Hierarchical Analysis of Chemical Process System: Modeling and Optimization of Large-Scale System

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Abstract

The complexity of chemical process systems and related spatial systems is familiar to all those practicing in this field. This complexity is inherent in the nature of the chemical process system problems, the multi-objective attributes of chemical process systems problems and the interactive coupling within chemical process networks, including raw materials and human resources as related to their quantity and quality. The complexity is also due to the difficulties of retrieving, transmitting, processing and analyzing data and to those aspects of decision-making process such as the institutional, political, and economic aspects as well as the technical, environmental and social impacts.

The multiple goals of different parts of the overall system is inevitable and inescapable and it should be quantitatively analyzed. This fact will drive all those practicing in this field to adopt systems methodologies that are amenable to modeling, analyzing and optimizing these complex systems.

Many applications of system engineering methodologies to large-scale chemical process system are adopted here. In particular, the applications of the hierarchical-multi level approach to large-scale and complex chemical process systems are discussed. The resulting system approach in chemical processing development requires the optimal use of innovative research results from different professional discipline in university and industry and the cooperation between the user, government and chemical processing system constructors as well.

Keywords: Multi-objective Attribute; System Approach; Hierarchical Multi Level approach.

1. INTRODUCTION

The problems in chemical process system are often large enough to strain and exceed the abilities of a single team of engineers. These large problems are necessary to relegate the design responsibility to several more or less autonomous experts and each responsible for a part of the system. If one or more team of engineers are engaged with this kind of problem, the question to be asked is: “How is the effort of these teams to coordinate their activities so that their design will mesh together to form an optimal system?”.

Typically, the design of a chemical process system which is large with chemical plants around the country must be divided into numbers of sub processes which will purchase chemicals from each other and from the outside. And these facts leads to the implant prices that should be set to force the several designs so that the levels at which the efficiency of the large complex process system obtaining it maximum values. In an extremely large problem, the engineer must face the choices between an absolute need for reducing the size of the individual units and the reality that the careless optimization of the smaller units may not be in the best interest of the overall system. And the problem is how the efforts of those responsibilities for the subsystem are coordinated to achieve the system goal. The answer for this problem can be accommodated by multilevel optimization.

In chemical engineering design practice, the engineer deal with the large scale problem and a multilevel approach can be used to solve this kind of problem. A multilevel approach in which the responsibility for the engineering of each of the subsystems is assigned to individual engineering groups which is known as first-level are only responsible for the design of their subsystems. In doing their duties, they need not concern themselves with the design of any other portion in the process. And

at the second level, the coordinating groups is responsible for the overall system behavior and this level is divorced from the need for considering all the details of the subsystems. They are charged only for assuring the cooperation of the other groups in achieving the system goal.
The communication must be maintained between this two levels by supply, demand and price parameters. This two levels model can be extended to more than two levels model and this extension will be discussed in this paper.

2. THE STRUCTURE OF GENERAL HIERARCHICAL MODELING

In this section we will discuss the structure of general hierarchical modeling for large scale design problem and the chemical processing model. The first will be discussed in short while the second will be discussed in long.

2.1. Large Scale Design Problem

In this subsection we will see how the dilemma appears in a large processing system design and how we can handle it. The dilemma of a large processing system optimization can be handled by multilevel approach. In this approach we should know what it means with subsystems, and subsystem optimization and thus, the forced cooperation.

The Dilemma of A Large System In a large processing system design, a practical limit exists on the number of detail for which the single group of engineers can be held responsible. Usually, large processing system exceeds this limit and hence, there is a need for tearing the large system into a number of smaller subsystems. This tearing make possible to allocate the responsibility for the design of subsystems among a number of engineering groups. We see the responsibility for the design of a chemical processing system distributed among the raw material handling and separation design group, fractionation system design group, the waste treatment systems design group, and so forth, the original system being to large for one group to handle all of the details in the design.

The realization of tearing a large system into a number of subsystems may restrict the original problem, and the optimization is achieved only if it is free and no interaction is allowed among all subsystems in the system with its surroundings. This is the source of the dilemma. Thus, it need an approach to optimize the large design problem and the promising tool is a multilevel approach.

The Subsystems Our focus attention now on the design of the large system and the system has been divided into individual subsystems which interact via the state variable χ, which might be the flow rates of the products and intermediates. The design goal is to select the detailed designs for subsystems that maximize the overall system objective function, F, consisting of the contributions F_1, F_2, …, F_n from the subsystems. For example, the subsystem 1 might be, the profit calculated from the value of chemicals sold by the subsystem to the surroundings, less the manufacturing costs and the appropriate charges for capital invested in the subsystem. Since there is no way of assessing the values of implant transfer of material or energy, no charge is assigned to such implant transfer.
During the development of the objective function of each subsystem, internal transfer are considered to be free and unlimited, and in this way the subsystem are torn free from the system. Within its domain of responsibility, each group at the first-level has the following:
(1) The contribution to the overall system objective by the subsystem
(2) The design details δ of the subsystem in which each group is the sole authority.
(3) The state variables χ which connect the system with other subsystems.

Then, the large processing system may be written as

$$\max_{\delta_1,\delta_2,\ldots,\delta_n} \left(F_1 + F_2 + \ldots + F_n\right) \tag{1}$$

With the responsibility assigned to the subsystems group at the first-level as follows

- The Objective Function:

$$\left.\begin{array}{ll} F_1(\chi_1,\chi_2,..,\chi_n,\delta_1) & for\ \ Group\ \ I_1 \\ F_2(\chi_1,\chi_2,..,\chi_n,\delta_2) & for\ \ Group\ \ I_2 \\ \bullet\ \bullet\ \bullet & \\ \bullet\ \bullet\ \bullet & \\ F_2(\chi_1,\chi_2,..,\chi_n,\delta_2) & for\ \ Group\ \ I_n \end{array}\right\} \quad (2)$$

- The Design Detail

$$\left.\begin{array}{ll} d_1(\chi_1,\chi_2,..,\chi_n,\delta_1)=0 & for\ \ Group\ \ I_1 \\ d_2(\chi_1,\chi_2,..,\chi_n,\delta_2)=0 & for\ \ Group\ \ I_2 \\ \bullet\ \bullet\ \bullet & \\ \bullet\ \bullet\ \bullet & \\ d_2(\chi_1,\chi_2,..,\chi_n,\delta_2)=0 & for\ \ Group\ \ I_n \end{array}\right\} \quad (3)$$

The expression for the design detail of subsystem 1, for example, is a shorthand expression of all the tools are elected to bear by Group I_1. This group design relation states that for a given a given design detail δ_1, and for given state variables $\chi_2,..,\chi_n$; the behavior the group for this area can be predicted by the group due its responsibility related to the system and assign a value to output χ_1, and this may require the efforts of the team of engineers aided by computing facilities.

Sub-optimization. The optimization of any subsystem by itself, without interaction with other parts of the system will give no optimal strategy for the system. Thus, there must be cooperations among the groups of process system designer and it is needed to have a new coordinating group to assign suitable sub-optimization goals to the subsystems to force their cooperation.

Such cooperation can be accomplished by requiring that each subsystem buy its input state variables from the other subsystem and sell its output state variables to the other subsystems at assigned prices. While attempting to solve their own sub-optimization problem under coordination of the coordinating group, all first-level groups are led to cooperate in solving the system problem. In this case, the task of the coordinating groups is to assign and adjust prices of these state variables.

For example, consider system of three subsystems: 1, 2 and 3. Sub-system 1 buy the input state variable from subsystem 3, χ_3, and sell its output state variable, χ_1, to subsystem 2. Sub-system 2 buy its input from and sell its output to the surrounding. Sub-system 3 buy its input state variable, χ_2, from subsystem 2 and sell its output to the surrounding. If φ_1, φ_2, and φ_3 are the implant prices to be prescribed by the second-level coordinating group, then this example shows that: being required to buy and sell from within, the first-level groups will pursue the maximum of the new objective functions:

$$\left.\begin{array}{ll} \max\limits_{\chi_3,\delta_1}(F_1+\varphi_1\chi_1-\varphi_3\chi_3) & for\ \ Group\ \ I_1 \\ \max\limits_{\chi_3,\delta_1}(F_2+\varphi_2\chi_2-\varphi_1\chi_1) & for\ \ Group\ \ I_2 \\ \max\limits_{\chi_3,\delta_1}(F_3+\varphi_3\chi_3-\varphi_2\chi_2) & for\ \ Group\ \ I_3 \end{array}\right\} \quad (4)$$

Now, we can make a few observations. The first-level groups have additional variables to manipulate during sub-optimization, i.e., the amount of input state variable. Hence, for given prices each subsystem will demand certain of its input state variable as an attempt to achieve local maximum goal. In other hand, that demanded by one subsystem must be supplied by another, while the prices which force the equality of supply and demand are still unknown.

Intuitively, we can expect that the system will operate efficiently when all implant supplies and demands are equal and this also happen to the large class of optimization problems which exhibit properties of continuity and differentiability. For this class of optimization, the sub-problems are extracted from the Lagrangian of the original problem as will shown later in this paper. Thus the theory of Lagrange multipliers can be used to validate the criteria of the sub-optimization design.

The first level subsystem group now set forth its tentative design based on the assumption that the implant material is available at free of charge. And the second-level coordinating group compares the supplies and demands and attempts to design artificial implant prices for the state variables. These activities will cause the first-level groups to readjust their tentative design toward the condition where the demands of each subsystem equal the supplies given by other system.

These facts had been indicated above, i.e., the first-level groups communicate with coordinating group of the second level via supply and demand variables and the second-level coordinating group communicates via price parameters. Here is the procedure for the coordination of first-level groups:

Step 1. Supply the sub-optimization goals
Step 2. Propose the tentative designs
Step 3. Supply and demand data
Step 4. If the tentative designs are fit together, then stop. Else, repeat step 1.

After receiving supply and demand data, the coordinating group should make an adjustment of the price parameter to more equate the supplies and demands on the next round. Then, the coordinating group must analyze these data and find a new set of prices for the next round. The attack results in solving the minimization problem

$$\min_{\{\varphi_1,\varphi_2,\varphi_3\}} \left\{ \sum_i \left| \chi_i^{demand} - \chi_i^{sup\,ply} \right| \right\} \tag{5}$$

Problem indicated by eq. (5) can be solved using direct search approach.

When the demand of a commodity exceeds the supply, commodity value will increase in marketplace and it provides more incentive to produce and less incentive to consume. Thus, this situation tends to drive the supply toward the demand in the future and this situation suggests a price adjustment for the system coordination problem. The new price is now estimated by

$$\varphi_i^{new} - \varphi_i^{old} = \kappa_i \left(\chi_i^{demand} - \chi_i^{sup\,ply} \right) \qquad for \quad i = 1,2,3... \tag{6}$$

where κ_is are constants of proportionality. These constants determine the rate of convergence of the price adjustment scheme. When the demand exceeds the supply then the prices tend to rise. But if the supply exceeds the demand then the prices tend to fall.

2.2. Chemical Process System

The modeling of chemical process systems, where the quality is the main theme, results in large dimensions model. The fact that the product quality cannot be expressed by one-dimensional state variable, nor can there be a unique representation of chemicals as the product of the chemical processing system. There cannot be a unique representation of a chemical quality, its characteristics and properties are the combination of impurities contained in the chemical, temperature, pressure etc. Moreover chemical process system always consists of the chemical resource and treatment system. This system will affect the quality of chemical and it is important that the chemical quality also cannot be expressed as a one-dimension state variables. Like a chemical, we cannot have a unique representation of water quality, since the chemical characteristics and properties are the result of a combination of indicators such as organic material, temperature, BOD, chlorides, phosphates, nitrates, algae, etc.

Nevertheless, in a chemical processing system, some measures of chemical characteristics one considers, the more accurate a description of the chemical quality one gets, and consequently, the more complex one's system model becomes.

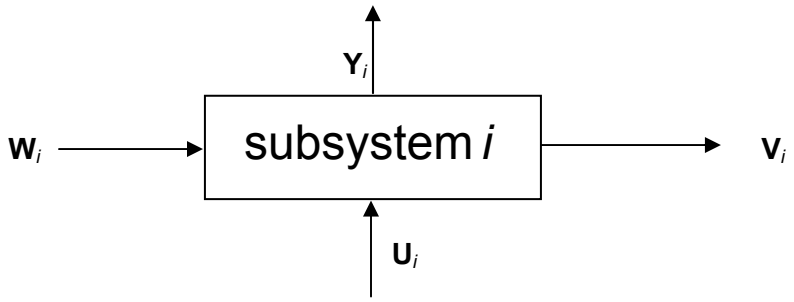

Figure 1. Model for Subsystem *i*.

A general mathematical model is developed here first. Each case where chemical effluent is discharged directly into the product tank, into the packaging plant, or into a bypass pipe leading to a subsequent chemical plant, constitutes a special case of the general model.

Consider a chemical processing system (CPS). Let $\mathbf{U}_i$ be the the *i*-th chemical input vector to the CPS, $i = 1,2,\ldots..,N.$

$$\mathbf{U}_i^T = \{U_{i1}, U_{i2}\ldots\ldots U_{im}\} \tag{7}$$

where U_{i1} represents the chemical quantity and $U_{i2}\ldots..U_{im}$ represent different chemical characteristics, e.g., temperature, density, heat capacity, etc.

It is convenient to decompose the CPS into *N* subsystems, each of which includes one chemical input $\mathbf{U}_i$ (see Figure 1). Let

$\mathbf{W}_i$ be the input vector coming into the *i*-th subsystem from other subsystem
$\mathbf{V}_i$ be the output vector of the *i*-th subsystem going to other subsystems, and
$\mathbf{Y}_i$ be the output vector of the *i*-th subsystem leaving the system

Where $\mathbf{W}_i$, $\mathbf{V}_i$, and $\mathbf{Y}_i$ are of the same dimensionality as $\mathbf{U}_i$, i.e., m-dimension and the vector sum $\mathbf{W_i + U_i}$ is meaningless and is not equal to $\mathbf{V_i + Y_i}$.
It is assumed that the subsystems outputs $\mathbf{V_i}$ and $\mathbf{Y_i}$ can be represented by the following functions:

$$\mathbf{V_i = \Xi_i(U_i, W_i)} \tag{8}$$

$$\mathbf{Y_i = \Psi_i(U_i, W_i)} \tag{9}$$
$i = 1, 2,\ldots, N$

where

$$\mathbf{\Xi_i^T = \{\ \Xi_{i1},\ \Xi_{i2},\ldots\ldots,\ \Xi_{im}\}}$$

$$\mathbf{\Psi_i^T = \{\ \Psi_{i1},\ \Psi_{i2},\ldots\ldots,\ \Psi_{im}\}}$$

We see that not all components of the functions $\mathbf{\Xi_i}$ and $\mathbf{\Psi_i}$ are known to chemical quality experts. And this constitutes no limitation to the model, because if the functional relationship of any component of $\mathbf{U_i}$ is known, we can add that component. The presence or absence of a component of $\mathbf{U_i}$ has a strong effect on the model. With the greater the number of components of $\mathbf{U_i}$ that are considered and analyzed, we will have the more accurate and representative mathematical model, assuming that all needed data are available.

More general formulation is required in order to handle branching in the CPS under consideration. This general formulation is made where more than one input from other subsystems enters the *i*th subsystem. The approach taken here for hierarchical multi-level optimization would be much simpler without introducing branching in the CPS. And without loss of generality, it is assumed that no branching will occur.

Suppose

$$\mathbf{H_i(U_i,W_i,Y_i)} \le 0 \qquad i = 1, 2 \ldots, N \tag{10}$$

be the vector of constraints to be satisfied by the *i*th subsystem , i = 1,2,....N and $\mathbf{H_i(U_i,W_iY_i)}$ are K-dimensional continuous functions. The physical, legal, economic, and other system constraints and also equality constraints are represented by equation (10).

The sum of the treatment cost functions of each system $F_i(\mathbf{U}_i,\mathbf{Y}_i)$ is the overall CPS treatment cost functions, F, that is :

$$F = \sum_{i=1}^{N} F_i(\mathbf{U}_i, \mathbf{Y}_i) \tag{11}$$

It is assumed that the cost function F_i for the *i*th subsystem is an explicit function of the effluent input $\mathbf{U}_i$ and the output $\mathbf{Y}_i$. It is assumed that the functions $F_i(\mathbf{U}_i,\mathbf{Y}_i)$ are continuous. The assumption that the cost function of $F_i(\mathbf{U}_i,\mathbf{Y}_i)$: depends only on $\mathbf{U}_i$ and $\mathbf{Y}_i$ can be replaced by a more general cost function which depends on all $\mathbf{U}_i$ and $\mathbf{Y}_i$, I = 1,2,....N. This will require a further decomposition of the CPS treatment cost function by introducing pseudo-variables.

Systems Decomposition Assume that there are existences of a regional authority that has control over chemical processing facilities. Also that each subsystem may develop its own chemical processing facility and its development should be economically justified by the optimization procedure.

In the two-level optimization procedure, the CPS is decomposed into N "independent" subsystem. At the first level, each subsystem is separately and independently optimized. In the second level, the subsystems are joined by coupling variables which are manipulated by second level controllers in order to arrive at the optimal solution for the whole system. These controllers are the system model Lagrange multipliers.

The optimization problem for the overall system can be summarized as follows:

$$\left.\begin{array}{c} min\left\{F = \sum_{i=1}^{N} F_i(\mathbf{U}_i, \mathbf{Y}_i)\right\} \\ \text{Subject to} \\ \mathbf{V}_i = \boldsymbol{\Xi}_i(\mathbf{U}_i, \mathbf{W}_i) \\ \mathbf{Y}_i = \boldsymbol{\Psi}_i(\mathbf{U}_i, \mathbf{W}_i) \\ \mathbf{H}_i(\mathbf{U}_i, \mathbf{W}_i, \mathbf{Y}_i) \\ \mathbf{W}_{i+1} = \mathbf{V}_i \\ i = 1,2,...,\mathrm{N} \end{array}\right\} \tag{12}$$

where $\mathbf{W}_{N+1} = \mathbf{V}_N$ is the chemical leaving the CPS.

Form the Lagrangian L:

$$L = \sum_{i=1}^{N} F_i(\mathbf{U}_i, \mathbf{Y}_i) + \sum_{i=1}^{N-1} \lambda_i^T [\mathbf{V}_i - \mathbf{W}_{i+1}] + \sum_{i=1}^{N} \rho_i^T H_i(\mathbf{U}_i, \mathbf{W}_i, \mathbf{Y}_i) \tag{13}$$

Where λ_i are m-dimensional Lagrange multipliers; i = 1,2,.... N - 1, and are *k*th dimensional generalized Lagrange multipliers, i = 1,2,..N

Substituting the values for $\mathbf{Y}_i$ and $\mathbf{V}_i$ from eqs (2),(3) yields

$$L = \sum_{i=1}^{N} F_i(\mathbf{U}_i, \boldsymbol{\Phi}_i) + \sum_{i=1}^{N-1} \lambda_i^T [\boldsymbol{\Xi}(\mathbf{U}_i, \mathbf{W}_i) - \mathbf{W}_{i+1}] + \sum_{i=1}^{N} \rho_i^T H_i(\mathbf{U}_i, \mathbf{W}_i, \mathbf{Y}, \boldsymbol{\Phi}_i) \tag{14}$$

It should be noted that

$$\sum_{i=1}^{N-1} \lambda_i^T [\boldsymbol{\Xi}(\mathbf{U}_i, \mathbf{W}_i) - \mathbf{W}_{i+1}] = \sum_{i=1}^{N-1} \lambda_i^T \boldsymbol{\Phi}_i(\mathbf{U}_i, \mathbf{W}_i) - \sum_{i=2}^{N} \lambda_{i-1}^T \mathbf{W}_i \tag{15}$$

Then L is then decomposed into N independent subsystems:

$$L = \sum_{i=1}^{N} L_i(\mathbf{U}_i, \mathbf{W}_i, \rho_i, \lambda_i) \tag{16}$$

where

$$L_i = F_i(\mathbf{U}_i, \mathbf{\Psi}_i) + \lambda_i^T \mathbf{\Xi}_i(\mathbf{U}_i, \mathbf{W}_i) - \lambda_{i-1}^T \mathbf{W}_i + \rho_i^T H_i(\mathbf{U}_i, \mathbf{W}_i, \mathbf{\Psi}_i);\ i = 1,2, \ldots, N \tag{17}$$

and also by definition,

$$\lambda_N^T \mathbf{\Xi}_N(\mathbf{U}_N, \mathbf{W}_N) \equiv 0 \tag{18}$$

$$\lambda_1^T \mathbf{W}_1 \equiv 0 \tag{19}$$

Thus we have defined, λ_i for $i = 1, 2, \ldots, N$

The Lagrangian L has a saddle point at $(\mathbf{U}_i^0, \mathbf{W}_i^0, \boldsymbol{\rho}_i^0, \boldsymbol{\lambda}_i^0)$ if

$$\mathbf{U}_i^0 \quad \text{and} \quad \mathbf{W}_i^0 \text{ minimize } L(\mathbf{U}_i^0, \mathbf{W}_i^0, \boldsymbol{\rho}_i^0, \boldsymbol{\lambda}_i^0) \tag{20}$$

and

$$\mathbf{W}_{i+1}^0 - \mathbf{\Xi}_i(\mathbf{U}_i^0, \mathbf{W}_i^0) = 0 \tag{21}$$

$$\mathbf{H}_i[\mathbf{U}_i^0, \mathbf{W}_i^0, \mathbf{\Psi}(\mathbf{U}_i^0, \mathbf{W}_i^0)] \le 0 \tag{22}$$

$$(\rho_i^0)^T \mathbf{H}_i[\mathbf{U}_i^0, \mathbf{W}_i^0, \mathbf{\Psi}(\mathbf{U}_i^0, \mathbf{W}_i^0)] = 0 \tag{23}$$

$$\rho_i^0 \ge 0 \tag{24}$$

for $i = 1,2,.....,N$

with the assumption that the Kuhn-Tucker constraints qualifications hold. A saddle point for the Lagrangian , L, given by equation (10) satisfies the following inequalities:

$$L(\mathbf{U}_i^0, \mathbf{W}_i^0, \rho_i, \lambda_i) \le L(\mathbf{U}_i^0, \mathbf{W}_i^0, \rho_i^0, \lambda_i^0) \le L(\mathbf{U}_i, \mathbf{W}_i, \rho_i^0, \lambda_i^0) \tag{25}$$

If the saddle point exists, $\mathbf{U}_i^0$ and $\mathbf{W}_i^0$ will minimize L, while λ_i^0 and ρ_i^0 maximize L. This fact is important for the coordination between the two levels of optimization in this problem because of the Lagrangian formulation. Note that ρ_i not a vector of pseudo variables but it is a vector of Lagrange multipliers associated with the inequality constraints.

$$\lambda = [\lambda_1 \quad \lambda_2 \quad \ldots \quad \lambda_N] \tag{26}$$

$$\rho = [\rho_1 \quad \rho_2 \quad \ldots \quad \rho_N] \tag{27}$$

Since λ and ρ has been assumed to be known at the first level, then the first level optimization will consist of obtaining $\mathbf{U}_i$ and $\mathbf{W}_i$ which minimize the corresponding i-th subsystem Lagrangian.

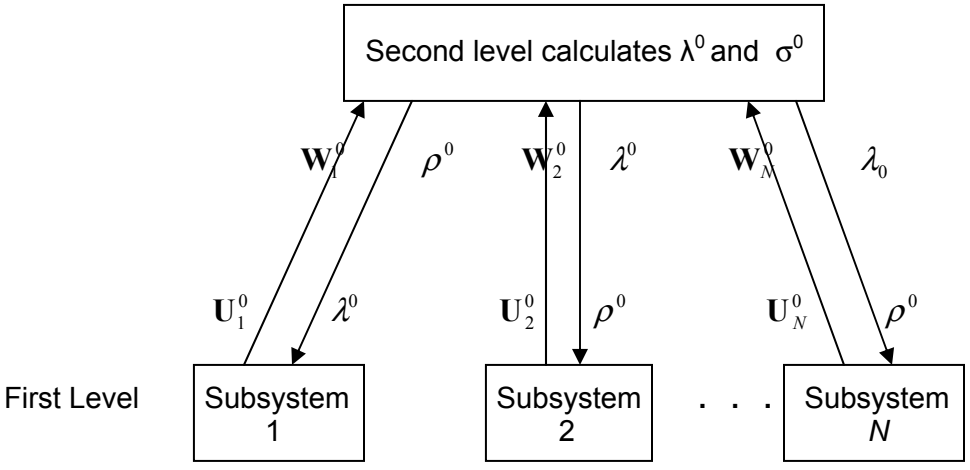

Figure 2. Schematic diagram of Two-level Optimization

With known values of $\mathbf{U}_i^0(\boldsymbol{\lambda}, \rho)$ and $\mathbf{W}_i^0(\boldsymbol{\lambda}, \rho)$ from the first level, the Lagrangian L of the whole CPS is maximized with respect to ρ and $\boldsymbol{\lambda}$ and this occur at the second level. This is an iterative procedure which terminates when convergence is achieved.

Economic Interpretation of λ_i The Lagrange multipliers λ_i associated with the equality constraints $\mathbf{W}_{i+1} = \mathbf{V}_i$ are of special interest. The two-level optimization approach studied in this paper is analogous to the operation of a perfectly competitive economic system. The λs are prices determined by the regional authority for the pollution caused by the subsystem. In turn, each subsystem must have a capability to determine its own policy on whether to pay the price specified by the regional authority for causing the degradation of the quality of the water body due to the waste effluent from the chemical processing plant or to invest its money in developing local waste chemical processing plants which in turn will improve the quality of its effluent discharge. If the total cost of improving the quality of the system by the regional authority as a whole is minimized, then the optimal policy for each subsystem can be reached and this is both economically and socially desirable.

Ideally, the regional authority should have the power to review engineering plans for individual plants to ensure that the polluters (users) can do with their claimed treatment efficiency.

3. TWO-LEVEL STRUCTURE

In this section we will discuss two-level structure for chemical processing system and water treatment system.

3.1. THE CHEMICAL PROCESS SYSTEM

The following formulation of the mathematical model is made for single chemical processing system called subsystem, then it is extended for *N* subsystem. The observed Chemical Process System is the pure chemical processing system and it does not includes waste water treatment system.

Based on the concept developed in the preceding section (see Figure 1) we will develop a general model for this system. The raw materials and energy enters the subsystem-*i* and they are imported from outside or from the other subsystems. For example, the optimal operation of steam reforming of hydrocarbon unit is of utmost concern to the industry. This is because steam reforming of hydrocarbons has established it self as the most economic and preferred process of the production of synthesis and hydrogen gas and the large value addition involved in the process as well as its high energy consumption coupled with energy cost.

The choice of feed stock for chemical processing system is largely by location, availability, and the local energy policy.

In this paper, a rigorous general model taking into account the presence of reactant, energy and catalysts used. There after, optimal operating conditions for the complete plant are obtained by considering simultaneous maximization of the main product and export flow rate and minimize the reactor heat duty for a fixed reactant feed rate. Reactor heat flux profile is considered a decision variable in optimization, thus predicting an optimal heat flux for Pareto- optimal solution.

In order to achieve at the best result, before develop the model, process description must be studied carefully. With this description, the model can be developed and thus followed by formulation of the optimization problem. For example, consider an urea producing plant (see for example Reference No. 1). Hydrogen is made from natural gas using high and low temperature converters, Hydrogen and steam is produced. Large part of Hydrogen is used for producing ammonia through a ammonia synthesis loop. Ammonia is then used to manufacture urea. Hydrogen, steam, and ammonia will also be exported to the other plants such as nitric acid plant, formic acid plant and hydrogen peroxide plant.

The profitability of operating a hydrogen plant will depend on the revenue generated from the sale of hydrogen and steam. When the generalized cost values can be obtained, these factors then can be combined into single parameter, the profitability function, to be minimized during optimization. Thus the optimization problem for hydrogen plant, the simultaneous maximization of the flow rates of product hydrogen, F_{hydrogen}, and the exported steam, F_{steam}, and this should be considered first.

The consumption of furnace fuel should also be considered as the third objective function to be minimized. The inclusion of consumption of furnace fuel, poses a difficulty due to the way in which the requirement of furnace fuel is determined in the model. By integrating the heat flux on the reformer tubes along the tube length, we can find the total heat duty required by the reformer, Q_R. Thus the minimization of Q_R, should be considered third objective function. Thus the objective functions of the optimization are

$$\left.\begin{array}{ll} Maximize & F_{hydrogen} \\ Maximize & F_{hsteam} \\ Minimize & Q_R \end{array}\right\} \tag{28}$$

The operating temperature, i.e., the catalyst tube wall, should not exceed 1200 K, because the reformer tube metal will creep under thermal stress, resulting in rupture (see Reference No. 8) and this can be expressed by the following equation

$$T_{W,max} \leq 1200 \text{ K} \tag{29}$$

Another constraint is based on thermodynamic consideration, to prevent the reversal shift reaction, i.e., the ratio of H_2O to hydrogen is to maintained in specified level say 0.3

$$\left[\frac{y_{H_2O}}{y_{H_2}}\right] \geq 0.3 \tag{30}$$

Two remaining constraints are the duties of heat exchanger and the total feed rate to the unit must conform to design margins. They are

$$Q_E \leq \alpha\, Q_{E,}\, max \tag{31}$$

and

$$F \leq \alpha\, F_{max} \tag{32}$$

where α is a specified constant.

The objective function Q_R is constrained by the fraction of the total reformer duty, Q_{SR}, supplied by furnace fuel, Q_{FF}, i.e.,

$$\frac{Q_{FF}}{Q_{SR}} = \beta \tag{33}$$

where β is a specified constant and it is based on the typical industrial values. (see Reference No. 6)

The axial heat flux profile of the reformer is a function of tube length x. The side fired system has many burners at varying height to provide greater flexibility in controlling the heat input to the reformer. For industrial application, the typical heat flux profile is quadratic with a dominant peak near the entrance. Two parabolic functions of are included are used to model the sections of the tube preceding and following the position, x^*, which the maximum flux occurred. Those functions are

$$q = A + B\left(\frac{x}{x^*}\right) + C\left(\frac{x}{x^*}\right)^2, \qquad z \leq z^* \tag{34}$$

and

$$q = A + B + C + D\left(\frac{x - x^*}{L}\right) + E\left(\frac{x - x^*}{L}\right)^2, \qquad z > z^* \tag{35}$$

The decision variables are taken from the operation of steam reformer, i.e., the variables that fully determine the operation of the steam reformer. These variables are the temperature at the inlet of steam reformer, $T_{\text{Reformer, in}}$, pressure at the inlet of steam reformer, $P_{\text{Reformer, in}}$, steam to carbon ratio at the inlet of steam reformer, $(S/C)_{\text{in}}$, hydrogen to carbon ratio at the inlet of steam reformer, $(H/C)_{\text{in}}$, the axial location in reformer tube where the maximum heat flux occurs, x^*. While A, B, C, D, and E are the coefficient of eqs. (34) and (35). These decision variables are described by the following bounds

$$T_{\text{Reformer, lower}} \le T_{\text{Reformer, in}} \le T_{\text{Reformer, upper}}, \quad (36)$$

$$P_{\text{Reformer, lower}} \le P_{\text{Reformer, in}} \le P_{\text{Reformer, upper}}, \quad (37)$$

$$(S/C)_{\text{in, lower}} \le (S/C)_{\text{in}} \le (S/C)_{\text{in, upper}} \quad (38)$$

$$(H/C)_{\text{in, lower}} \le (H/C)_{\text{in}} \le (H/C)_{\text{in, upper}} \quad (39)$$

$$A_{\text{lower}}\ \text{kcal m}^{-2}\text{h}^{-1} \le A \le A_{\text{upper}}\ \text{kcal m}^{-2}\text{h}^{-1}, \quad (40)$$

$$B_{\text{lower}} \le B \le B_{\text{upper}}\ \text{kcal m}^{-2}\text{h}^{-1}, \quad (41)$$

$$C_{\text{lower}}\ \text{kcal m}^{-2}\text{h}^{-1} \le C \le C_{\text{upper}}, \quad (42)$$

$$D_{\text{lower}}\ \text{kcal m}^{-2}\text{h}^{-1} \le D \le D_{\text{upper}}, \quad (43)$$

$$E_{\text{lower}}\ \text{kcal m}^{-2}\text{h}^{-1} \le E \le E_{\text{upper}}\ \text{kcal m}^{-2}\text{h}^{-1}, \quad (44)$$

and

$$x_{lower} \le x^* \le x_{upper}, \quad (45)$$

while the remaining decision variable is the adiabatic HT shift converter :

$$T_{\text{Reformer, lower}} \le T_{\text{Reformer, in}} \le T_{\text{Reformer, upper}}, \quad (46)$$

The subscript 'upper' denotes the upper limit and 'lower' denotes the lower limit of each decision variables, respectively.

Now, the problem of optimization for the hydrogen plant can be written as

$$\left.\begin{array}{l} \textit{Maximize} \quad F_{hydrogen} \\ \textit{Maximize} \quad F_{steam} \\ \textit{Minimize} \quad Q_{SR} \\ \textit{Subject to} \quad T_{W,max} \le 1200 \\ \left(\dfrac{y_{H_2O}}{y_{H_2}}\right) \ge 0.3 \\ Q_{E_i} \le \alpha Q_{E_{i,masx}} \qquad i = 1,2 \\ F \le \alpha F_{max} \\ \dfrac{Q_{FF}}{Q_{SR}} \ge \beta \end{array}\right\} \quad (47)$$

Equation (47) is the multi-objective optimization problem and it can be solved numerically by the methods available. The use of the surrogate worth trade-off method, after decomposition will lead to the problem of hierarchical multi-level optimization. (See Reference No.3)

3.2. WATER SYSTEM: INDUSTRIAL AND NON INDUSTRIAL USES

The following formulation of the mathematical model is made for the river which is polluted by nearby process industries. Suppose we have a river is segmented into *r* reaches, *p* of which are associated with polluters who discharge organic wastes into the stream (see Figure 3) Since data are available only for dissolved oxygen standards, the model is a relatively simple one. We will make a relation to transform minimum dissolved oxygen standards for each reach into a set of linear inequalities relating upstream treatment levels to downstream decisions.

Model Formulation The constraints require that the supply of available oxygen for the organic decomposition process in each reach (that available above the quality standard requirement) must be equal to or exceed the demand imposed by BOD loads discharged into that reach and all reaches preceeding it. Thus, for reach *i* it is required that:

$$d_{i1}b_1(1 - x_1) + d_{i2}b_2(1 - x_2) + \ldots + d_{ii}b_i(1 - x_i) \le \sigma_i \quad (48)$$

where

b_j = gross biological oxygen demand (BOD) load introduced at the beginning of the *j* th reach that has a polluting input (kg/day).
x_j = percentage of b_j removed through treatment by the *j*th polluter
d_{ij} = kgs of oxygen demanded by the decomposition of a pound of BOD discharged by the *j*th polluter in reach *i*
σ_i = amount of dissolved oxygen available for decomposition process (total available less standard requirement) in reach I per unit of flow.

The system of inequality constraints Eq.(48) can be rewritten more compactly as follows:

$$a_{i1}x_1 + a_{i2}x_2 + \ldots + a_{ii}x_i \geq c_i \qquad (49)$$

where

$$a_{ij} = d_{i1}\, b_j$$

and

$$c_i = a_{i1} + a_{i2} + \ldots + a_{ii} - \sigma_i$$

In addition, other restrictions on x_j's are $w_R < x_j < T_{upper}$, j = 1,….,R, which ensure that all discharges be subjected to at least primary treatment. In general, primary treatment involves chlorination, filtering, and settling to reduce bacteria and remove bulky solids. Such sewage treatment usually remove about $100w_R$ % of the gross BOD waste load. Also 100 T_{upper} % is assumed to be the upper treatment limit.

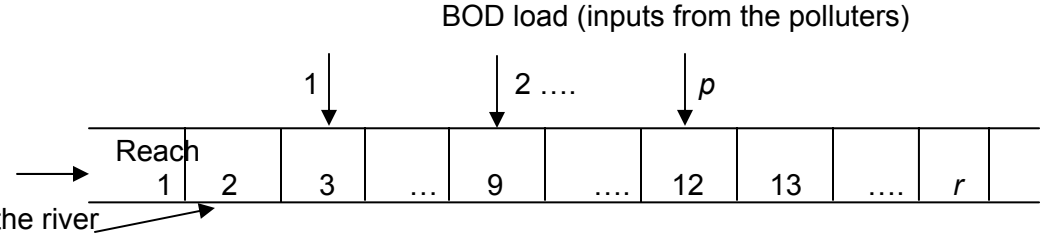

Figure 3. The decomposition structure of a river

If $f_i(x_j)$ is the treatment cost function of the *j*th polluter. Then the optimization problem for the River takes the following forms:

$$\min \sum_{p=1}^{P} f_p\left(x_p\right) \qquad (50)$$

subject to

$$\begin{aligned} a_{11}x_1 &\geq c_1 \\ a_{21}x_1 + a_{22}x_2 &\geq c_2 \\ \cdots & \\ a_{r,1}x_1 + a_{r2}x_2 + \ldots + a_{rp}x_p &\geq c_R \end{aligned} \qquad (51)$$

and

$$w_R \leq x_j \leq T_{upper} \qquad j = 1,2,\ldots, p \qquad 52)$$

where

$$f_j(x_j) = \gamma_{j1}\, x_j^2 + \gamma_{j2}\, x_j + \ldots + \gamma_{jm} \qquad j = 1,2,\ldots, p$$

and γ_{jk} are known constants. Values for the constants a_{ij}, c_i, γ_{jk} are available.

There are two types of second level coordination schemes are presented for the decentralized decision-making process. The first assumes knowledge of the local treatment cost functions by the regional authority while the second assumes no such knowledge.

Pseudo-Decentralized Decision Process For this type of decision process, we assumed that the regional authority, RA, has a complete knowledge of the local treatment cost function. The basis of the multi level scheme utilized in this section is duality in non linear programming and the saddle point concepts. The optimization problem represented by Equation (50)-(52) will be called the primal problem. This problem forms the Lagrangian function $L(\mathbf{X}, \lambda)$ for the primal problem as follows:

$$L(\mathbf{X}, \lambda) = \sum_{i=1}^{p} f_j(x_j) + \sum_{j=1}^{r} \lambda_i \left(c_j - \sum_{i=1}^{p} a_{i1} x_i \right) \tag{53}$$

where λ_i are Lagrange multipliers $j = 1,2, ..., r$

$$\lambda^T = [\lambda_1, \lambda_2, \ldots\ldots \lambda_r]$$

$$\mathbf{X}^T = [x_1, x_2, \ldots\ldots x_p]$$

Lets define a dual function $G(\lambda)$ as follows:

$$G(\lambda) = \min L(\mathbf{X}, \lambda) \tag{54}$$

where

$$S = \{w_R \le x_i \le T_{upper} \qquad i = 1, 2, \ldots, p \}$$

Then the dual function $G(\lambda)$ is defined over the domain D, where

$$D = \{\lambda ; \lambda \ge 0: G(\lambda) \text{ exists } \}$$

Since, for all $\lambda \ge 0$, $L(\mathbf{X}, \lambda)$ is continuous in $\mathbf{X}$ for all $\mathbf{X} \in S$, and S is closed and bounded, by the Weierstrass theorem, $G(\lambda)$ exists. Thus

$$D = \{\lambda ; \lambda \ge 0\}$$

Suppose

$$F(\mathbf{X}) = \sum_{j=1}^{p} F_j(x_j)$$

And the dual problem can be written as

$$\min_{\lambda \in D} G(\lambda) \tag{55}$$

The Lagrangian $L(\mathbf{X}, \lambda)$ possesses a saddle point at $(\mathbf{X}^0, \lambda^0)$ if and only if $\mathbf{X}^0$ solves the primal problem and λ^0 solves the dual problem. Thus

$$F(\mathbf{X}^0) = G(\lambda^0) \tag{56}$$

This preceding argument suggest that it is possible to decompose the problem into subsystem, solve them to obtain the firs-level solution, and coordinate these subsystems by choosing the multipliers, λ, to solve the dual for the second-level solutions so that their combined solutions solve the primal. The coordinator will have the task of maximizing G, subject to λD, If the Lagrangian $L(\mathbf{X}, \lambda)$ of the primal problem is separable in $\mathbf{X}$.

Since each $f_j(x_j)$ is a function of a single variable x_j and the coefficient terms λ_i are linear, $L(\mathbf{X}, \lambda)$ is readily decomposed into p independent subsystems

$$L(\mathbf{X}, \lambda) = \sum_{j=1}^{p} L_j(x_j, \lambda) + L_0(\lambda) \tag{57}$$

where

$$L_j(x_j, \lambda) = f_j(x_j) - \left(\sum_{i=1}^{r} \lambda_i a_{ij} \right) x_j \qquad j = 1, 2, \ldots, p \tag{58}$$

and

$$L_0(\lambda) = \sum_{j=1}^{r} \lambda_j c_i \qquad (59)$$

Note that : for this case $L(\mathbf{X}, \lambda)$ additively separable with respect to x_js and L_0 (λ) is a function of λ only, and is taken care of at the second level.

The outline of multilevel structure of the optimization problem is depicted by Figure 4. From the figure we see that at the first level, λ is assumed to be known. This means that the first level optimization consists the procedure of obtaining $x_j(\lambda)$ which minimizes the corresponding jth subsystem Lagrangian , L_j, subject to $w_R \le x_j \le T_{upper}$

G(λ) is evaluated at the second level, with known values of x_j(λ)'s from the first level. The new multipliers λ are chosen so that G(λ) is increased. The same procedure is repeated until G(λ)is maximized. ($\mathbf{X}^0$, λ^0) is the optimal solution to the system, if, upon termination of the procedure, λº solves the dual and some Xº is primal feasible. It can be also noted that in this case the primal value is the same as the dual's.

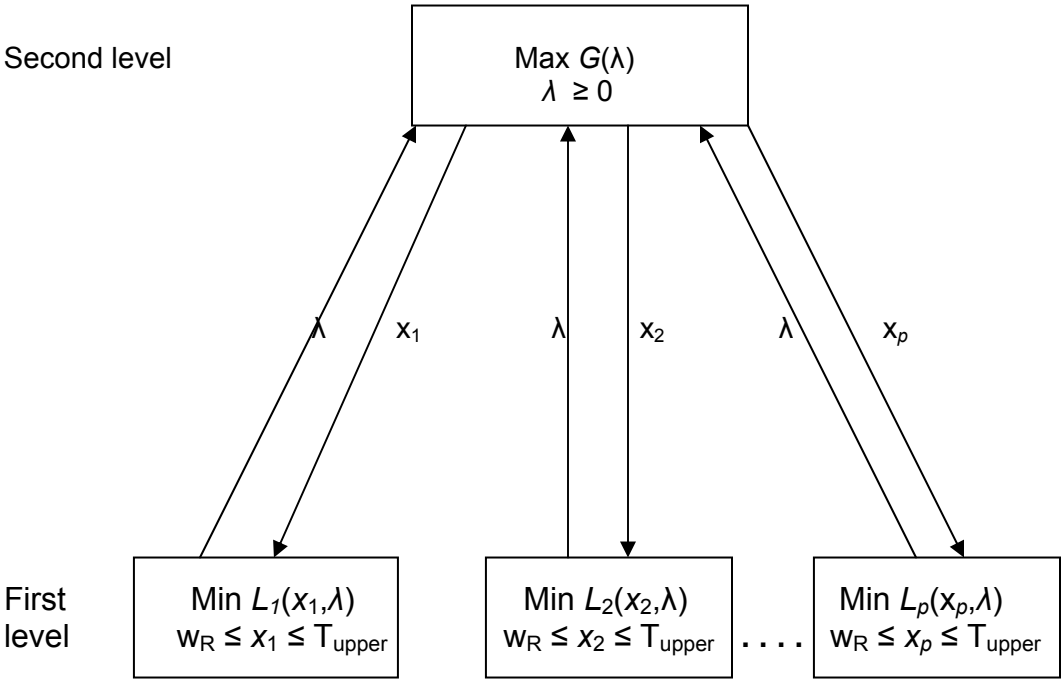

Figure 4. The two-level optimization structure

For general classes of problems, the existence of a saddle point cannot be guaranteed. But, problems with convex objective and constraint functions under generous conditions must have a saddle point.

Computational algorithm and Economic interpretation of the level procedure

1. Set k = 0. Choose initial values $\lambda^{(k)} > 0$. Set k = 1, go to Step 2
2. Solve the first level with $\lambda = \lambda^{(k)}$, obtaining a solution $X(\lambda^{(k)})$ subject to $w_R \le X \le T_{upper}$
3. Form the dual function $G(\lambda^{(k)}) = (X(\lambda^{(k)}), \lambda^{(k)})$ by adding the first level sub Lagrangians and $L_0(\lambda)$.Calculate the gradient $\nabla_\lambda G\left(\lambda^{(k)}\right)$whose elements are

$$\left.\frac{\partial G}{\partial \lambda_i}\right|_{\lambda^{(k)}} = c_i - \sum_{j=1}^{p} a_{ij} x_j \qquad i = 1,2,...,r$$

4. Define a direction of search $\mathbf{d^k}$ by

$$d_i^{(k)} = \begin{cases} \left.\dfrac{\partial G}{\partial \lambda_i}\right|_{\lambda^{(k)}}, & \lambda_i^{(k)} > 0 \\ max\left\{0, \left.\dfrac{\partial G}{\partial \lambda_i}\right|_{\lambda^{(k)}}\right\}, & if \quad \lambda_i^{(k)} = 0 \\ \\ i = 1,2,...,r \end{cases}$$

Choose a new vector $\lambda^{(k+1)}$ by

$$\lambda^{(k+1)} = \lambda^{(k)} + t_k \, \mathbf{d}^{(k)} \tag{58}$$

where

$$\mathbf{d}^{(k)} = [d_i^{(k)}, d_2^{(k)}, \ldots\ldots, d_r^{(k)}]$$

The step size t_k is selected so that it maximizes $G(\lambda^{(k)} + t_k d^{(k)})$ subject to $t_k \geq 0$ and $\lambda^{(k+1)} \geq 0$. For this selection of optimal t_k , a Fibonacci-Search technique can be employed.

5. If $G(\lambda^{(k+1)})$-$G(\lambda^{(k)}) <$`ε (i.e., the convergence is achieved) then stop. Else, set $k = k + 1$ and return to Step 2.

An interesting economic interpretation will come to existence when we use the gradient algorithm in the two-level optimization procedure. The economic interpretation of first-level subsystems is that it represents the costs to each local polluter. While the social total cost of river basin-wide regional authority (RA) was the second level economic interpretation.

The local polluter have to plan their treatment levels (x_j's), minimizing their costs and report them to the RA according to the λ^* announced by the RA. After responses is given by the local polluter, the RA forms the dual function which is the sum of the first –level minimum :

$$G(\lambda) = \sum_j^p L_i\left[x_j(\lambda), \lambda\right] + L_0(\lambda) \tag{59}$$

The gradient component of G at λ^* is given by

$$\left.\frac{\partial G}{\partial \lambda_i}\right|_{\lambda^*} = c_i - \sum_{j=1}^p a_{ij} x_j \qquad i = 1,2,...,r \tag{60}$$

which are actually the slacks of the inequality constraints Eq (31) and may be viewed as excess demands for oxygen in each reach. By step 4 , the gradient algorithm requires that λ_i^* be increased if excess demand is positive and decreased otherwise, unless $\lambda_i^* = 0$ .This is a familiar price-adjustment rule of fundamental economics. Thus, upon solving the second level, the RA has a new measure of the economic value (marginal cost) associated with supplying the ith reach with an additional pound of oxygen per day. These are the Lagrange multipliers λ_i. Note that λ_i^* are non-negative and that, for those constraints they are binding, they are positive.

Each local polluter's has the problem of the following form

$$\min_{w_R \leq x_j \leq T_{upper}} \left\{ f(x_j) - \sum_{i=1}^r \lambda a_{ij} \right\} \qquad j = 1,2,...,p \tag{61}$$

The term $f(x_j) - \sum_{i=1}^r \lambda a_{ij}, \quad j = 1,2,...,p$ in Eq (36) can be viewed as the cost, for which the jth polluter is responsible, in abating the chemical pollution. This interpretation comes from the fact that $a_{ij} = d_{ij}$ represents the oxygen demand in reach i to meet the untreated waste effluent load incurred by the jth polluter, the term $\sum_{i=1}^r \lambda_i a_{ij}$. Hence, the $\sum_{i=1}^r \lambda_i a_{ij}$ is the tax (effluent charges) imposed by the RA for the pollution caused by the jth polluter. Each polluter can determine whether to pay the specified tax by the

regional authority for causing the degradation of the quality of chemical or to invest his money in developing a local waste water treatment plant to decrease his taxes.

Computational analysis Computational analysis is summarized as follows:

1. The iteration started with initial Lagrange multipliers, λ_1, λ_1, …, $\lambda_{r-1} = 0$ and λ_5 is finite number less then ten.
2. The slow convergence after a few rapid initial iterations is characteristics of the steepest descent method used. Other accelerated gradient methods are recommended for practical calculations. In particular, since the dual problem is quadratic in the Lagrange multipliers, the gradient methods of Fletcher and Powell, and Fletcher and Reeves, applied at the second level would find the optimal solution in fewer iterations
3. There does not exist a standard programmed code for the multilevel approach and one must program one's own for each problem. However, since the whole problem is decomposed into subsystems, programming logic is quite simple and easy to "debug"

Complete Decentralized Decision Process In forming this model, it is assumed that the regional authority has no knowledge of the local treatment cost functions, $f_j(x_j)$, $j = 1, 2, \ldots, p$ and this situation often arises when private industries are not interested in releasing proprietary information regarding their industrial processes.

Now, as as in the preceding section, let us form the system Lagrangian $L(\mathbf{X}, \lambda)$ as

$$L(\mathbf{X}, \lambda) = \sum_{j=1}^{p} f_j(x_j) + \sum_{i=1}^{r} \lambda_i \left[c_i - \sum_{j=1}^{p} a_{ij} x_j \right] \tag{62}$$

and may be rearranged to yield

$$L(\mathbf{X}, \lambda) = \sum_{j=1}^{p} f_j(x_j) + \sum_{i=1}^{r} \lambda_i c_i - \sum_{i=1}^{r} \sum_{j=1}^{p} a_{ij} x_j \tag{63}$$

Taking summations over j, we have:

$$L(\mathbf{X}, \lambda) = \sum_{j=1}^{p} f_j(x_j) + \sum_{j=1}^{p} \left[\sum_{i=1}^{r} \frac{\lambda_i c_i}{p} - \sum_{i=1}^{r} a_{ij} x_j \right] \tag{64}$$

An appropriate grouping of terms can be applied to the Subsystem Lagrangians, $L_j(x_j, \lambda)$, thus we have

$$L(\mathbf{X}, \lambda) = \sum_{j=1}^{p} L_j(x_j, \lambda) \tag{65}$$

where

$$L_j(x_j, \lambda) = f_j(x_j) + \sum_{i=1}^{r} \frac{\lambda_i c_i}{p} - x_j \sum_{j=1}^{r} \lambda_i a_{ij} \tag{66}$$

In the last equation (39), the jth user views the $L_j(x_j, \lambda)$s as the performance function to be minimized by him at the first level.

Computational algorithm The computational procedure for is described in Fig 5. The algorithm is essentially a steepest ascent description of the law of supply and demand. The following gives an outline of the computational procedure.

The Regional Authority (second level) initially specifies zero tax rates, i.e., $\lambda_i = 0$, for all i chemical processing unit. The p discharges respond at the first level with the minimum level of $100w_R$ % removal of BOD. The RA receives this information and checks the r constraints for violations by substituting the first level, minimizing values of x_j into the constraint set. If some violations occur and finite related components of the tax vector λ are increased, using step size option No 2 and transmitted to the first level of the second iteration.

The tax for each chemical processing unit is affected by the total vector of tax rates. All upstream decisions will be affected by a single increase associated with the last (r^{th}) reach. Hence, a number changes should bring about a dramatic response. This occurs while some dischargers respond with

near-maximum levels of treatment efficiency, and the constraints are satisfied. The taxes thus decreased because feasibility has been reached. The Computational procedure can be outlined by the following algorithm (See Figure 5).

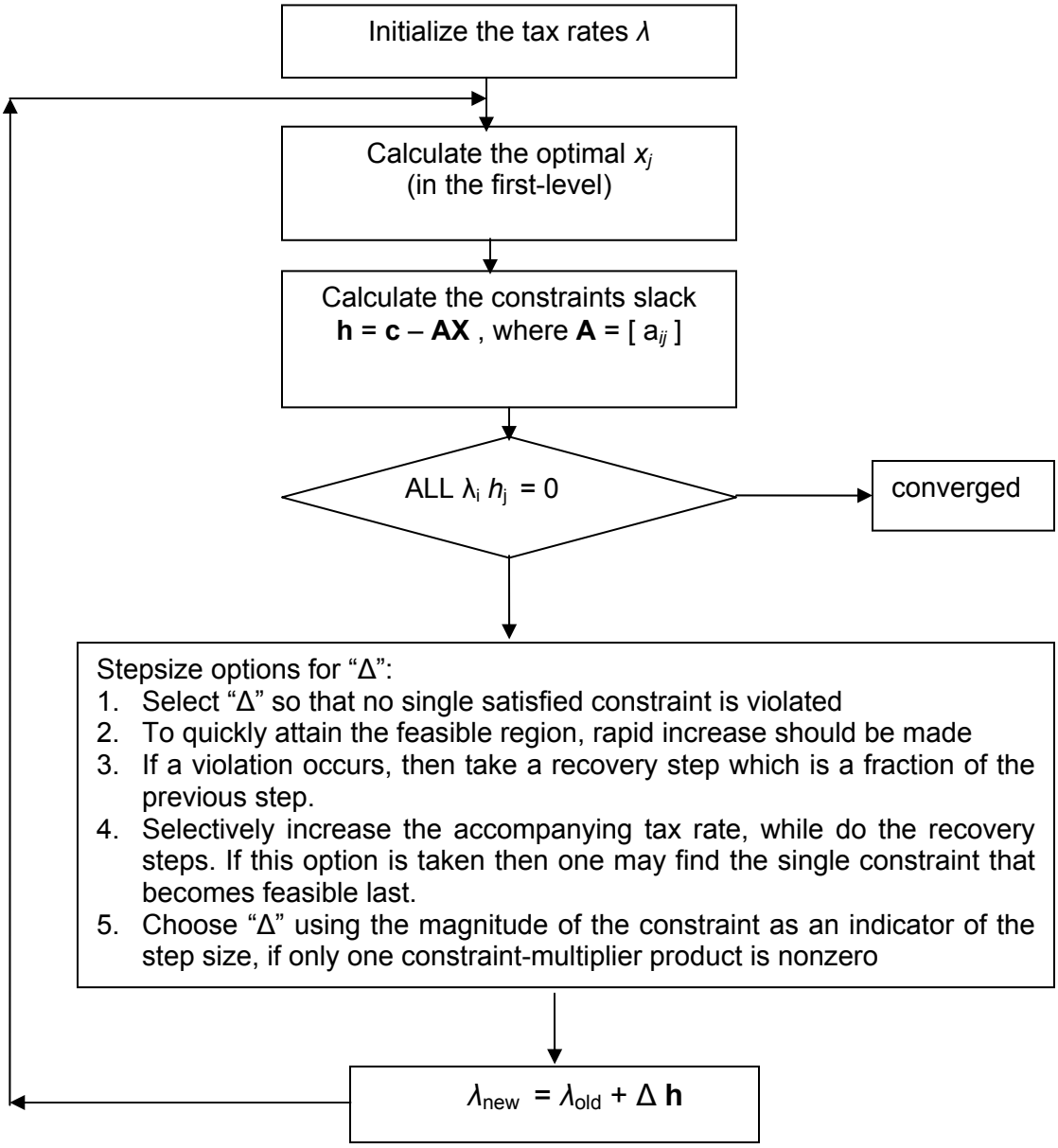

Figure 5. Computational Procedure

The above algorithm can be outlined as follows. By examining the constraint slacks for each i Determine reach l which is the closest to violate the constraints so that the absolute values of h_ls is less than that of h_is, i.e.,

$$l = i \quad \text{so that} \quad |h_l| < |h_i| \quad \text{for all } i \tag{67}$$

where

$$h_i = c_i - \sum_{i=1}^{r} a_{ij} x_i \tag{68}$$

Then reduce the tax rate at the kth reach to zero :

$$\lambda_k \text{ (new)} = \lambda_k\text{(old)} + \Delta h_k = 0 \quad (69)$$

This condition is enforced by solving for the unknown stepsize :

$$x = -\lambda_k\text{(old)}/h_k \quad (70)$$

This is the essence of step size option No. 1 in Fig. 5. New tax rates are calculated and transmitted to the first level, which then respond with new treatment levels.

The second level (RA) checks for new violations: however, at this iteration, none exist. The convergence criterion that all $\lambda_i h_i$ products be zero is next checked. There are now some finite nonzero $\lambda_i h_i$ products. Since the constraints are satisfied, option 1 is used again. Furthermore, this procedure of forcing tax rate components to zero is successfully repeated until less nonzero products remain when the constraints are again violated. Recovery steps (option No. 3) are made until the critical constraint (i.e., the constraint that upon recovery steps is the last to become feasible) is found to be the twelfth .This tax rate is then selectively raised (option No. 4). The constraints are once again satisfied and the algorithm attempts to force all $\lambda_i h_i$ products to zero. Finally, there is only one nonzero product remaining. The tax rate is then fine-tuned (option No. 5) by considering the constraint magnitude which is being driven to zero.

Computational analysis. The following observations can be made concerning the computational procedure.

1. The optimal treatment efficiencies are the least sensitive factors in the model.
2. The level of taxing is of median sensitivity and was chosen for the stopping criteria (as $\lambda_i h_i = 0$).
3. It would have been better to enter the feasible region less vigorously. This might save many iterations.
4. Selective increase of a single tax should have been a higher magnitude to reduce repeated increases of the same tax component.
5. The most difficult task was to select the step sizes for the different step size options.

4. THREE-LEVEL STRUCTURE OF CHEMICAL PROCESSING SYSTEM

In the previous section we have discussed the two-level structure and the capacity of the regional system is not considered as a variable to be optimized. This is the reason why we extend this two-level structure of optimization to the three-level structure. Thus, we can state the new regional problem as follows. Find an optimal processing configuration for meeting the quality standards of products considering the possibility of a regional waste treatment plant, while simultaneously determining the pollution taxes to achieve this configuration when the Regional Authority does not necessarily know the treatment cost.

In this section we will not repeat the detailed mathematical formulation developed in previous section here because the three-level hierarchy can be constructed with only a minor extension. Again the chemical processing system is decomposed into *n* subsystem and the water system of the river is decomposed into *r* reaches. In the water system, at the head of each reach is an effluent discharge from a polluter or change in the hydraulic characteristic of the river, such as turbidity, surface area exposure or the inflow of tributary.

Solution Procedure We have assumed that the Regional Authority does not necessarily know the treatment cost functions of the chemical processing plants (the individual polluters), the optimization problem must decomposed into sub-problems in order to facilitate its solution.

In this case The Dantzig-Wolfe decomposition cannot be applied because the optimal taxing structure, the optimal regional plant size and regional treatment level must also be determined.

When we apply the hierarchical multi level approach, the overall optimization problem must be decomposed into a set of hierarchically ordered sub-problems and the solution of this sub-problems are then coordinated so as to obtain an optimal solution to the original problem.
Any optimization technique may be used in this level because there is no restriction as to how the sub-problems at the first-level can be solved. In this approach, the second and the third-level controller must be chosen more carefully.

Three levels approach of optimization are introduced for the solution of the regional problem. Individual polluters or chemical processing plants are at the first level. Regional treatment plant is at the second level, while the third level is occupied by Regional Authority. Figure 6 illustrates how the decomposition works, how the information exchanged between levels and how this information is updated and coordinated so that the optimal solution to the problem is obtained.

The function of Regional Authority (third level function's) is to propose a tax structure to the lower levels and this tax structure is based on marginal cost to society of adding an additional kilogram of waste chemical (for chemical processing plant) or adding additional kilogram of dissolved oxygen into each reach of the river (for water resource system). The marginal cost are the Lagrange multipliers, i.e., the shadow prices of the binding constraints of the overall optimization problem. It means that if a constraint is not binding, i.e., there is no excess of waste chemical to the regional plant (for chemical processing plant) or there is a excess of dissolved oxygen in that reach (for water resource system), there is no tax on the reach. For water resource system, the BOD load discharged untreated by the regional plant is taxed in the same manner as the local plants are charged. The solution process is initiated by the Regional Authority by estimating all of the shadow prices and then determines tax structure based on these shadow prices. The obtained tax structure is then sent down to the lower levels for processing and it will be discussed later in this paper. This tax structure is processed by the lower levels and the results are passed back up to the Regional Authority as optimal treatment levels. These treatment levels is used by Regional Authority to check the river or the effluent of the treatment plant quality constraints to determine whether the previous taxing structure was too high, i.e., there is no binding constraints, too low where some constraints are violated, or optimal that is no constraints are violated but some constraints binding. The new tax structure must be developed if the previous tax structure is not optimal. The development of the new tax structure must be based on the previous tax structure. For this problem, the new tax structure is updated by a gradient search technique using updated step sizes to converge toward the optimal solution. (see for example Reference No. 7).
The second level function is to determine an optimal regional plant treatment level and optimal regional plant size., and to issue charges based on the regional treatment cost to the polluter (chemical processing plant).

The second level assumes a given regional plant size based on the prediction of which chemical processing plants or polluters ship their waste water or waste chemical to the regional plant. This action is taken based on the given tax on the regional plant which is determined by the third level. The second level then computes an optimal regional treatment level and results on the regional treatment cost. The regional treatment cost is then divided among the chemical processing plants (the polluters) assumed to shipping their wastewater or waste chemicals to the regional plant on the basis of the total wastewater or waste chemicals shipped. The tax on the regional plant is divided among the chemical processing plants assumed to be using the regional facilities on the basis of BOD and COD load shipped to the regional plant. This cost information is then sent down to the first level and the first level then uses this additional information to determine which chemical processing plants (polluters) actually would ship their waste to the regional plant. The information is then returned to the second level where the process stops and all information is passed up to the third level. This process of returned information to the second level occurs if the previous prediction of which the chemical processing plant (polluters) will ship to the regional plant is correct. But, if the previous prediction is not correct or if the difference is greater then a specified tolerated error, the prediction is updated on the basis of the result obtained. The new regional plant size is determined, also a new optional regional treatment cost is calculated and the process is repeated until the predicted plant size and the actual

number of chemical processing plants who do the ship agree. In this case, the predicted plant size is the prediction when chemical processing plant will ship.

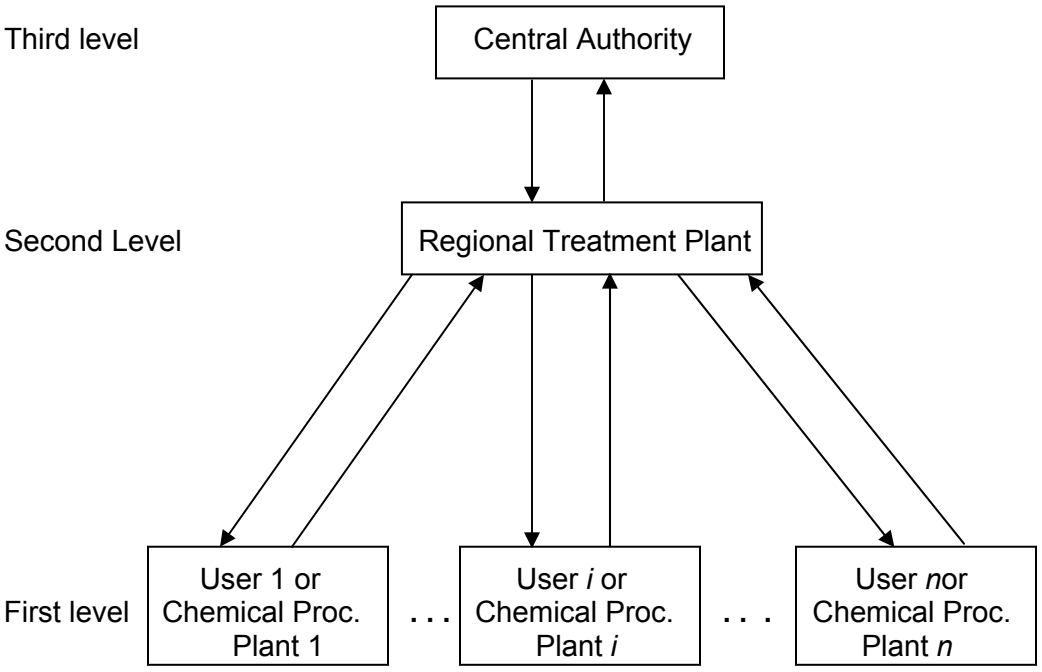

Figure 6. Three-level structure

In this problem, the routine to be used to update the prediction of the regional plant size is a modified Gauss-Siedel routine. The optimization problem at the first level was solved by satisfying the Kuhn-Tucker condition for stationary. The treatment level determined in this manner was not allowed to violate the treatment level constraints.

To determine the optimal treatment cost for each chemical processing plant, is the first-level optimization function and it involves determining whether or not to ship to the regional plant and what is the optimal local treatment level. Thus, the optimal treatment cost policy can be determined by solving the following minimization problem.

Min(cost of local treatment + local tax + cost of regional treatment +
cost of piping to regional plant + regional tax) (71)

Assuming that the waste is treated at the local plant to each chemical processing plant, the first level determines optimal local treatment level. This occurs if a given regional treatment cost and the regional tax is determined by the second level while a local tax is determined by the third level. Upon using this treatment level, the local treatment cost and local tax are computed for each chemical processing plant. This local cost is then compared to the cost of regional waste treatment for each plant. The most economical treatment method is selected and the resulting information is passed back up to the higher levels. Figure 6 illustrates the three-level optimization technique in solving this kind of problem. This three level approach can be expanded to include several regional treatment plans.

5. CONCLUSION

In practice, chemical processing system is a large scale industrial problem and it has been decomposed into subsystems and then optimized empirically or using rigorous mathematical base. In

two-level approach, the responsibility for the engineering of each subsystems is assigned to the individual engineering groups which is called first-level. The groups of the first level are only responsible for the design of their subsystem and they need not directly concern themselves with the sign of any other groups. The responsibility of for the overall system behavior is the responsibility of the coordinating group. This second-level group is divorced from the need of considering the details of the subsystems. They are charged only for assuring the cooperation between other groups in the first-level in achieving the system goal.

The two-level optimization scheme as discussed in Sec 3 can be extended to include three or more levels of optimization. In waste water treatment system, the user, i.e., the polluters such as chemical processing plant etc, is offered the options: (1) to treat his effluent locally, or (2) to ship it to the co-op treatment plant or (3) to ship it to a regional treatment plant. And three-level optimization discussed in Sec 4 is used for this extension.

The hierarchical approach via the three-level optimization scheme provides an important tool in chemical quality as well as water quality management in chemical processing system, whether in the stage of planning and design, operation or development. Since the chemical processing problems are hierarchical in their nature, mathematical models constructed to represent these problems should have the same structure. By providing the suitable coordination scheme among the subsystems in the hierarchy, the multi-level approach can handle such hierarchical models. This, however, makes the approach desirable and tractable.

6. REFFERENCES

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