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Hierarchical Optimization in isotope separation - Gaseous diffusion : Plant - Cascade - Stage - Principios and applications

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The large scale system represented by a gaseous diffusion plant model, and its hierarchical mathematical structure are the reasons for a decomposition method, minimizing the total cost of enrichment. This procedure has been used for years in the optimization problems of the french projects.

INTRODUCTION

1. Theoretical studies, laboratory work, pilot experiments, economical and industrial analyses have been pursued in France since several years in the gaseous diffusion field. This results in a relatively complex model simulating a plant with good accuracy. The hierarchical structure of the mathematical model leads to a decomposition technique of the global plant system, authorizing a practical utilisation. In particular the optimization of a large number of variables is possible by this multilevel approach. There is an increasing amount of research in the area of decomposition techniques of large scale systems and some general applications have been recently widely publicized (Mesarovic and Pestel). This communication is devoted to the specific decomposition method of a gaseous diffusion plant model, which has been effectively used for optimizing real projects. More than twenty variables have been optimized using this method, requiring a reasonable calculation time on a computer. The first part of this paper will introduce the method of multi-level decomposition. Then the application to a gaseous diffusion plant will be described. The third part will present a direct optimum-seeking algorithm, specifically developed for this problem, and treating mixed variables (discrete and continuous), with discontinuities in the objective function and constraints. This algorithm is used for two out of the three sub-optimizations, the whole procedure being programmed for a computer. The paper is concluded with remarks on possible extensions of this method.

Theoretical introduction to multi-level decomposition

2. Optimization of a large process is sometimes impossible to perform in a single integrated way because of the complexity, non linearity and the large number of degrees of freedom involved. The optimum-seeking methods dealing with all the variables simultaneously, do not work, or at best consume too much time.

For handling such complex problems, several new optimization methods are being developed (Lasdon, Mesarovic, Wilde, Wismer) and systems analysis and decomposition have recently received world wide applications. The successful way of solving this kind of problems involves the decomposition of the large scale system into a number of smaller sub-systems, each one containing its own goals and constraints. Then the sub problems may be solved specifically because their size is amenable to precise solutions. But it is clear that these sub-problems are interrelated, and the main difficulty is to ensure coordination between the various parts for assuming overall optimal result. In fact, optimizing a sub-system without paying attention to the effect of interaction would be detrimental to other parts, so that the overall performance would be worse than without any optimization. This optimization problem finds an equivalent in the actual design field, where some large industrial process exceeds the ability of a single team of engineers. The solution is to allocate the responsibility among several specific teams, and to coordinate properly their efforts to achieve the final goal.

3. Depending upon the structure of the model, several different decomposition techniques are available. Calculus of variations, linear programming, dynamic programming, maximum principle are some of these tools. We are interested here in the hierarchical structure, that is a vertical arrangement of sub systems which comprise the overall system, in which a given level controls or coordinates the units on the level below it and in turn is controlled by the units on the level above it. The figure 1 is extracted from Mesarovic and illustrates the vertical interactions. The optimization of this system is accomplished by introducing new variables, called pseudo-variables or coordinating variables. Then each level is separately and independently solved using the optimization techniques properly suited to the nature of the sub problem.

The sub-systems are then joined together by coordinating variables, treated by second level controllers, to induce the first-level systems into choosing the solutions which in fact correspond to an overall system optimum. A good example illustrating the decomposition and multi-level approach is given by Barnett. Let us consider a company with N departments, each having a manager reporting to the president of the company. The sole objective of the i th manager is to maximize the performance function of his own department by acting on his own decision variables. The president's objective is to maximize the performance of the company as a whole. He succeeds by imposing internal prices for "sellings" and "buyings" between the departments to control supplies and demands for interdepartment products. The company's overall optimal policy is achieved through an interactive procedure. The separate optimization of each department does not necessarily imply the overall maximization of the company's performance, unless the performance of each department is coordinated at a higher level, i.e. by the president.

4. In the field of isotopic separation, it is easy to discover interacting parts, each involved in a specific goal. But the unit separative cost, would not be minimized without coordinating the sub-systems. A preliminary example could be given, decomposing the gaseous diffusion process into two basic stage components, i.e. barrier and compressor (fig.2). Of course the best barrier and the best compressor must be adapted one to the other so that the two design teams involved in their development have to take into account their interaction when acting on their own decision variables. This is easily obtained by the coordinating variable P , pressure level, whose optimum choice has to be made at the upper level of overall stage performance (fig.3), represented by the specific energy consumption $W/\Delta U$ in this oversimplified example. (The real case would of course involve many other components and parameters).

Application of the decomposition method to a gaseous diffusion plant model

5. The starting formulation for the general optimization problem could be the following: "Define the optimal C_D plant for producing given products P 's at given enriched enrichments N_p 's, choosing every free design and operating variable for that plant and its components, in order to minimize the product cost C_P , for given technical and economical data" (see fig.4). An alternate and even more usual way to define the purpose of the plant lies in its separative capacity ΔU . It is shown in the literature (Benedict, Cohen, Von Halle, and others) that the separative capacity is directly proportional to the amount of product, as shown in the relation:

$$\Delta U = P \left[V(N_p) + \frac{N_p - N_F}{N_F - N_W} V(N_W) - \frac{N_p - N}{N_F - N} V(N_F) \right] \quad (1)$$

where $V(N) = (2N-1) \log \frac{N}{1-N}$ (value function).

The expression in brackets in (1) is a function of the external assays: $E(N_p, N_F, N_W)$, with only one free variable: the tails assay N_W . So, when N_W is imposed or optimized, it is equivalent to use separative capacity or production to describe the plant. (The figure 5 illustrates the relation (1)). The overall optimization is performed at three levels, from the highest to the lowest, namely: plant, cascade and stage.

6. Plant level. It is convenient to consider two parts in this level: tails assay and intermediate assays.

6.1 The determination of the tails assay N_W , gives the best compromise between the natural uranium feed cost and the separative work cost, which minimizes the product cost. A conventional formulation is

$$C_p = \frac{1}{P} \left[C_0 P + C_\Delta \Delta U \right] \quad (2)$$

in which C_p unit product cost ($C_p = C_T/P$)
 C_0 unit feed cost
 C_Δ unit separative work cost

Using the two material balance equations and the separative capacity equation (1), we obtain

$$C_p = C_0 \frac{N_p - N_W}{N_F - N_W} + C_\Delta \left[V(N_p) + \frac{N_p - N_F}{N_F - N_W} V(N_W) - \frac{N_p - N}{N_F - N} V(N_F) \right] \quad (3)$$

This optimization has only one decision variable N_W , so the solution can be given in an analytic form, using the necessary condition on the derivative:

$$\frac{dC_p}{dN_W} = 0, \text{ leading to the expression} \quad (4)$$

$$\frac{C_0}{C_\Delta} = V(N_F) - V(N_W) - (N_F - N_W) \left(\frac{dV}{dN} \right)_{N_W} \quad (5)$$

Thus the unit cost C_p will be a minimum when the condition (4) is satisfied, for a given value of C_Δ . Figure 6 gives some values of the optimal assay N_W versus C_0/C_Δ . But the unit separative work cost C_Δ depends on the value of N_W . So one has to deal with the second plant sub-level.

6.2 The determination of the intermediate assays N_j , gives the minimum of C_Δ , for a fixed value of N_W . It can be seen on figure 7 that for a plant having N -cascades in series (Cohen's squared-off profile), there are $N-1$ intermediate assays as degrees of freedom (decision variables), under certain restrictions concerning the number of stages of each cascade. For operation, maintenance as well as start-up considerations, all stages are gathered, depending upon their reliability, up to 20 in a cell, which is the least operating unit (pressure level and power distribution, bypass system for outage). This condition is handled in a subsequent design calculus, examining the different combinations of integer numbers of cells, surrounding the unrestrained solution.

An alternate and better way is to replace the assays as decision variables, by the numbers of cells in each cascade. These variables may only assume integer values, but this is correctly done by the algorithm described in part 3 of this paper. The sub-problem has the objective function:

$$C_{\Delta j} = \left[\left(\sum_j C_{\Delta j} \Delta U_j \right) + PE \right] / \Delta U, \text{ where } (6)$$

$C_{\Delta j}$, unit separative cost for cascade j ,

is obtained as a function $C_{\Delta j} = f(N_j)$ from the lower level.

ΔU_j , the real separative capacity for cascade j is given by the formula

$$\Delta U_j = \theta_j [V(N_j + 1) - V(N_j) + (N_j^w - N_j + 1) V'(N_j + 1) - (N_j^w - N_j) V'(N_j)] \quad (7)$$

with

θ_j transport stream

N_j^w transport assay

$$V'(N) = \left(\frac{dV}{dN} \right)_N$$

In the case of a plant with only a production at the top

$\theta_j = P$ et $N_j^w = N_p$ in the enriching sections
 $\theta_j = -W$ et $N_j^w = N_w$ in the stripping sections.

PE are the plant annual expenses, which are not allocated to the cascades. They include studies, engineering fees, ancillaries, general site investments and so on. They are sometimes referred to as "indirect expenses", and are expressed by a multiplying factor applied to the total direct expenses.

ΔU , the total separative capacity, is fixed by the first part (c-1).

So at this level, the problem is to minimize

$$C_{\Delta} = \left[\left(\sum_j C_{\Delta j} (N_j) \times \Delta U_j (N_j) \right) + PE (\Delta U) \Delta U \right] \quad (8)$$

with respect to the $N-1$ variables N_j , $j=2, \dots, N$.

7. Cascade level. Determination of the cascade sizes l_j , furnishing the minimum values for the $C_{\Delta j}$, for fixed values of the N_j . Several parameters, for the cascade j , must be defined (figure 9):

D_j annual expenses for the cascade

τ_j number of stages

a_j annual expenses per stage

c_j enrichment factor

L_j stage flow

$\beta_j = a_j / c_j$ reduced expenses per stage

$l_j = c_j \times L_j$ reduced flow

$s_j = c_j \times \tau_j$ reduced number of stages

The cascade sub-problem has the objective function (for each cascade):

$$C_{\Delta j} = D_j / \Delta U_j = (a_j \tau_j + CE_j) / \Delta U_j \quad (9)$$

Or using the reduced parameters

$$C_{\Delta j} = \frac{1}{\Delta U_j} \left[\frac{a_j}{c_j} \times c_j \tau_j + CE_j \right] = \frac{1}{\Delta U_j} [\beta_j \cdot s_j + CE_j] \quad (10)$$

where

β_j , reduced expense per stage, is obtained as a function $\beta_j = f(l_j)$ from the lower level

s_j is given by the usual expression.

$$s_j = \frac{1}{\Delta \phi_j} \text{Tanh}^{-1} \left[\frac{N_{j+1} - N_j}{(N_{j+1} \cdot N_j)^{1/2} (1 + \epsilon_j) - 2N_{j+1} N_j - 2N_j^2 \epsilon_j} \right] \quad (11)$$

$$\phi_j = \theta_j / l_j \text{ and } \Delta \phi_j = 1 + 2\phi_j (1 - 2N_j^w) + \phi_j^2$$

CE_j are the cascade annual expenses which are not allocated to the stages. They could concern for instance some sub-control stations, inter-cascades junctions and facilities.

ΔU_j is fixed by the upper level

(with the θ_j et N_j^w).

So at this level one has to minimize for each cascade:

$$C_{\Delta j} = \frac{1}{\Delta U_j} [\beta_j(l_j) \times s_j(l_j) + CE_j(\Delta U_j)] \quad (12)$$

with respect to the variable l_j .

An important remark: the optimum profile

In practice the U_j cascade sub-model is more complicated and takes into account variations of the cascade size l_j , in order to further minimize the $C_{\Delta j}$. Without entering into a detailed demonstration, it is possible to appreciate the economical interest of size variations or modulation.

Let x be the modulation factor (variable within technological constraints along the cascade: $x(N)$ between N_j and N_{j+1}).

l_j be the design size value.

Then $l_j^x = x \cdot l_j$ is the operating value - Clearly the cascade j is not any more a square section, but a profiled one. The cascade sub-problem is then to minimize

$$C_{\Delta j} = \frac{1}{\Delta U_j} \left[\int \beta \, ds + CE_j \right] \quad (\text{cascade } j)$$

that is to minimize, with respect to

$\{l_j, x(N)\}$ in which $x(N)$ is the profile

$$C_{\Delta j} = \frac{1}{\Delta U_j} \left[\int_{N_j}^{N_{j+1}} \beta_j [l_j, x(N)] \times \frac{ds}{dN} \times dN + CE_j(\Delta U_j) \right] \quad (13)$$

where $\frac{ds}{dN}$ is the reciprocal of the fundamental differential equation (Cohen)

$$\frac{dN}{ds} = 2N(1-N) - \frac{\theta}{l} (N^2 - N) \quad (14)$$

This integral minimization is known as an optimal control problem. A complete presentation of the resolution technique would be beyond the scope of this paper. Nevertheless Figure 9 illustrates the difference between the ideal profile (IP) described by Cohen, and the economically optimum profile (EOP). The important point is to notice that the optimum profile EOP becomes identical to the ideal one when the reduced expense β is directly proportionnal to the operating reduced flow: $\beta = a \cdot l^2$, (or $a = a \times l \cdot c^2$). In this case the equation (13) becomes:

$$\min C\delta_j = \frac{1}{\delta U_j} \left[\sum_{N_j}^{N_{j+1}} a \cdot I_k \frac{da}{dN} dN + DC_j (\delta U_j) \right] \quad (15)$$

This is the total cascade flow integral, the minimum of which defines the ideal profile.

8. Stage level. Determination of the stages internal parameters λ_j , giving the minimum

values of the f_j , for fixed values of the l_j . One must first define some additional terms:

δU_j separative capacity of one stage ($\delta U = \frac{1}{2} Lr^2$)

$C\delta_j$ unit separative work cost of one stage ($C\delta = a/\delta U$)

Notice first that the two following sub-problems are equivalent (i.e. have the same solution):

$$\min \left\{ \lambda \right\} \beta_j \quad \text{for fixed } l_j$$

$$\text{and } \min \left\{ \lambda \right\} C\delta_j \quad \text{" "}$$

$$\text{This results from } C\delta_j = \frac{2 \beta_j}{l_j}$$

Thus the stage sub-problem has the objective function (for each kind of stage j):

$$C\delta_j = \frac{a_j}{\delta U_j} = \frac{a(\lambda_i^j)}{\frac{1}{2} L (\lambda_i^j) c^2 (\lambda_i^j)} \quad (\text{fixed } l_j) \quad (16)$$

in which l_j is fixed by the upper level, and with respect to the λ internal variable

$$\left\{ \lambda_i^j \right\}, i = 1, \dots, m$$

The annual expense a has four components:

- investments amortization
- power cost
- operating costs
- eventually a return coming from by-products (mainly energy).

Let us introduce the following concepts (all applied to the kind of stage j):

- I Total investment.
- I_k k th item in the total investment ($1 = \sum I_k$).
- τ annual rate of return, depending upon the amortization period, the rate of interest.
- e annual aggregate maintenance factor (may be split in the same number of items than the investment).
- Φ Total electric power consumed.
- W Total electric annual consumption.
- p unit cost of electricity.
- oc annual operating costs, including manpower.

Using these conventions, the stage criterion can be written in the usual form:

$$C\delta = \frac{a}{\delta U} = \frac{(\tau+e) I + pW + OC}{\delta U} \quad (17)$$

$$\text{or } C\delta = (\tau + e) I/\delta U + p W/\delta U + OC/\delta U \quad (18)$$

where the specific components appear

$$\left. \begin{array}{l} I/\delta U \text{ specific investment} \\ W/\delta U \text{ specific energy consumption} \\ OC/\delta U \text{ specific operating cost} \end{array} \right\} \text{ per stage}$$

Without entering into any detail, some indications on the determination of the objective function $C\delta$ in the case of a single stage may be given:

- The total stage investment is divided into 10 items, as indicated in figure 10, expressed as functions of the internal variables:

$$I^j = \sum_{k=1}^{10} I_k^j \quad \text{and} \quad I_k^j = f(\lambda_i^j)$$

Every cost item has a particular cost equation, derived from estimations, quotations, industrial prices and trends. The cost equation may present discontinuities or even may not be defined in a range of some variables. But basically, a cost function is expressed in the form

$$I = a(n) \cdot \lambda^n$$

(see for instance Mårtensson or Ebel and Pasquier).

Where λ is one size variable (flow or physical dimension)

a is an exponent, indicating a size effect.

In the CD industry, λ ranges from 0.6 to 1.

$a(n)$ is a function of the number of items to be built or manufactured, taking eventually into account a series effect.

- The power requirement. It is calculated from the compressors performances (pressure ratios and flows) and the various efficiencies and losses: thermodynamic, drive motor, power distribution. Stage auxiliaries must be taken into account.

- The operating costs consist mainly of labour (not an important component in a highly automated process), and spares.

- The enrichment factor depends on three kinds of internal variables:

- . stage arrangement and design variables (stage flowsheet, diffuser parameters)
- . operating variables (pressures, temperature)
- . barrier characteristics (dimensions and performances).

For a single stage, the classical formulation is given in Massignon:

$$c = co \cdot f(\theta) \cdot S \cdot Z \quad \left(c = \frac{R'}{R} - 1 \right) \quad (19)$$

with $co = 43 \cdot 10^{-4}$ ideal enrichment factor

$$f(\theta) = \frac{1-\theta}{\theta} \log \frac{1}{1-\theta} = \text{flow cut factor} \quad (20)$$

A single stage is characterized by the cut value $\theta = 1/2$, giving $f(\theta) = 0.693$

$$S = (1-K) \exp \left[-(1-K) P/P_c \right] \text{ Separation efficiency} \quad (21)$$

with P = fore pressure

K = back pressure/fore pressure

P_c = barrier characteristic

$$Z = 1 - \frac{Va\delta}{D_{12}} \text{ aerodynamic efficiency} \quad (22)$$

with Va velocity of gas through the membrane
 D_{12} molecular diffusivity

$\delta = A Re^{-b}$

Re = Reynolds number

A = function of some barrier characteristics.

9. The general strategy used to optimize the overall plant performance by the multi-level decomposition method, is summarized in fig.11. For a given set of assumptions concerning the productions and enriched assays of the plant, the number of cascades to introduce, the type of stage flow-sheet and some basic and economical data, technological options and constraints, the procedure followed is initiated in the following sequence, from the lowest to the highest level :

10. For any given arbitrary value of l (guessimate in the expected range for each cascade), the stage-level sub-optimization is made, using the optimum-seeking algorithm (described in part 15).

Note : minimize $C_{Sj} = f(\lambda_j)$ for the fixed value of $l_j = l_0$, is performed via the Lagrange's method of multipliers, giving

$$\min \{ \lambda_j \} [C_{Sj} - \lambda (l_j - l_0)] \quad (23)$$

The results are memorized as

$$C_{Sj}(l) \text{ or } \bar{E}(l).$$

11. The cascade level utilizes the $C_{Sj}(l_j)$ function as input data, and must solve the problem : $\min \{ l_j, \bar{x} \} C_{Sj}$, for some given values of N_j . Results are stored (here \bar{x} stands for the optimal modulation profile).

12. The plant level receives the results $C_{Sj}(N_j)$ as input data, and has to minimize $C_A = f(N_j)$ versus some values of N_0 . The result is memorized : $C_A(N_0)$.

13. The final optimization is to minimize $C_p = f(N_0)$. This part is straightforward using the equation (5).

14. In some typical computations 5 cascades are obtained with only 3 different stage sizes (fig. 7-2). This cascading has been compared to others and proved to be the best. In each stage the internal parameters λ_j could range from 4 to 7. The total number of decision variables are in this case :

λ_j	---	$3 \times (4 \text{ to } 7) =$	12 to 21
l_j	---		3
N_j	---		4
N_0	---		1
			20 to 29

Note : The whole procedure is implemented in a computer code, and is easily utilized. Because of the direct search algorithm and the optimal control problem, the time consumption is large but acceptable for the dimension of the problem.

An optimum-seeking algorithm

15. At the stage level, some of the variables to be optimized have discrete values, such as the number of barriers to be arranged in the diffusers.

At the cascade level, an integer number of multi-stages groups (cells) must be obtained. This number must be even if two rows of cells are to be built. Moreover the objective functions may have discontinuities : for instance above a given value of the compressed flow, the type of compressor drive has to be changed, introducing a step in the cost function. Another case would be the choice of different barrier types depending upon temperature and pressure levels. Another characteristic of the model is to use eventually non-analytical data, such as numerical tables instead of functions. A special optimum seeking algorithm has been developed to deal with these characteristics. It is of the mixed integer direct search programming type. Based on random exploration of the feasible space, the method does not need derivatives' calculations but requires only the values of the objective function for the trial variables. The use of a random exploration may be proved useful as in the following example :

Consider the objective function to maximize $f(\vec{x}) = f(x_1, \dots, x_n)$ where \vec{x} is defined over the m -space E . Define $A \subset E$ best part of E , if

$$\left. \begin{array}{l} \forall \vec{x} \in A \\ \forall \vec{y} \in E-A \end{array} \right\} f(\vec{x}) > f(\vec{y})$$

$$\text{Introduce } a = \frac{\text{measure}(A)}{\text{measure}(E)}$$

The probability for one random trial in the m -space E to miss A , will be $1-a$, and for n independant trials $(1-a)^n$. So if $p(A)$ is the probability for at least one trial out of the n -series to belong to A , then $p(A) = 1 - (1-a)^n$

$$\text{that is } n = \frac{\log(1-p(A))}{\log(1-a)} \quad (24)$$

Taking $a = 1/100$, a 500 trials series will hit at least one time the A sub-space, with a probability higher than 99%. A flow chart is given on fig.12, indicating one simplified but effectively used version. This method is not very fast, thus it is advisable to choose properly the driving parameters of the computation: initial exploration zone, number of trials N_T , rate of convergence RC , precision PR .

Possible extensions of the method

16. The multi-level decomposition proved to be useful in the G D plant optimization model. A rather natural extension of this work is to consider another upper level, above the plant : the isotope separation complex. Receiving from the plant level the functions $C_{Pn}^n(P_n, N_{Pn}^n)$ and C_{Dn}^n , the complex level may allocate productions and assays between the n plants to minimize a new overall objective B , total benefit of the whole complex (fig.13). In this case the plants are not operated independently, but in a related way, or overlap operation. Moreover another extension would take into account the time dynamics, involving capacity increases, new plants start-ups, new technology break through, the objective function being then the maximum discounted benefit over the period under consideration. The capacity extension is examined in another contribution to this conference (Coates)

CONCLUSION

The multi-level decomposition method has been applied in this paper to a GD plant optimization. This technique, which is applicable to other enrichment processes or to associations of processes, furnishes successively the sub-results for each level, while insuring their proper coordination for the final goal.

This procedure has been followed extensively either entirely or partly. Indeed, it is not necessary to take full computations at the highest level to appreciate the effect of technical results leading to improvements in the formulation. On the contrary, parameters such as the economic environment, having a deep effect on the project, must be brought up at plant (or complex) level.

In the case of a gaseous diffusion plant, the model enabled the influence on the enrichment cost of the successive improvements obtained in the R and D programs to be permanently assessed. Present studies deal with dynamic optimizations of enrichment capacity increases.

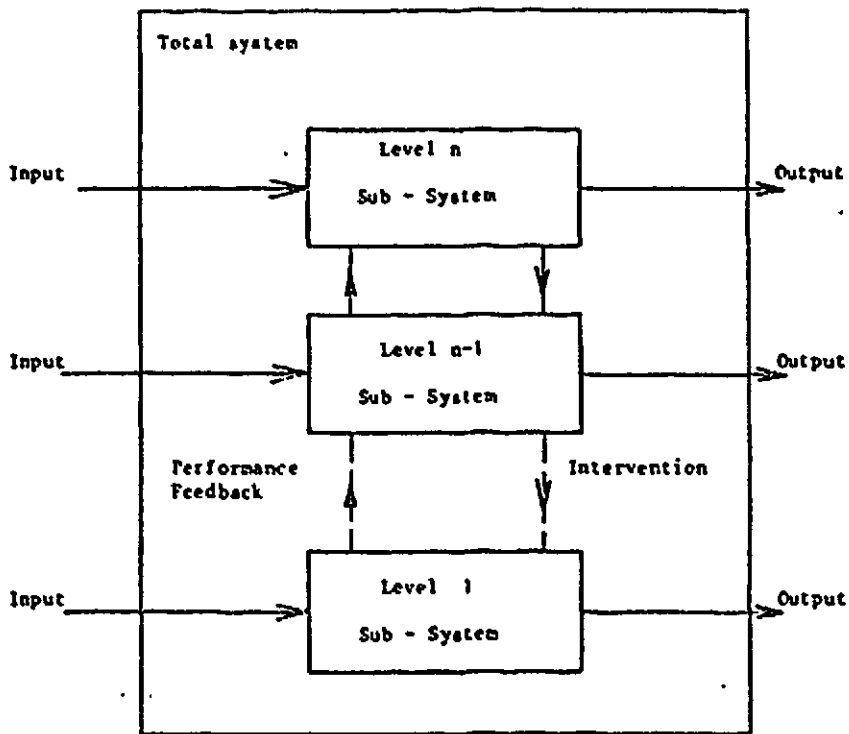
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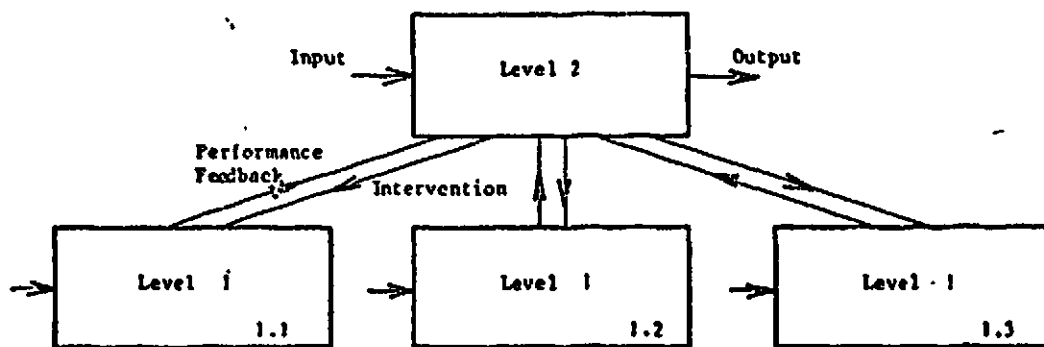
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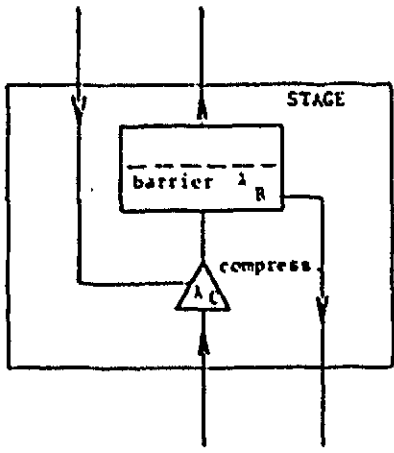


1.1 Vertical arrangement in multi-level decomposition (from Mcserovic)

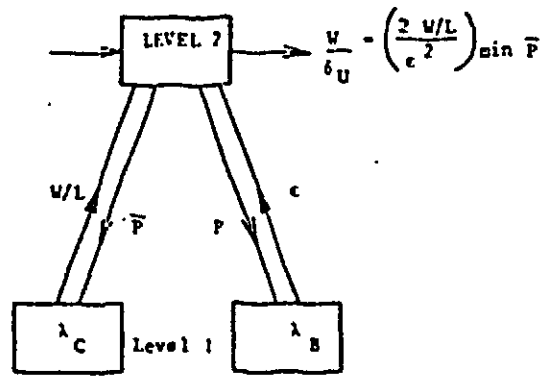


1.2 Example of multi-goal two-level system

Fig.1.



2.1 Basic GD stage components



2.2 Functional representation

Fig 2.

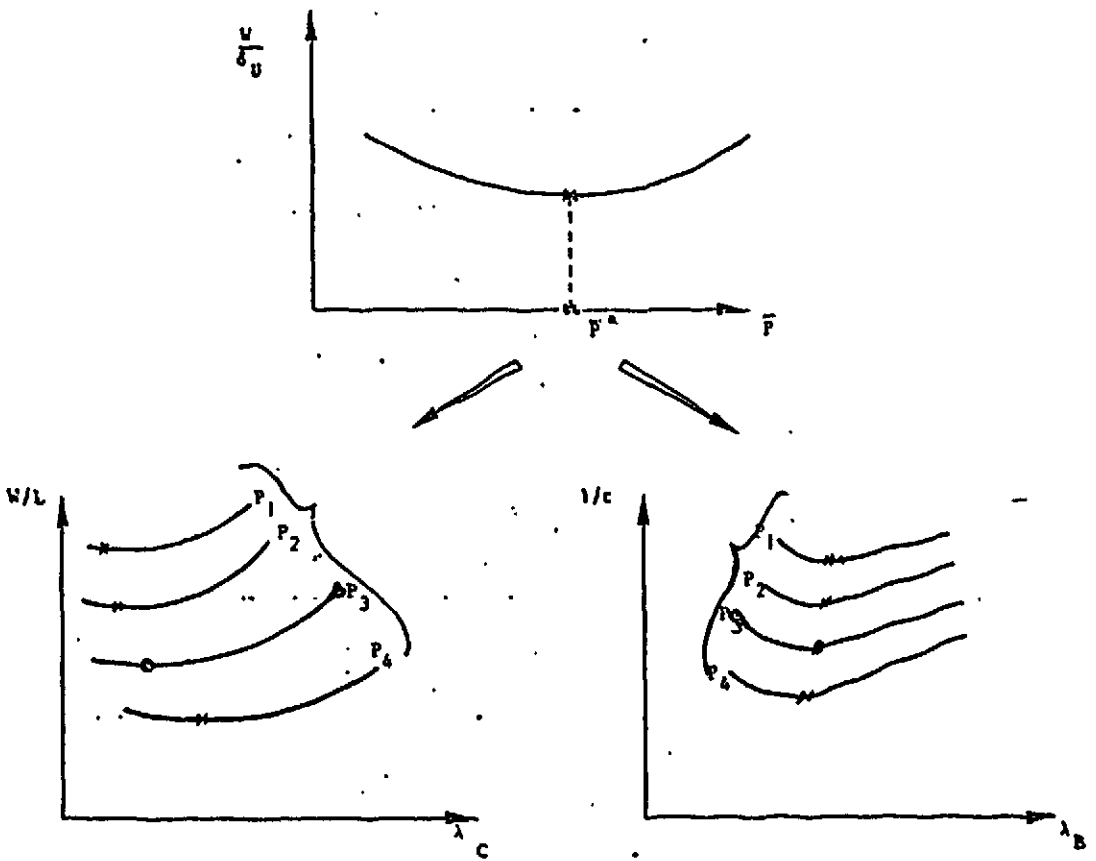


Fig.3 Illustration of the \bar{P} optimisation

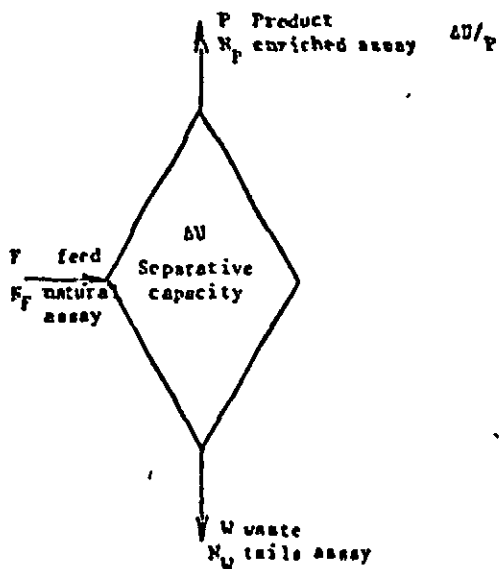


Fig.4 Gasous diffusion plant schematic representation .

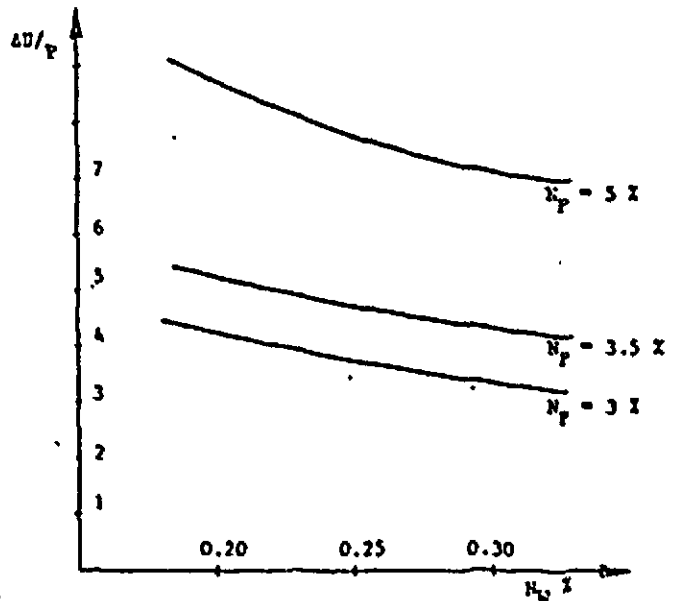


Fig.5 Separative capacity requirements

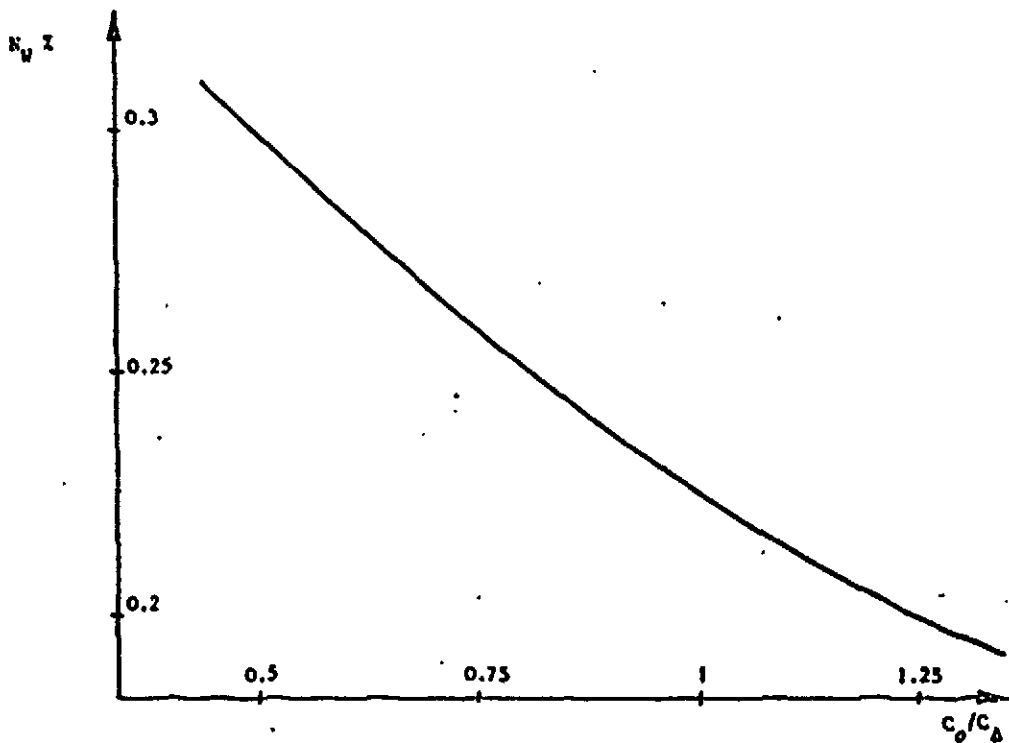
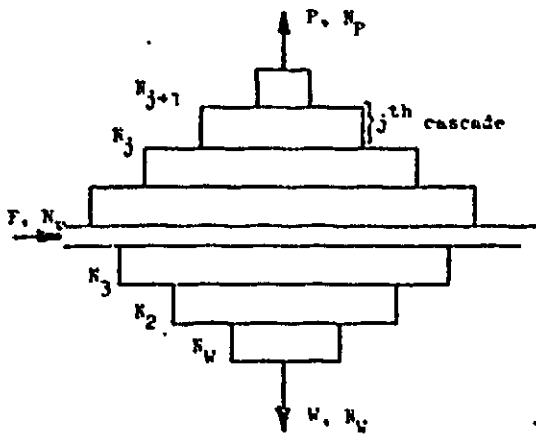
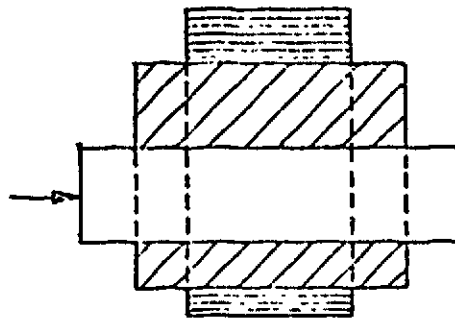


Fig.8 Optimal tails assays versus Co/CA



7.1 Squared-off plant



7.2 5 cascades - 3 stages sizes plant

Fig. 7.

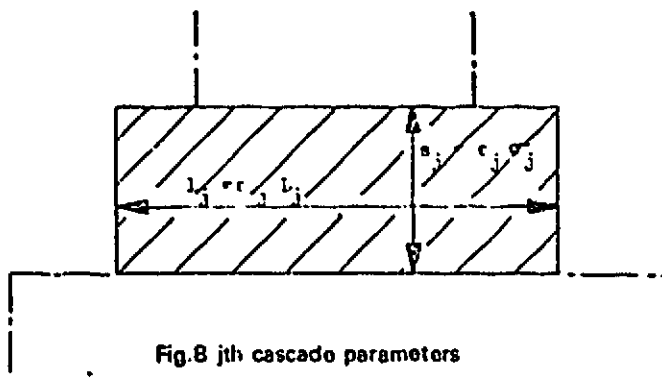


Fig.8 jth cascade parameters

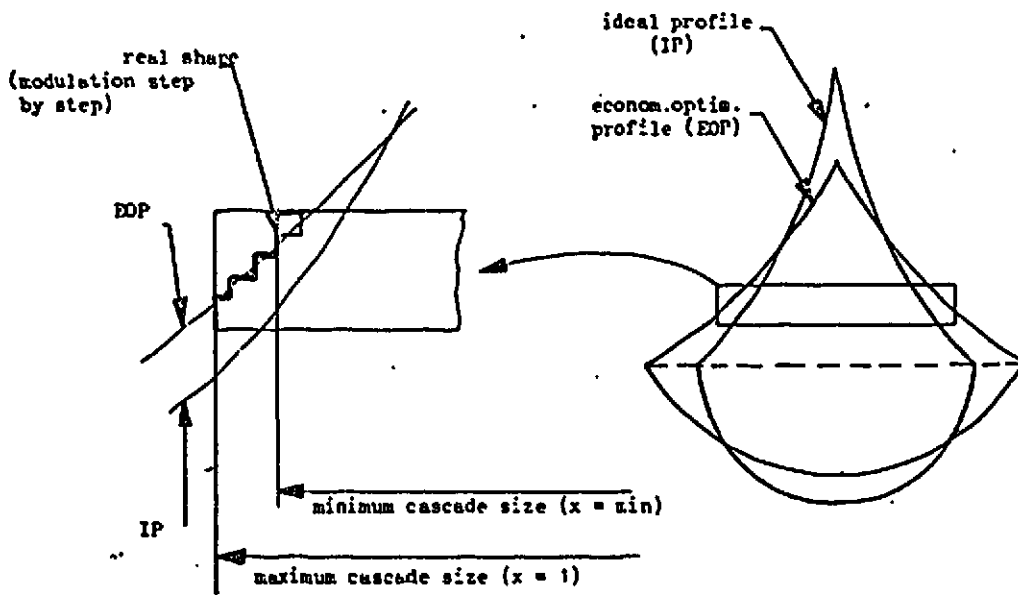
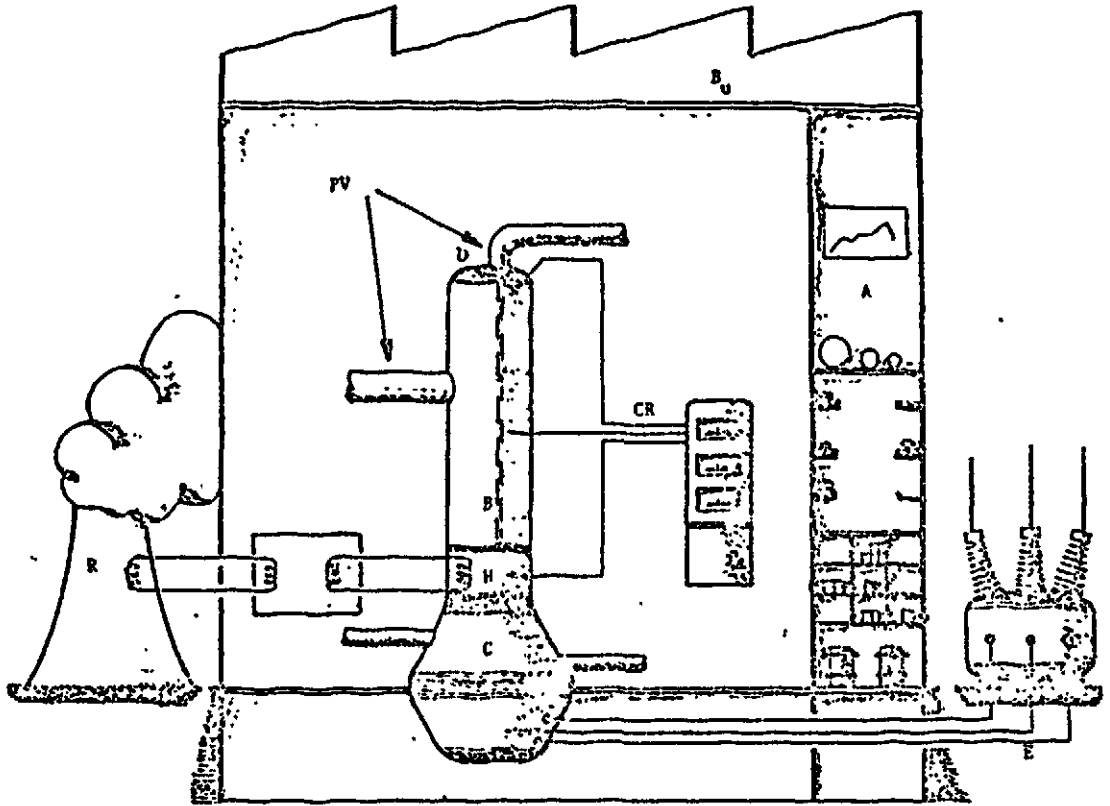


Fig.9 Size modulation



- B barriers
- D diffuser
- C compressor
- H heat exchanger
- R heat rejection (or recuperation)
- FV piping and valves
- CR control - regulation
- E electrical distribution
- Bu buildings
- A auxiliaries

Fig.10 Stage cost components

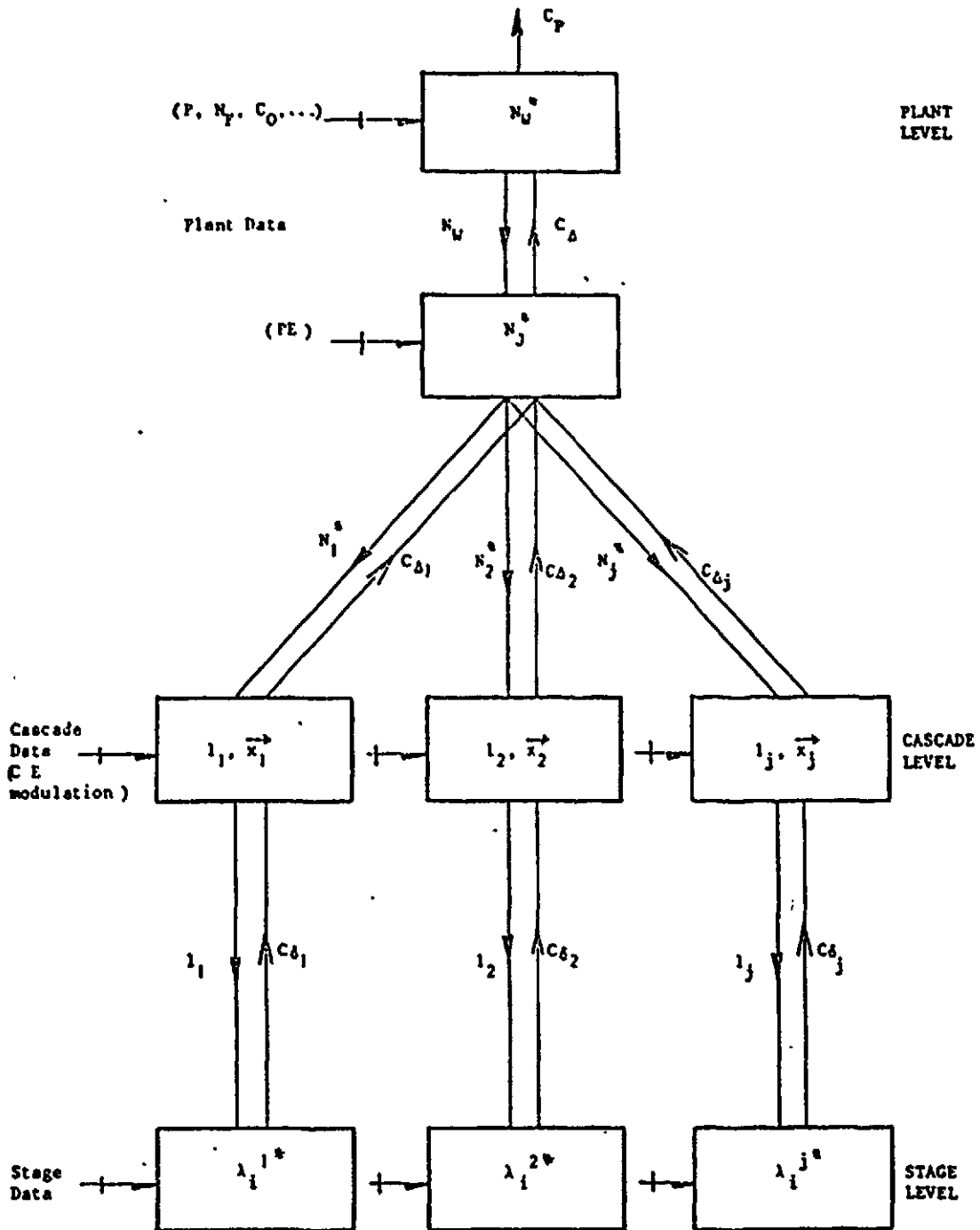


Fig.11 General plant optimization strategy

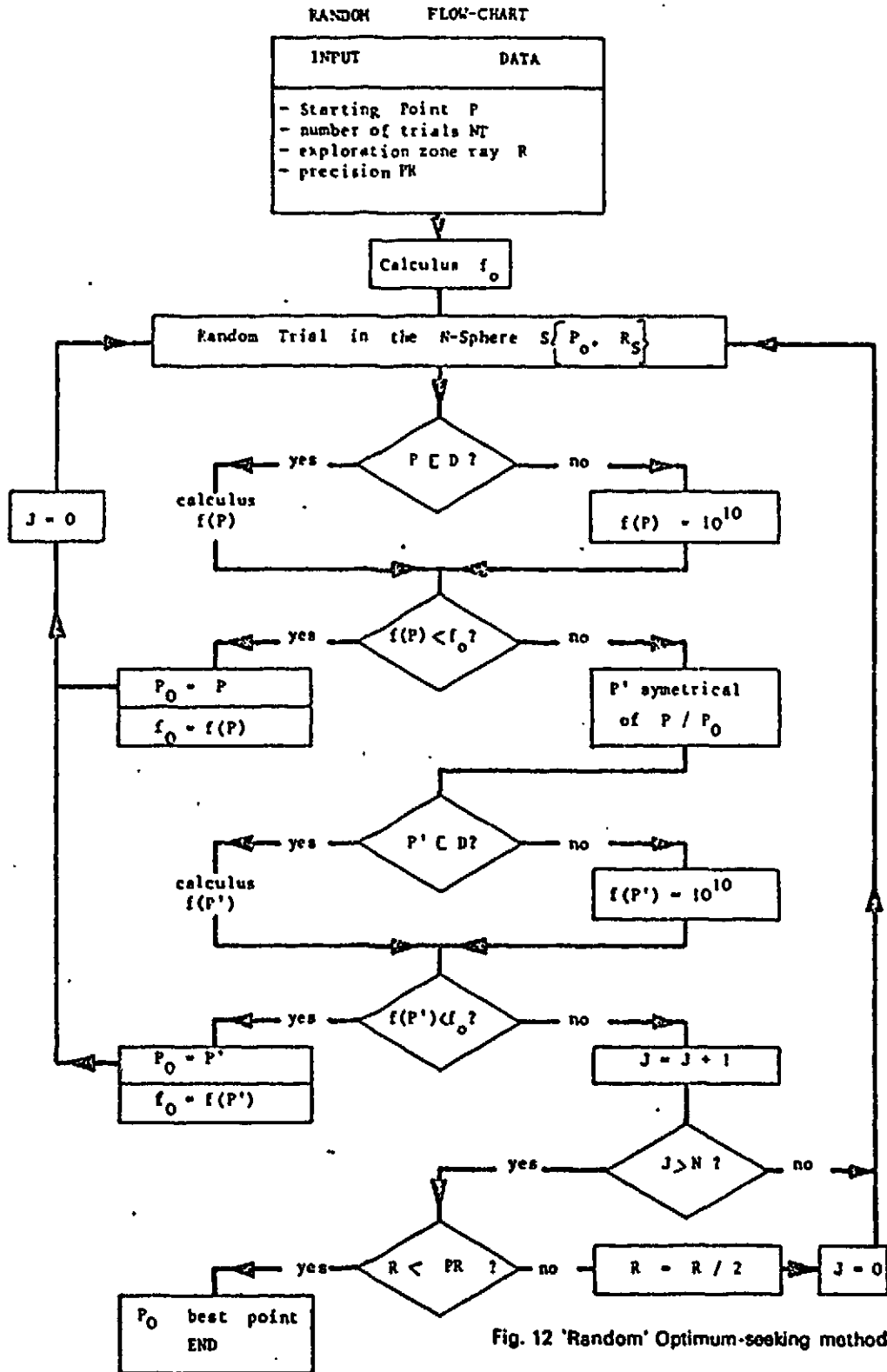


Fig. 12 'Random' Optimum-seeking method

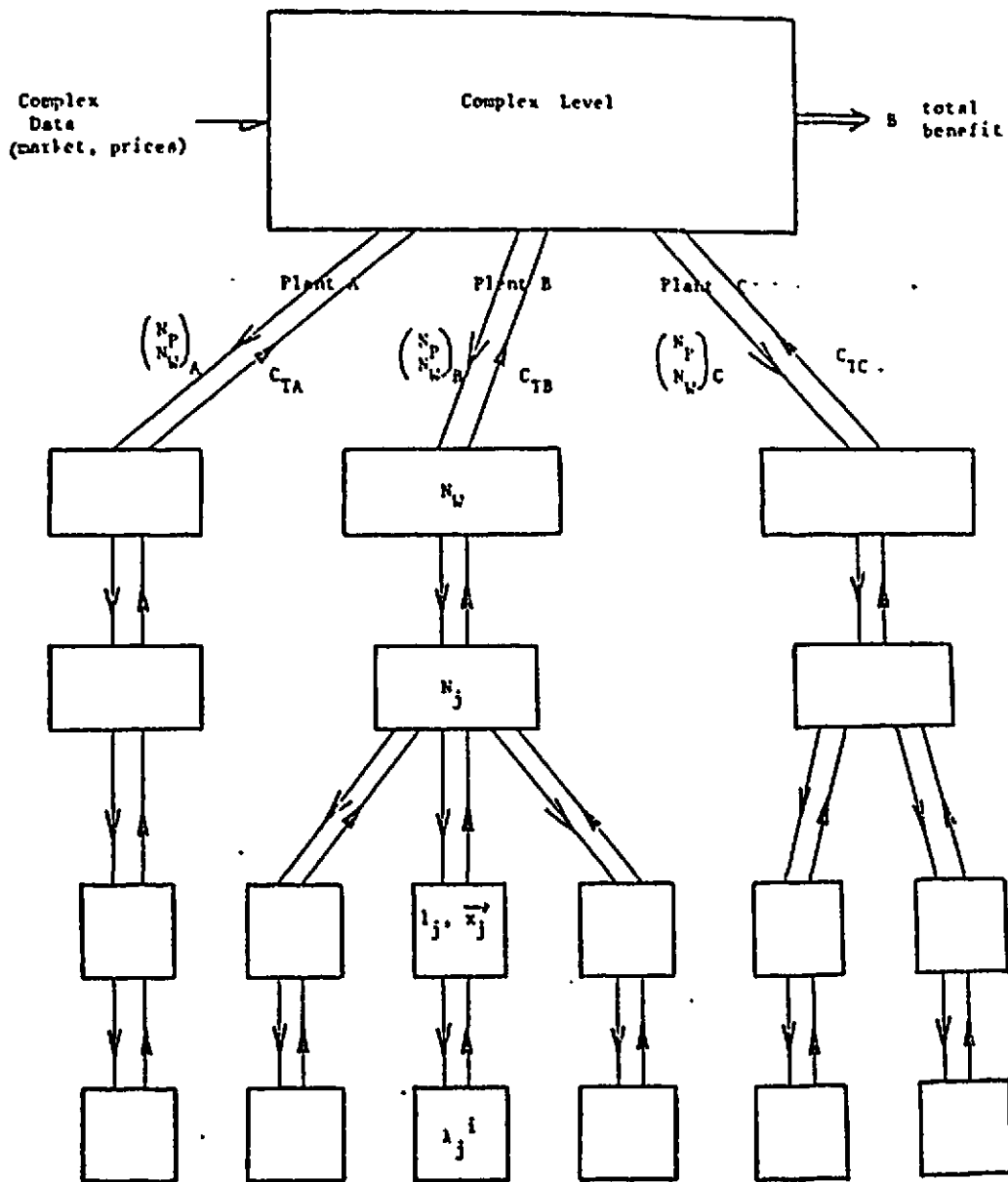


Fig 13 Model extension example

