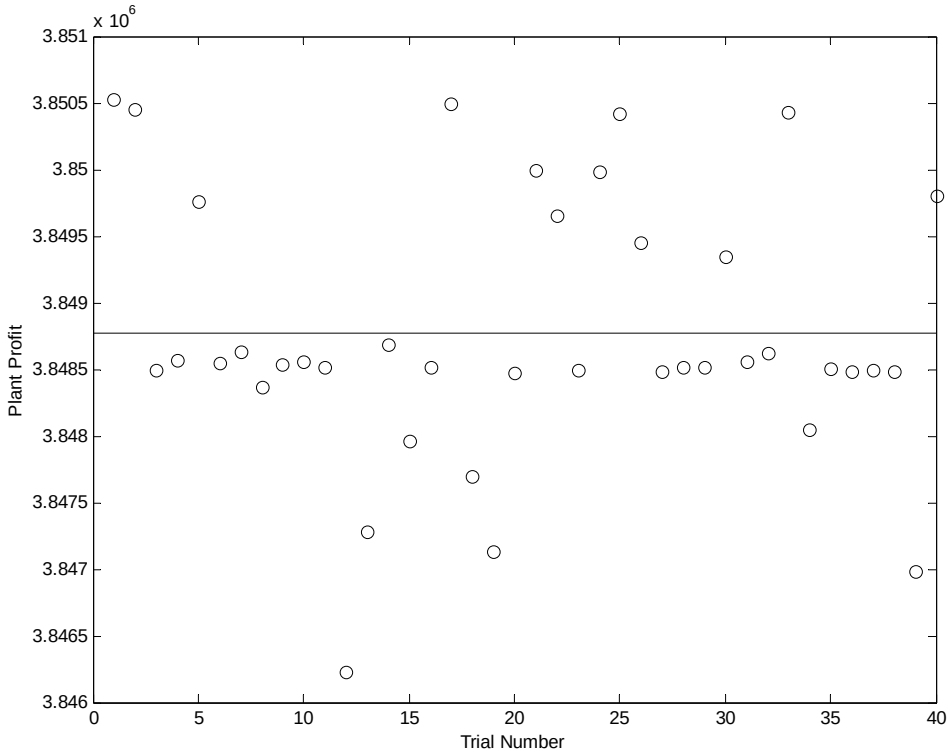


Fig. 20. Convergence error of the flowsheet at the normal operating condition.

$$\begin{aligned} &\text{Minimize:} \quad q = \frac{1}{2} x^T H x + f^T x + c \\ &\text{Subject to:} \quad 0.1 \le x_1 \le 0.3 \\ &\qquad\qquad\quad 400 \le x_2 \le 500 \\ &\qquad\qquad\quad 270 \le x_3 \le 310 \\ &\qquad\qquad\quad -8 \le x_4 \le 0 \end{aligned} \tag{48}$$

The sub-optimization problem can be solved by the QP since there is no nonlinear constraint involved to this problem.

The GQSA is applied three times to each profit maximization problem in order to increase the possibility of finding the global optimum. Table 34 shows the best solution for each problem and the evaluated profit of the co-producers under optimal operating conditions. The results verifies that the profit of the co-producers may have a different value based upon the applied objective to the optimization problem. When the objective of the optimization problem is to maximize either the plant-wide profit or the Plant's profit, both optimization problems produce almost the same result for the optimal operating condition as well as for the plant-wide profit and for the co-producers' profits. That is because the portions of the gas and liquid products assigned to the Plant are equivalent to each other. The plant-wide profit that is defined as the summation of all co-producers' profits, in other words, is the summation of all profits from gas and liquid products. Since the Plant's profit is 25% of the plant-wide profit, they are directly proportional to each other. However, when the objective of the optimization problem is to maximize the profit of either Supplier 1 or Supplier 2, the maximum plant-wide profit cannot be realized. Also, other co-producers should give up some of their profits, which

Table 33. Parameters for the GQSA

Genetic Algorithm	- Number of generations = 100 - Number of binary digits in genes = 12 - Population size = 60 - Number of new offsprings in each generation = 30 - Operation probability of mutation = 0.05 - Operation probability of random = 0.05 - Operation probability of crossover = 0.90 - Probability of the random selection of parents in crossover = 0.05 - Probability of the roulette wheel selection of individuals for the next generation = 0.70 - Probability of the random selection of individuals for the next generation = 0.30
Quadratic Search	- Factor for the number of data (ω) = 1.5 - Number of past generations for quadric modeling = 10
Hyper-cube Initialization	- Space coverage (τ_c) = 0.60

Table 34. Results of natural gas plant economic optimization

Objective	Optimal Solution
Plant-wide Profit	x^* = (0.1117, 400.00, 284.20, -8.00) **Plant-wide Profit = $3,930,000** Plant's Profit = $982,500 Supplier 1's Profit = $1,678,300 Supplier 2's Profit = $1,269,200
Plant's Profit	x^* = (0.1095, 400.00, 283.39, -7.88) Plant-wide Profit = $3,930,100 **Plant's Profit = $982,530** Supplier 1's Profit = $1,677,400 Supplier 2's Profit = $1,270,200
Supplier 1's Profit	x^* = (0.1019, 400.00, 292.89, 0.00) Plant-wide Profit = $3,829,300 Plant's Profit = $957,320 **Supplier 1's Profit = $1,708,100** Supplier 2's Profit = $1,163,900
Supplier 2's Profit	x^* = (0.1001, 400.20, 270.05, -8.00) Plant-wide Profit = $3,895,300 Plant's Profit = $973,830 Supplier 1's Profit = $1,638,700 **Supplier 2's Profit = $1,282,800**

can be obtained under the operating condition for the maximization of the plant-wide profit.

We can conclude from this observation that the Plant will fairly operate the turbo-expander plant without any monitoring because the Plant can have its maximum profit under the operating condition maximizing the plant-wide profit. Also, it may be anticipated that the two suppliers agree this operating condition in order to maximize the plant-wide profit because some of the plant-wide profit as well as other co-producers' profits should be sacrificed when the plant is operated in order to maximize one of their profits.

7. CONCLUSION

Natural gas plants can be characterized by multiple owners for the raw natural gas streams and processing facilities as well as multiple products. Due to these characteristics, a proper cost allocation method is necessary for taxation of the profits from natural gas and crude oil as well as for cost sharing among gas producers. However, the cost allocation methods used most often in accounting, such as the sales value method and the physical units method, are inappropriate for natural gas processes because of a lack of a relationship between product price and processing cost, multiple split-off points, and a logical and common physical attribute.

Wright and Hall (1998) have proposed the DBM based upon engineering principles and Wright *et al.* (2001) applied this idea to a natural gas process. This first application illustrated that the DBM can be a reliable cost allocation technique for natural gas processes. However, there have been limitations in the application of the DBM because of its modeling technique, which determines oversimplified models and does not consider infeasible regions.

To solve these problems, we have developed a rigorous modeling technique for the DBM based upon a Taylor series approximation. This modeling technique not only employs a generalized modeling procedure applicable to a wide variety of equipment, but it is also more easily implemented on a computer system. Also, we have investigated a cost allocation framework composed of the determination of the virtual flows, the equipment modeling technique, and the evaluation of cost allocation for extending the application of the design benefit method to other scenarios, particularly those found in

the petroleum and gas industries. As these individual procedures can be implemented on a computer system, the proposed framework can easily be developed as a software package, and its application can be extended to large-scale processes.

In order to illustrate the potential application of the proposed cost-allocation framework, we have investigated the optimization framework for the application to natural gas plant economic optimizations where cost allocation results are involved. The optimization framework can provide co-producers sharing raw natural gas streams and a processing plant not only with the optimal operating condition but also with valuable information that can help to evaluate their contracts. The profit evaluation results corresponding to new operating conditions can be a means of monitoring plant operations to the co-producers. Also, the careful analysis of the co-producers' profit status can provide the co-producers with important information for renewing and reevaluating the contractual agreement.

For the optimization framework, we have developed the GQSA composed of a general genetic algorithm and a quadratic search. Natural gas plant economic optimization problems need a lot of process flowsheet convergences characterized by discontinuity and non-convexity in order to collect process information required to compute their objective functions. As each process flowsheet convergence requires an expensive computation, it is extremely important to develop an efficient search algorithm that requires a smaller number of objective function evaluations. However, typical gradient-based optimization techniques as well as general genetic algorithms may not work properly in this application because of the characteristics of process flowsheet

optimizations. As the GQSA inherits the advantages of both genetic algorithms and quadratic search techniques, it is able to find the global optimum with a high possibility for discontinuous as well as non-convex optimization problems but also usually has a much faster convergence speed than general genetic algorithms. Because of these features, the GQSA can become a suitable technique for solving optimization problems including process flowsheet optimization.

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VITA

Won-Hyouk Jang was born in Chunnam, Korea, on 23 May 1969. He received his Bachelor of Science and Master of Science in chemical engineering from Hanyang University, Korea in February 1991 and February 1993, respectively. Upon graduation, he worked at Choheung Chemical Co. in Seoul, Korea as a process engineer until June 1996. After that, he joined Kolon Engineering & Construction Co. in Kyunggi, Korea as a control system engineer before attending the Department of Chemical Engineering at Texas A&M University in August 1999.

His permanent address is:

116-15 18/10 Shinlim 2-Dong, Kwanak-Ku

Seoul 151-012, Korea