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Studies in the Synthesis of Control Structures for Chemical Processes

Part I: Formulation of the Problem. Process Decomposition and the Classification of the Control Tasks. Analysis of the Optimizing Control Structures.

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Part I of this series presents a unified formulation of the problem of synthesizing control structures for chemical processes. The formulation is rigorous and free of engineering heuristics, providing the framework for generalizations and further analytical developments on this important problem.

Decomposition is the underlying, guiding principle, leading to the classification of the control objectives (regulation, optimization) and the partitioning of the process for the practical implementation of the control structures. Within the framework of hierarchical control and multi-level optimization theory, mathematical measures have been developed to guide the decomposition of the control tasks and the partitioning of the process. Consequently, the extent and the purpose of the regulatory and optimizing control objectives for a given plant are well defined, and alternative control structures can be generated for the designer's analysis and screening.

In addition, in this first part we examine the features of various optimizing control strategies (feedforward, feedback; centralized, decentralized) and develop methods for their generation and selective screening. Application of all these principles is illustrated on an integrated chemical plant that offers enough variety and complexity to allow conclusions about a real-life situation.

SCOPE

During the last ten years, numerous works have dealt with the design of control systems to regulate specific unit operations (e.g., distillation), to bring a system (e.g., a reactor) back to the desired operating point in some optimal fashion, to guarantee optimal profiles in nonhomogeneous reactors, etc. The interactions between different pieces of equipment in a chemical plant are complex, and do not allow us to regard plant control as a simple extension of unit operations control. These interconnections decrease the number of degrees of freedom, and great care must be taken not to over- or under-specify the control objectives in a process.

All available control theories assume that measured and manipulated variables have been selected, thus not answering one of the basic questions an engineer is facing when designing a plant. Rules of thumb and experience guide the designer's choice of measured and manipulated variables. Naturally, without a systematic procedure, there is no guarantee that all the feasible alternatives are explored, and even less that the best possible structure is chosen. The lack of sound techniques for solving those problems has been criticized frequently, and

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is mainly due to the absence of a proper mathematical formulation and a clear statement of the objectives. We propose to determine the general underlying foundations of present day pragmatic control structure synthesis, and to demonstrate how theoretical results can be used to improve empirical procedures.

Any design method has to allow for engineering judgment between automatized steps. There are several important complicating factors that have not been dealt with in previous work (Govind and Powers 1976, Umeda et al. 1978):

1. The disturbances expected to enter the process during operation have to be defined and their impact on the performance evaluated; only then can the need for a certain controller be established. (This makes process control different from control in other disciplines where the disturbances can generally only be described in a noise-like manner).

2. Many control objectives are a straightforward consequence of the requirements imposed by product quality, safety, etc., but the definition of economic objectives in terms of controlled variables is by no means trivial.

3. Often the variables of interest cannot be measured directly, and the proper secondary measurements have to be selected.

4. Problem size can easily get overwhelming, and without proper decomposition methods, a solution becomes intractable.

All these questions are explicitly addressed here. Part II of this series will deal with applying an extended concept of controllability and observability to the synthesis of feasible alternative regulatory control structures. Finally, in the third part, the problem of selecting the most appropriate secondary measurements and associated estimation problems will be treated.

CONCLUSIONS AND SIGNIFICANCE

The multilayer-multiechelon approach of hierarchical control theory is useful in organizing the control structure synthesis problem for chemical processes. Quantitative measures are developed to allow the decomposition of the control tasks and the concrete formulation of regulatory and optimizing control problems for a chemical plant. Decomposition criteria are proposed for partitioning the process into subsystems. These new quantitative criteria are useful in determining the framework within which alternative process control structures will be generated. An analysis of the fundamental features of the various optimizing control strategies (feedforward, feedback, centralized, decentralized), reveals criteria for selecting the optimizing control structure for a given chemical plant. The developed criteria are local in character, and can be generated from the steady-state flowsheet of a chemical process. The application of the developed concepts to an integrated chemical plant produces all the information that a designer would need, to formulate the control synthesis problem and generate feasible control structures.

SYNTHESIS OF CONTROL STRUCTURES

Articles and seminars evaluating the current status of process control and suggesting future research have been flourishing (Foss 1973, Kestenbaum *et al.* 1976, Lee and Weekman 1976, Foss and Denn 1976). A central point often is the unavailability of a method for synthesizing control structures for a complete plant.

Considering how many papers have been written on control of a single unit operation like distillation, plant control has been discussed only a few times (Buckley 1964, Govind and Powers 1976, Umeda *et al.* 1978) because of its inherent complexity. A similar evolution can be historically observed—from the analysis of individual unit operations and chemical reactors to the synthesis of integrated process flowsheets. Here, we lay the foundations for the synthesis of process control structures by merging the methods of process design and the theoretical developments of control science.

A control structure is composed of the following elements:

- a set of variables which are to be controlled to achieve a set of specified objectives,
- a set of variables which can be measured for control purposes,
- a set of manipulated variables, and
- a structure interconnecting measured and manipulated variables.

The essential purpose of chemical process control is to develop a dynamic structure of measured and manipulated variables so that certain processing objectives will be satisfied almost continuously. These objectives usually vary according to the process, characteristics of the environment, and general management policy, which will be determined, in turn, by present and future economic conditions.

Difficulties arise because, in certain cases, a variable will be both manipulated and controlled (e.g., ratio control of input streams). This implies that the various feasible sets of controlled, measured and manipulated variables and the interconnecting structure, cannot be selected independently, but rather should be considered simultaneously. To make matters more complicated, the optimal operating conditions change as a function of the external disturbances. Maarleveld and Rijnsdorp (1969) have demonstrated that the optimum operation of a plant switches discontinuously from one process constraint to another. Industrial experience also indicates that such operational policy is quite common and economically sound. It is clear though, that switching the operation of a plant from one given set of constraints to another implies a change in the plant's regulation structure.

While regulation is the principal control objective, the adopted regulatory control structure may not allow smooth, safe and reliable transition of the plant's operation to a new point for better economic performance. This conflict can be resolved by systematically formulating the regulatory and optimizing control structures, and is treated here. Further, if technically possible and economically justifiable, one will measure the controlled variables. Otherwise, secondary measurements will be chosen, in conjunction with estimation techniques to infer the value of the unmeasured control objectives. The estimator will be part of the structure interconnecting the measurements and the manipulated variables.

Apart from the macroscopic structuring difficulties, we face a variety of local problems. Defining the lowest degree of model complexity necessary to answer the posed questions is the initial task. Then, we develop preliminary control structures which are feasible from an engineering and mathematical structural point of view, and follow with an evaluation where more detailed static or dynamic models are required. The complexity of the encountered physicochemical systems makes checks for interaction and effects of nonlinearity necessary. Combining the isolated subgroups into an overall system decreases the number of degrees of freedom, and overspecification has to be carefully avoided.

We present here an outline of the steps to a suitable control structure. This sequence serves at the same time as a guide to the following articles of this series.

Definition of the Control Objectives

Always, we must start with a qualitative formulation of the control objectives for a given plant. Many will be determined by the specific nature of the process involved. General rules can not, nor need be given.

In the first category of control objectives are those related to the operational feasibility. They are always a function of process variables, which are to be kept within certain specified bounds, in spite of uncontrolled influences on the process. The origin of these requirements may be product quality specifications, safety considerations, operational requirements, environmental regulations etc.

The second category of objectives is derived from economic considerations. These enter only if, after satisfying the first class of objectives, manipulated variables are left to adapt the operating conditions to stay at the most profitable point of operation. A feedforward adjustment of the manipulated variables in an optimal fashion is one such method, but is relatively complex and unreliable. Alternatives will be discussed here, e.g. translating the feedforward optimizing structure into a feedback scheme, which is easier to implement. Along with classifying the objectives goes a classification of the control tasks, into regulatory and optimizing ones.

Decomposition of the Process

The decomposition of the process is not dictated by any computational considerations. On the contrary, it is part of the design strategy, very much in the same way as it was used for *process flowsheet synthesis* (Rudd 1968, Masso and Rudd 1969), optimization (Lasdon 1970), optimal control (Bailey and Ramapriyan 1973) etc. Process decomposition reveals the aggregates of unit operations and chemical reactors which must be centrally controlled. Note that the process decomposition can be directed towards developing the independently controlled groups of units, in terms of regulation or optimization. Both criteria can be applied to the same process simultaneously and nearly independently. Although this may sound contradictory, as it will be pointed out later, a process decomposition for regulatory purposes will be feasible within the bounds of the groups established from the process decomposition for optimizing control purposes.

The process decomposition for optimizing control purposes will be discussed here, (Part I) while the process decomposition for regulatory control will be explored in Part II.

To split a process into subprocesses which are optimized separately, one must be able to decompose the overall objective function linearly, and one part of it must be associated with every subsystem. The minimal size of a subsystem is usually dictated by that restriction. For optimization, the magnitude of the subproblems has to be balanced against the effort to coordinate solutions. In addition, the solution should not be too sensitive to the exact satisfaction of the interconnection constraints. Otherwise, the required coordination algorithm has to be too involved.

Selection of Measurements

The first class of control objectives (product quality, safety, regulations, etc.) dictates directly the measurements which should be made for monitoring the process. The second class (economic performance) can be translated into feedback loops under certain conditions to be described later, thus requiring additional measurements. These primary, theoretically desirable measurements, are not always available. Often, they have to be substituted by secondary ones.

Measuring secondary variables allows us to estimate the primary ones on the basis of a process model. The choice of secondary measurements and the associated estimation problem can roughly be regarded to be independent of other decisions. (Loosely speaking we could invoke the separation principle of optimal control as a foundation of that statement.) Selection criteria for secondary measurements and the development of a dynamic estimation scheme is the objective of Part III.

The complete set of measured variables for a feasible control structure must satisfy the extended conditions of structural observability, which are developed in Part II. This includes the question of augmenting the set of measurements to obtain a structurally observable system. From the above discussion, it can be seen easily that alternative sets of measured variables will be developed during the synthesis of control structures. Which of these sets is the "best" is the central question in selecting the control structure for a chemical process. We will attempt to answer this question in the Parts II and III of this series.

Selection of the Manipulated Variables

Selecting the manipulated variables will affect response capability to the external disturbances and the ability to keep the control objectives at the desired levels almost continuously. The more manipulated variables available, the better will be the control of the process. Structural aspects of the processing system and of the equations describing the physicochemical processing units are of paramount importance in establishing feasible sets of manipulated variables. Certain manipulated variables will be more desirable than others, from an engineering point of view. Govind and Powers (1976) have listed a number of qualitative features that the selected manipulated variables should satisfy, the product of numerous discussions with practicing engineers. Among these are reliability, ease of operation, startup and shutdown, to avoid the manipulation of "unpleasant" streams (solids, slurries) and of variables which influence a large number of other variables.

Interconnecting the Measured and Manipulated Variables

Solutions to this problem will again be guided partly by engineering and cost, partly by control theoretical considerations. For example, if we insist on using single loop controllers only, our sets of manipulated variables must be chosen to result in the minimum possible interaction between the loops. If we allow for the possibility of multivariable control, be it decoupling, modal or optimal control, we gain more freedom. An interesting comparison and evaluation of the different techniques is presented by Edgar (1976). Virtually all the past control studies were directed toward the design of the multivariable control scheme, and they will not be elaborated on further.

THE SYNTHESIS OF PROCESS CONTROL STRUCTURES WITHIN THE FRAMEWORK OF HIERARCHICAL CONTROL

The theoretical development of hierarchical control structures has been discussed in a variety of articles over the last decade. Here, we only outline the basic ideas.

Much of the theoretical development can be found in the book by Mesarovic (1970a), and a collection of papers on related issues edited by Wismer (1971). Qualitative introductory outlines are given by Lefkowitz (1966, 1975) and Mesarovic (1970b), while a systematic quantitative treatment of the control and coordination of hierarchical systems, is given by Findeisen *et al.* (1979). Some of the unsolved problems which have prevented application of the schemes are presented by Bailey and Malinowski (1977). Views from industry are expressed by Bernard and Howard (1970), Tinnis (1976) and Bernard (1966). The basic reference for multilevel optimization methods is Lasdon's book (1970). For our purposes, i.e. the systematic and organized development of control structures for chemical processes, we found the framework of the multilayer-multiechelon concept to be very meaningful, convenient, and having the potential for further development. Let us elaborate further on this, and on how it affects the synthesis of control structures.

Multilayer Decomposition

During chemical plant operation, the basic goal is to optimize an economic measure of the operation (e.g. minimize operating cost, maximize profit), while at the same time satisfying certain equality or inequality constraints (quality and production specifications, environmental regulations, safety etc.). This optimization must be achieved in the presence of external disturbances which enter the plant. Thus, we formulate the optimization problem to reflect these attitudes during the operation of a chemical process

$$\underset{m}{\text{Minimize}} \int_0^T \bar{\Phi}(y, m, d)dt \tag{1}$$

subject to

$$\dot{x} = g'(x, m, d) \quad \text{state equations} \tag{2}$$
$$x(0) = x_0$$
$$g''(x, m, d) \leq 0 \quad \text{feasibility constraints} \tag{3}$$
$$y = h(x, m, d) \quad \text{outputs from the process.} \tag{4}$$

where $x \in R^n$ is the vector of state (dependent) variables
$m \in R^l$ is the vector of manipulated (independent) variables
$d \in R^m$ is the vector of external disturbances
$y \in R^r$ is the vector of process outputs.
and $\bar{\Phi}$ is the operating cost (performance function) of the process.

Plant control is required because of external disturbances d. Their stochastic nature makes solving the resulting nonlinear stochastic control problem (1) an impossible task. If we partition the disturbance vector in the following fashion (which can always be done by an appropriate change of the coordinate system), a manageable degree of complexity can be reached

$$d_1 \in R^{m_1} \text{ such that } \lim_{t\to\infty} E\{d_1\} = \bar{d}_1 \neq 0, \; d_1(0) = d_{10}$$

$$d_2 \in R^{m_2} \text{ such that } \lim_{t\to\infty} E\{d_2\} = \bar{d}_2 = 0, \; d_2(0) = d_{20}$$

where

$$d^T = (d_1^T, d_2^T).$$

This partition into a stationary (d_2) and a nonstationary (d_1) disturbance component is discussed in more detail in Part III.

The disturbance model underlying d_1 has its poles on the imaginary axis, while the poles of the model for d_2 lie strictly in the left half plane. This strict partition into d_1, d_2 is rarely possible from experimental observations alone. A suitable criterion is to assume the poles of the disturbance model, which are several times slower than the time constant of the system, to be effectively zero. The partition defines implicitly two-time scales, the basis of the "temporal hierarchy" (Findeisen 1976) in the control activities on a chemical plant. The disturbance components d_2 are "fast" varying. They are irrelevant for the long term optimization of the process, because their predicted value is essentially zero after a short time. Regulatory control is used to suppress their influence.

On the other hand, d_1 contains persistent and/or periodic disturbances which have to be included in the long term optimization. Without much error, we can neglect the time averaging of the objective function (1) and reformulate it in mathematical terms employing a pseudo steady state assumption.

1) Optimizing Control:

$$\underset{m}{\text{Minimize}} \quad \Phi(y, m, \bar{d}_1)$$
$$\text{subject to} \quad g'(x, m, \bar{d}_1) = 0 \tag{P1}$$
$$g''(x, m, \bar{d}_1) \leq 0$$
$$y = h(x, m, \bar{d}_1)$$

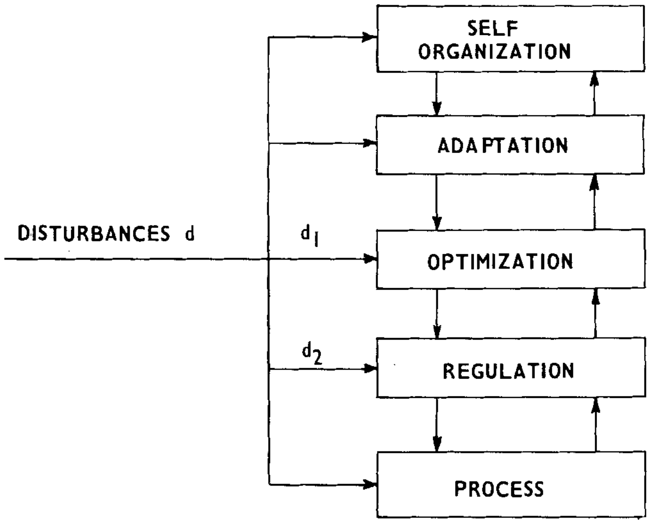

Figure 1. Multilayer decomposition of the control tasks.

where $\bar{d}_1 = E\{d_1(T_0)\}$; $d_1(0) = d_{10}$ and the time period, T_0, is large enough for the prediction to be approximately constant and the plant dynamics to be negligible. The optimum solution of the problem (P1) is

$$x^* = x(m^*, \bar{d}_1)$$
$$y^* = y(m^*, \bar{d}_1)$$

2) Regulatory Control:

$$\underset{m}{\text{Minimize}} \int_{t_0}^{t_1} \{(y - y^*)^T W_1 (y - y^*) + (m - m^*)^T W_2 (m - m^*)\}dt$$

$$\text{s.t.} \quad \dot{x} = g'(x,m,d)$$

$$x(t_0) = x_0, \; x(t_1) = x^*(t_1)$$

$$y = h(x,m,d)$$

$$g''(x, m, d) \leq 0$$

where W_1 and W_2 are positive definite and symmetric weighting matrices. A natural definition would be

$$W_1 = \left(\frac{\partial^2\Phi}{\partial y^2}\right)_{\substack{y=y^* \\ m=m^* \\ d=\bar{d}_1}} \text{ and } W_2 = \left(\frac{\partial^2\Phi}{\partial m^2}\right)_{\substack{y=y^* \\ m=m^* \\ d=\bar{d}_1}}$$

Note that $0 \leq t_0 \leq t_1 \leq T_0$, i.e. the time horizon for regulation is significantly shorter than for optimization.

The previous discussion indicates that the "multilayer structure" is a natural element of the control activities in a chemical plant and leads to a vertical decomposition of the control tasks. The first (lower) layer takes care of the regulation and allows the process to be considered at pseudo steady state. The second (higher) layer is responsible for determining the optimal set points under the influence of changing disturbances. For a general system, more layers can be realized (Figure 1), but they will not be discussed here.

Multiechelon Decomposition

The second type of decomposition is done horizontally, developing multiple echelons for control action in the chemical process. The plant is divided into interacting groups of processing units, for which the optimization is carried out separately. These are coordinated from time to time by a coordinator (see

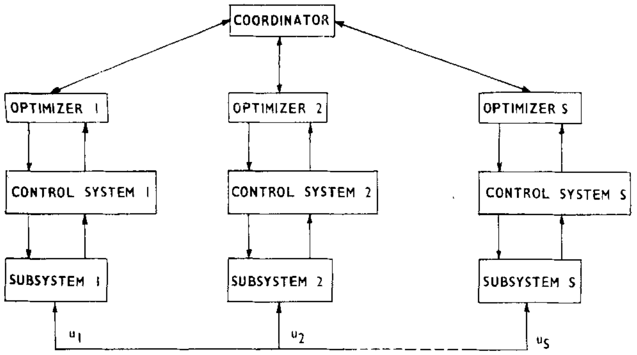

Figure 2. Multiechelon decomposition of the control tasks.

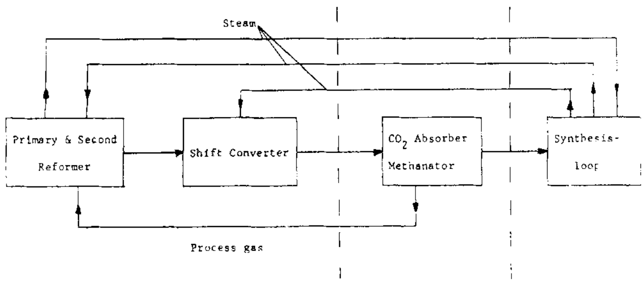

Figure 3. One possible decomposition of an ammonia plant.

Figure 2). This multiechelon decomposition is also a natural element arising from the structure of a chemical process.

Decomposing the process under steady state assumptions is necessary for the following reasons:

1. Developing an optimizing control strategy for an integrated plant often goes contrary to the designer's or the operator's intuition, which is to think in terms of groups of units with a common functional goal. Further, different aggregates of operating units will have different functional goals.
2. Solution of the on-line optimization problem every time an important disturbance enters the system can be overwhelming; decomposition facilitates its solution.
3. Synthesis of the regulatory control structure is also simplified, since it is concentrated within a group of units (subgroup, echelon) with a common functional goal.

As an example, consider an ammonia plant (Figure 3), where one possible process decomposition for optimization is demonstrated. Note that each subgroup of units has a very well specified and well understood operational objective. Thus, the operational goal of the first subgroup (the primary and secondary reformer and the shift converter) is to provide the hydrogen necessary for the ammonia synthesis. The goal of the second subgroup is to prepare the reaction feed of nitrogen and hydrogen at the desired stoichiometry, by removing the undesired components. The third subgroup is to achieve the desired conversion of the H_2 and N_2 to ammonia.

The decomposition of the process should be made in such a way that an involved coordination among the subgroups is not required every time a disturbance enters the system. Otherwise, it loses its attractive features. This, along with our desire to develop processing groups with functional uniformity, constitute the two basic design guidelines in decomposing the process for the optimizing control structure.

Before we proceed with the mathematical formulation of the multiechelon decomposition, let us simplify the notation of (P1). Some of the inequality constraints, g'', will be active at the optimum. Since all our considerations will be of a local nature, we hypothesize that the set of active inequality constraints does not change with changing disturbances. Then, we can combine the steady-state transformation equations (i.e. $g' = 0$) and the active inequality constraints into one vector f and upon substitution for y we obtain

$$\begin{aligned} &\min_{m} \quad \Phi(x, m, d) \\ &\text{s.t.} \quad f(x, m, d) = 0 \end{aligned} \qquad (P1') \qquad (5)$$

where

$$f^T = [g'^T, g_1''^T] \text{ with } g''^T = [g_1''^T, g_2''^T] \text{ and } g_2'' < 0.$$

We also omitted the subscript and superscript of $\bar{d}_1$ for simplicity because we will be dealing with non-stationary disturbances only. For the decomposition, we assume the function of the overall plant to be the sum of the operating costs of all processing units, that is,

$$\Phi = \sum_{i=1}^{s} \Phi_i(x_i, m_i, u_i, d_i) \qquad (6)$$

We have s processing units in the plant, and the subscript i denotes the states (x_i), manipulated variables (m_i) and disturbances (d_i) associated with processing unit i. Further, the set of constraints is assumed to be decomposable

$$f_i(x_i, m_i, u_i, d_i) = 0 \text{ for } i = 1, 2, \ldots, s \qquad (7)$$

The inputs u_i result from the interconnections of unit i with the other units of the processing system

$$u_i = \sum_{j=1}^{s} Q_{ij} y_j = Q_i y \qquad (8)$$

where Q_i is the incidence matrix describing the interconnection of unit i with the other units. (P1′) reflects the extreme situation of completely centralized data acquisition and decision making (control action). On the other hand

$$\underset{m}{\text{Min}} \quad \Phi = \sum_{i=1}^{s} \underset{m_i}{\text{Min}} \quad \Phi_i(x_i, m_i, u_i, d_i) \quad \text{s.t. (7), (8)} \qquad (P2)$$

represents complete decentralization down to the basic operating unit. (P1′) suffers from too much complexity, while in (P2) the extensive coordination between the subunits may be undesirable. The multiechelon decomposition criteria to be developed later supply quantitative means for judging the attractiveness of the different decompositions.

CLASSIFYING DISTURBANCES AND DECOMPOSING THE CONTROL TASK:

Formalizing the discussion in the last section we can state for *Disturbance Classification 1:* (a) the nonstationary "slowly varying" disturbances d_1 are candidates for optimizing control action, and (b) only regulatory action will be taken to deal with the remaining disturbances d_2.

Not all the slow disturbances will affect seriously the optimum economic performance of the process. It is therefore important to realize which disturbances are of economic interest and to act appropriately. Here, we establish a measure to classify the disturbances from an economic point of view and thus establish the optimization requirements for the control structure. Since the external disturbances d_i, $i = 1, \ldots s$ are considered constant in a particular optimization step, we can regard them as additional constraints on the process, i.e. $d_i = d_i^*$, $i = 1, \ldots s$. If we let λ_i be the Lagrange multipliers associated with the interconnections (8) and π_i the multipliers associated with the constraints $d_i = d_i^*$ then the sub-Lagrangian associated with unit i is defined as

$$l_i = \Phi_i(x_i, m_i, u_i, d_i) - \lambda_i^T u_i + \sum_j \lambda_j^T Q_{ji} y_i - \pi_i^T d_i \qquad (9)$$

The stationarity condition at the optimum, with respect to the disturbance d_i, yields

$$\pi_i = \left(\frac{\partial \Phi_i}{\partial d_i}\right)_{f_i=0} + \sum_{j=1}^{s} \lambda_j^T Q_{ji} \left(\frac{\partial y_i}{\partial d_i}\right)_{f_i=0} \qquad (10)$$

(The derivative is understood to be a constrained derivative such that $f_i = 0$ is satisfied.) The value of π_i denotes the impact of a small change in the disturbance d_i on the optimum performance of the overall system. This well known sensitivity concept carried by the Lagrange multipliers at the optimum point, is very helpful in classifying the disturbances for optimizing control.

Disturbance Classification 2: only disturbances with a serious impact on the objective function are considered for optimization purposes, as this is demonstrated by the value of the Lagrange multiplier π_i associated with each disturbance. The first term on the right-hand side of (10) shows the economic impact of the disturbance d_i on the subsystem i. The second term is a measure of the impact that occurs because the effects of the disturbance are propagated to other units of the system. Depending on the relative magnitude of these two terms we can decide where we should concentrate our control action.

Disturbance Classification 3: if the term $(\partial\Phi_i/\partial d_i)_{f_i=0}$, in (10) is of larger absolute value than $\Sigma\, \lambda_j^T Q_{ji}\, (\partial y_i/\partial d_i)_{f_i=0}$, then the disturbance has its major economic impact on subsystem i. Otherwise, the major impact is on the remaining plant.

Since the disturbances d_i are quite often unmeasured upon entering the system, the values of π_i help us decide which disturbances we should try to estimate as best as we can, to bring the system promptly to the new optimum point. Methods for selecting secondary measurements to estimate the important unmeasured disturbances d_i are presented in Part III. The sign of the multipliers π_i in conjunction with the direct measurement of the disturbances d_i, or their estimation through secondary measurements will help the optimizing controller decide the direction it should move to improve system performance. Computation of π_i from (10) is rather straight forward. The simplest way to obtain λ (if it is not known from a two-level optimization) is from the stationarity condition of the lagrangian with respect to the interconnection inputs u_i, i.e. the conditions

$$\frac{\partial l_i}{\partial u_i} = 0 \quad i = 1, \ldots s$$

yield the system of equations

$$\left(\frac{\partial \phi_i}{\partial u_i}\right)_{f_i=0} - \lambda_i^T + \sum_{j=1}^{s} \lambda_j^T Q_{ji} \left(\frac{\partial y_i}{\partial u_i}\right)_{f_i=0} = 0 \quad i = 1, \ldots s$$

which can be solved for λ (Westerberg, 1973). The constrained derivates $(\partial\Phi_i/\partial d_i)_{f_i=0}$, $(\partial\Phi_i/\partial u_i)_{f_i=0}$, $(\partial y_i/\partial d_i)_{f_i=0}$, $(\partial y_i/\partial u_i)_{f_i=0}$ can be obtained from simple perturbations on subsystem i only. The remainder of the plant is not included in those computations.

It is clear classifying the disturbances should be one of the first steps in developing a control structure. It helps decompose the control task into its regulatory and optimizing parts within the framework of multilayer control structures, and also determines the extent of each task. Further, the economic impact of the various slow disturbances entering the system (demonstrated by the values of the associated Lagrange multipliers) determines the extent of the optimizing control structure and provides the initial rigorous guidelines for its construction. In the next section, we discuss methods for decomposing the process along the multiechelon concept. We introduce design methods to structure the optimizing controllers (translation of the economic objectives into process control objectives, feedforward optimizing structures vs feedback structures etc.).

CRITERIA FOR THE MULTIECHELON PROCESS DECOMPOSITION

Consider the whole plant as one integrated system. Then the optimizing control problem was formulated as

$$\begin{aligned} &\min_{m} \quad \Phi(x, m, d) \\ &\text{s.t.} \quad f(x, m, d) = 0 \end{aligned} \tag{P1'}$$

Any feasible perturbation has to satisfy the conditions

$$\delta f = \frac{\partial f}{\partial x^T}\delta x + \frac{\partial f}{\partial x^T}\delta m + \frac{\partial f}{\partial d^T}\delta d \equiv J\delta x + C\delta m + D\delta d = 0 \tag{11}$$

and

$$\delta\Phi = \frac{\partial \Phi}{\partial x^T}\delta x + \frac{\partial \Phi}{\partial m^T}\delta m + \frac{\partial \Phi}{\partial d^T}\delta d \tag{12}$$

The matrix J is nonsingular if the constraint equations are independent, and (11) can be solved for δx. After substituting its value in (12) we obtain

$$\delta\Phi = \left(\frac{\partial \Phi}{\partial m^T} - \frac{\partial \Phi}{\partial x^T} J^{-1} C\right)\delta m + \left(\frac{\partial \Phi}{\partial d^T} - \frac{\partial \Phi}{\partial x^T} J^{-1} D\right)\delta d \tag{13}$$

With respect to the invertibility of the matrix J, vector f contains the transformation equations at steady-state ($g' = 0$). Since $\dim(g') + \dim(g_1'') > \dim(x)$, a number of variables m will depend on the solution $f = 0$. The number of these additional dependent variables is equal to $\dim(g') + \dim(g_1'') - \dim(x)$. Therefore, in the perturbation analysis above, the vector x should be viewed as the vector of all dependent variables—not only of the states. Similarly m represents the vector of all independent variables, excluding the ones which are defined from the equation $f = 0$.

With these remarks in hand, J is always square. It is also invertible, since $f = 0$ is a set of independent equations. At the constrained optimum, the vector of constrained derivatives (coefficient of first term in Eq. 13) has to vanish, while the coefficient of the second term is the vector of disturbance sensitivity coefficients. There are certain important conclusions that can be drawn from (13):

Using only first-order terms the manipulated variables have no effect on the objective. Any control policy will affect the second and higher order terms only. Only when the second-order term is significant compared to the first-order one, it makes sense to discuss optimizing control. In view of these two observations, let us consider the change $\delta\Phi$ in the objective function by including also second-order terms. This is given by

$$\delta\Phi = \left(\frac{\partial \Phi}{\partial d^T} - \frac{\partial \Phi}{\partial x^T} J^{-1} D\right)\delta d + \tfrac{1}{2}[(-J^{-1}(C\delta m + D\delta d))^T, \delta m^T, \delta d^T] \; H \begin{bmatrix} (-J^{-1}(C\partial m + D\delta d)) \\ \delta m \\ \delta d \end{bmatrix} \tag{14}$$

where H is the matrix of second derivatives of Φ with respect to the variables (x, m, d). The solution δm^* to the optimization problem

$$\min_{\delta m} \quad \delta\Phi(\delta m, \delta d) \tag{15}$$

can be obtained analytically from (14) by solving the stationarity condition,

$$\partial(\delta\Phi)/\partial\delta m = 0$$

Thus, we have

$$\begin{aligned} \delta m^* = &\left((J^{-1}C)^T \frac{\partial^2\phi}{\partial x^2}(J^{-1}C) - (J^{-1}C)^T \frac{\partial^2\phi}{\partial x\partial m} - \frac{\partial^2\phi}{\partial m\partial x}(J^{-1}C) + \frac{\partial^2\phi}{\partial m^2}\right)^{-1} \\ &\left(\frac{\partial^2\phi}{\partial m\partial x}(J^{-1}D) + (J^{-1}C)^T \frac{\partial^2\phi}{\partial x\partial d} - \frac{\partial^2\phi}{\partial d^2} - (J^{-1}C)^T \frac{\partial^2\phi}{\partial x^2}(J^{-1}D)\right)\delta d \end{aligned} \tag{16}$$

The value of δm^* can be substituted back into (14) and we find that the change $\delta\Phi$ after a disturbance has entered the process is given by

$$\delta\Phi(\delta d, \delta m^*) = \left(\frac{\partial \Phi}{\partial d} - \frac{\partial \Phi}{\partial x} J^{-1} D\right)\delta d + \tfrac{1}{2}\,\delta d^T M \delta d \tag{17}$$

where M is the appropriate matrix resulting from the substitution of (16) into (14). The change in the minimum of the performance index given by Equation (17) is what is achieved by perfect open-loop feed-forward optimizing control on the integrated undecomposed system. It will be used as basis for evaluating the alternative decomposition schemes.

When decomposing the process into subgroups, we try to achieve the least possible loss due to decomposition and poor coordination. This implies that we would like to decompose the process in such a way that after the disturbance has entered, we will optimize only each subgroup independently, and have little or no coordination among them. Because of imperfect coordination, the $\delta\Phi$ of the decomposed process will be different from that given for the integrated process by Equation (17).

Similar aspects of balancing imperfect coordination and resulting suboptimality are discussed by Bailey and Ramapriyan (1973) and Bailey and Laub (1976) in the context of optimal regulatory control. In these works, subsystems are formed to be "weakly coupled." Optimal feedback gains are computed for the separate systems in such a way that the sum of the quadratic performance indices of the subsystems is close to the value of the performance index obtained if one central optimal feedback law had been found.

A quantitative measure of "weak coupling" is also given in these works. Similar approaches have been adopted by others within the context of multiechelon control. This idea, though, is quite unsatisfactory for decomposing a chemical process for optimizing control for two reasons: (a) this notion of "weakly coupled" subsystems can be used for regulation where the dynamics are important, but not for the optimization we are after, and (b) the interpretation of the quadratic performance index in economic terms is often not justified in process control.

One possible and commonly applied coordination method is the Interaction Balance Method, where the Lagrange multipliers associated with the interconnections among the subsystems are adjusted by the coordinator. Schoeffler (1964) suggests accordingly to decompose the system so the interconnection multipliers are insensitive to entering disturbances. But, how to determine the insensitivity is not trivial, and even when it is found, it is not very informative, because small deviations from the correct multiplier value could have large effects on the objective.

Consider the chemical process decomposed into s subsystems through an arbitrary decomposition. The optimizing control problem is defined by problem (P2) earlier in this article. If the optimizing control is implemented in a decentralized manner, then for each subsystem we have

$$\underset{m_i,\ u_i}{\text{Minimize}}\ l_i$$

where l_i is the sub-Lagrangian for subsystem i and is of the form given by (9). Following the same approach as for the undecomposed system (second-order perturbation around the optimum point for each subsystem i), it is easy to show that the optimum change in the manipulated variables $m'_i = (m_i^T, u_i^T)^T$ of subsystem i, when disturbances d_i enter the system, is given by

$$\delta\tilde{m}'_i = \Bigg((J_i^{-1}C_i)^T \frac{\partial^2 l_i}{\partial x_i^2}(J_i^{-1}C_i) - (J_i^{-1}C_i)^T \frac{\partial^2 l_i}{\partial x_i \partial m_i} - \frac{\partial^2 l_i}{\partial m_i \partial x_i}(J_i^{-1}C_i) + \frac{\partial^2 l_i}{\partial m_i^2}\Bigg)^{-1} \Bigg(\frac{\partial^2 l_i}{\partial m_i \partial x_i}(J_i^{-1}D_i) + (J_i^{-1}C_i)^T \frac{\partial^2 l_i}{\partial x_i \partial d_i} - \frac{\partial^2 l_i}{\partial d_i^2} - (J_i^{-1}C_i)^T \frac{\partial^2 l_i}{\partial x_i^2}(J_i^{-1}D_i)\Bigg)\delta d_i \tag{18}$$

for $i = 1, 2, \ldots s$. Then, if $\delta\tilde{m}^T = [\delta\tilde{m}_1^T\, \delta\tilde{m}_2^T \cdots \delta\tilde{m}_s^T]$ we have

Decomposition Criterion 1: The relative loss caused by insufficient coordination upon the occurrence of a disturbance is given by

$$\Delta = (\delta\Phi(\delta d, \delta\tilde{m}) - \delta\Phi(\delta d, \delta m^*))/|\delta\Phi(\delta d, \delta m^*)| \tag{19}$$

The subsystems should be aggregated in such a way that this loss is tolerable and properly balanced against the coordination effort.

Decomposition Criterion 2: If

$$\delta\Phi(\delta d, \delta\tilde{m}) - \delta\Phi(\delta d, 0) > 0 \tag{20}$$

the chosen aggregation cannot be accepted because the decentralized control action without exact coordination leads to a worse performance than no control at all.

Note that $[\delta\Phi(\delta d, \delta\tilde{m}) - \delta\Phi(\delta d, \delta m^*)] \geq 0$. In (19) and (20), only the second-order terms of the two quantities have to be compared, the first-order terms being identical. $\delta\Phi(\delta d, 0)$ can be determined through measurements on the plant (no control action is taken after a disturbance has entered) and compared with the theoretically computed $\delta\Phi(\delta d, \delta m^*)$. Based on the difference a decision about reoptimization can be made.

Certain final comments are in order on the computational aspects of the criteria 1 and 2 for process decomposition:

1. The computation of the quantities in (19) and (20), following the algebraic procedure outlined before, can be a monumental task—even for medium-size plants. Various alternatives are available. Simple and approximate models for the operating units, the economic functions, and the operational constraints could be adopted. The order-of-magnitude approximation technique developed by Doherty, Douglas (1978) is an attractive alternative to simplify the computations.

2. Once a steady-state optimum flowsheet is available, the Lagrange multipliers for all the streams interconnecting the processing units are easily available. A sensitivity analysis of these multipliers to the external disturbances d, provides useful information for selecting the decomposition.

3. (19) and (20) do not have to be evaluated analytically, but they can be obtained from a perturbation analysis

$\delta\Phi(\delta d, \delta m^*)$:	Change in the objective Φ when a disturbance occurs and the integrated plant is reoptimized.
$\delta\Phi(\delta d, \delta\tilde{m})$:	change in the objective Φ when a disturbance occurs and only the immediately affected subsystem is reoptimized.
$\delta\Phi(\delta d, 0)$:	change in the objective Φ when a disturbance occurs and no control action is taken.

4. Criteria 1 and 2 were developed assuming deterministic disturbances. Consequently, the advantages of one decomposition over another depend on the particular disturbances. If the probability distribution of the disturbance amplitude is known, the following values

$$E\{(\delta\Phi(\delta d, \delta\tilde{m}) - \delta\Phi(\delta d, \delta m^*))/|\delta\Phi(\delta d, \delta m^*)|\}$$

and

$$E\{\delta\Phi(\delta d, \delta\tilde{m}) - \delta\Phi(\delta d, 0)\}$$

can be evaluated with a Monte Carlo simulation either of (14), or, via the perturbation approach discussed above, of the full system model. It should be mentioned that the computation for the Monte Carlo simulation can be greatly reduced by taking advantage of the quadrature approximation developed by Johns (1973), which is valid for normally distributed disturbances.

OPTIMIZING CONTROL STRUCTURES AND THE SELECTION OF SECONDARY CONTROL OBJECTIVES

In the previous section, we developed two criteria for the decomposition of the process for steady-state optimizing control. During this development, the following optimizing control strategies arose:

(i) Completely centralized optimizing control considering the whole plant as an integrated system. The optimum change of the manipulated variables under these conditions is given by Equation (16).

(ii) Decentralized optimizing control for each subsystem i, resulting from process decomposition and coordination of local optimizations. If the coordination is perfect, the optimum change of the manipulated variables is given again by Equation (16). The quality of the optimum attained by this strategy is the same as for the strategy (i) above.

(iii) Decentralized optimizing control for each subsystem i, without coordination of the local optimizations. In this case, the optimum change of the manipulated variables is given by Equation (18). This strategy is suboptimal, inferior to (i) and (ii) above. It has, though, the advantage of easier practical implementation.

All these strategies are of the feedforward type, since for the adjustment of the manipulated variables we assume that the disturbances are known without the benefit of feedback information.

Let us also assume the situation where the main loss resulting from the presence of a slow disturbance can be attributed to the severe deviation of one process variable from the normal steady state. Then, we can eliminate the open-loop optimizer altogether, and replace it with a simple feedback loop. A physical example of such a situation was presented by Maarleveld and Rijnsdorp (1970) in the constraint control of distillation columns. They found that depending on the throughput, pressure in the column has to be adjusted for economically optimal operation. Within a certain range of feed flowrates, the best operation requires the tray loading in the stripping section to be maximum. Instead of computing the optimal pressure for every specific throughput, we can simply adjust the condenser's cooling water flowrate (and with it the column pressure) so that the pressure drop over the stripping section (which is representative for the tray loading) is at its maximum allowed value. A simple feedback loop can be used for that purpose.

In attempting to synthesize a feedback optimizing control structure, our main objective is to translate the economic objective into process control objectives. In other words we want to find a function c of the process variables (in the above distillation example, c is the pressure drop) which when held constant, leads automatically to the optimal adjustment of the manipulated variables, and with it, the optimal operating conditions.

In more concrete terms, we look for control structures such that

if

$$c(m, d) = c_d \Rightarrow \Phi = \Phi^* \tag{21}$$

This means that by keeping the function $c(m, d)$ at the set-point c_d, through the use of manipulated variables m, for various disturbances d, it follows uniquely that the process is operating at the optimal steady state, denoted by an asterisk. Furthermore the relationship (21) implies that if

$$c(m, d) = c_d \Rightarrow \Phi = \Phi^* \Rightarrow m = m^* \text{ and } x = x^* \tag{22}$$

The unique dependence demonstrated by (22) requires the satisfaction of the implicit function theorem as Findeisen (1976) suggested. These arguments are detailed in Part II of this series, where the alternative regulatory control structures are developed. Ideally one tries to select c in such a way that some or all the elements of c are independent of the disturbances d.

In many cases we will not be able to find c so that relationship (22) is satisfied, or that c is independent of the disturbances d. In general, we look for feedback optimizing structures which satisfy the following approximation

$$c(m, d) = c_d = \Rightarrow \Phi \approx \Phi^* \tag{23}$$

i.e., holding certain process variables at their set points, keeps the objective function approximately at the optimum. The additional constraints $c(m, d) = c_d$ imposed on the system, generate "secondary" control objectives which will be satisfied through the development of appropriate regulators. Note that we use the declaration "secondary" to distinguish these objectives from the "primary" regulatory objectives arising from the production amount and quality specifications, the safety considerations, the environmental and other regulations etc.

A selection procedure for the process outputs c to be controlled such that (22) and (23) are satisfied can be derived along the following lines: The relationship $c(m, d) = c_d$ imposed additional constraints on the system, and consequently the vector $\bar{f}$ and the matrices J and D have to be augmented. Note that $\bar{f}$ is the augmented composite vector of equality constraints, i.e., $\bar{f}^T = [g'^T, g_1''^T, (c - c_d)^T]$. Further, $\bar{J} = \partial \bar{f}/\partial x^T C = \partial \bar{f}/\partial m^T$ and $\bar{D} = \partial \bar{f}/\partial d^T$. Also, comments made earlier for the square character and the invertibility of the matrix J apply similarly to the matrix $\bar{J}$.

A number of free independent variables m, equal to the number of constraints c, have to be transferred to the vector of dependent variables, x, because these variables are used to implement the feedback control law and cannot be manipulated freely. In the special case that dim (m) = dim(c)(i.e., there are no free variables left), (14) can be written as

$$\delta\Phi(\delta d, \delta\bar{m}) = \left(\frac{\partial\Phi}{\partial d^T} - \frac{\partial\Phi}{\partial\bar{x}^T}\bar{J}^{-1}\bar{D}\right)\delta d + \tfrac{1}{2}[(-\bar{J}^{-1}\bar{D}\delta d)^T, \delta d^T]H\begin{bmatrix}-\bar{J}^{-1}\bar{D}\,\delta d\\ \delta d\end{bmatrix} \tag{24}$$

where $\delta\bar{m}$ is the change in the manipulated variables resulting from the feedback control arrangement, $\bar{J}$ and $\bar{D}$ are the augmented Jacobian matrices.

Feedback Optimizing Control Criterion 1:

$$(\delta\Phi(\delta d, \delta\bar{m}) - \delta\Phi(\delta d, \delta m^*))/|\delta\phi(\delta d, \delta m^*)| \tag{25}$$

represents the loss from the use of feedback instead of open loop optimal control action. The controlled variables c should be chosen such that this loss is tolerable.

Feedback Optimizing Control Criterion 2: If

$$\delta\Phi(\delta d, \delta\bar{m}) \geq \delta\Phi(d, 0) \tag{26}$$

the particular feedback optimizing control scheme is worse than no control at all and does not represent a feasible alternative.

Remarks: (1) The different feedback control structures are expressed in different constraint vectors $\bar{f}$ and different Jacobians $\bar{J}$. $\bar{J}$ can be of significant size in a real situation and repeated inversion to determine the optimal set of controlled variables c might be prohibitive. A simplification results from matrix inver-

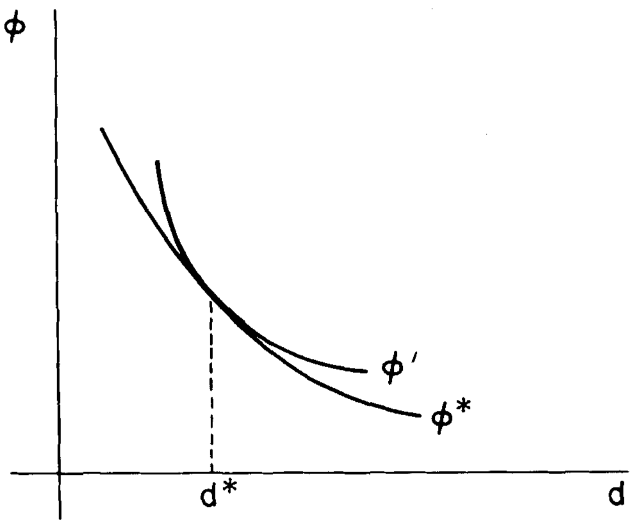

Figure 4. Optimal (Φ^*) and suboptimal (Φ') control policies with disturbance changes.

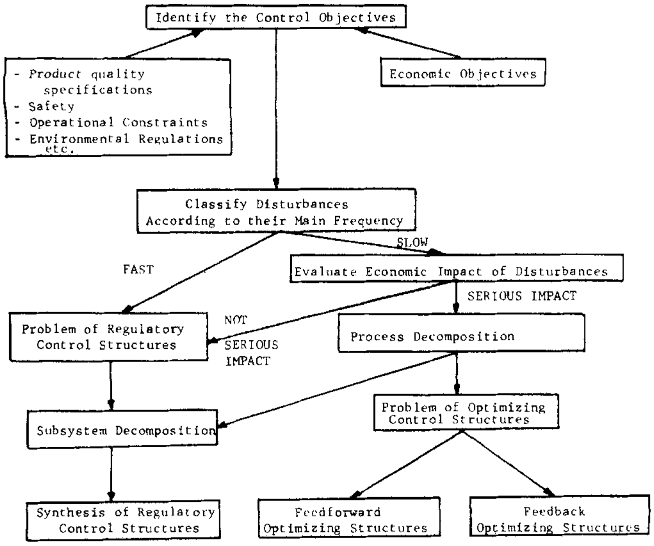

Figure 5. A diagram of the strategy employed during the synthesis of control structures.

sion by partition (Lottkin and Remage 1953). (2) $\delta\phi(\delta d, \delta\overline{m}) - \delta\Phi(\delta d, \delta m^*) \geq 0$. (3) If $\dim(c) < \dim(m)$, (25) and (26) depend on the manipulated variables chosen for the feedback laws. (4) In (25) and (26), only the quadratic terms have to be compared, the linear ones being identical.

The function of optimizing control can be understood better in a schematic diagram. One possible situation is depicted in Figure 4. The plant has been optimized for the disturbance d^*. The rate of change of the objective with a change in the disturbance d is given by the Lagrange multiplier π and is *independent* of the control policy. If the second-order terms of Φ' and Φ^* at $d = d^*$ are small compared to the first-order terms, then it is probably best not to use optimizing control at all, and to leave the manipulated variables unchanged for a change in the disturbances. If they are not negligible but if their difference is small, then the control policy yielding Φ' (e.g., feedback optimizing control or decentralized optimization without recoordination) is a permissible suboptimal one.

To summarize, we have presented diagramatically the strategy adopted for the synthesis of control structures for chemical processes in Figure 5.

NUMERICAL EXAMPLE

Here, we demonstrate the various developments of the previous sections on an integrated gasoline polymerization plant at the Shellburn Refinery (Shell Canada Ltd., Burnaby, B.C. Canada). This plant has been the subject of various studies for optimal process design (Gaines and Gaddy 1976) and for process operation optimization (Friedman and Pinder 1972). This plant offers relative complexity and integration which warrants a systematic analysis and synthesis of the potential control structures.

Process Description

The process is the Universal Oil Products solid phosphoric acid catalyst process. The product is gasoline from light hydrocarbons. Figure 6 is the flow diagram of the plant. The feed is mainly light olefins and paraffins, which are preheated and then enter the polymerization reactors, where dimerization of olefins takes place. The high exothermicity of the reactions requires propane quench to provide interstage cooling between catalyst beds. The reactor's effluent goes through a sequence of distillation columns to separate propane, butane and the gasoline as product streams. The information flow is shown in Figure 7, and is similar to the modular flowsheet used by Friedman (1972).

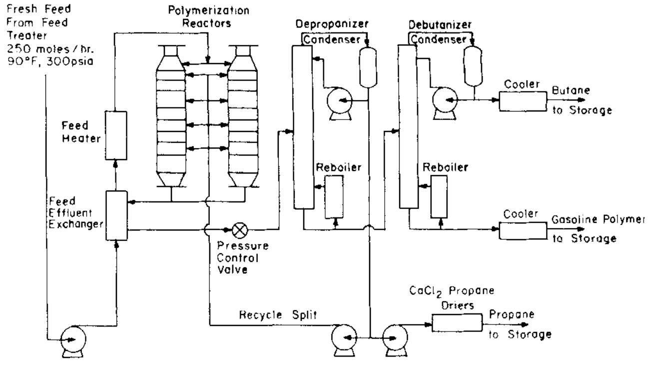

Figure 6. Flow diagram of the polymerization plant.

TABLE 1. OPTIMAL STEADY-STATE DESIGN CONDITIONS FOR THE POLYMERIZATION PLANT

Feed

Temperature: 305 K	recycle split s_p = .4647
Pressure, PSIA: 330	
(2.277×10^6Pa)	quench splits
Composition:	$s_1 = 0$
Propane: 57.45	$s_2 = 0$
I-Butane: 50.00	$s_3 = .6525$
N-Butane: 45.00	$s_4 = .3475$
I-Pentane: 7.5	Depropanizer
	Pressure = 363 psia (2.5×10^6Pa)
N-Pentane: 2.5	Debutanizer
	Pressure = 110 psia (758 kPa)
Propylene: 42.55	
Cis-2-Butene: 10	Reactor Bed Temperatures
Trans-2-Butene: 7.5	T_3 = 815°R (453 K)
I-Butene 25	T_5 = 925°R (513 K)
TR-2-Pentene 2.5	T_7 = 945°R (525 K)
Total 250 moles/hr.	T_{19} = 944.9°R (524.6 K)

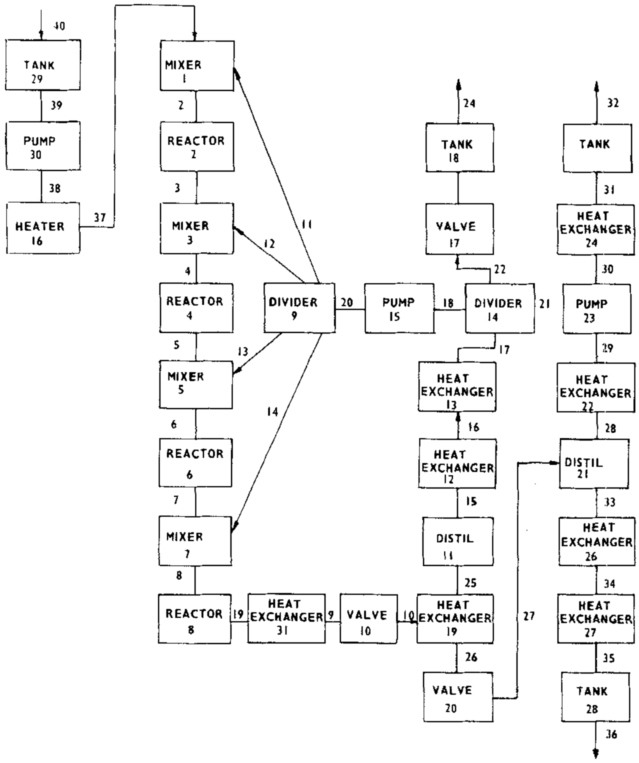

Figure 7. The modular representation of the polymerization plant.

TABLE 2. OPTIMAL VALUES OF THE λ_i'S FOR CRITICAL INTERCONNECTIONS

Components	λ_{19}	λ_{20}	λ_{26}
Temperature	−6.594	29.26	151.1
Pressure	−9.055	0	−29.3
Propane	1,774.2	1,517.6	2,746.1
I-Butane	4,096.1	3,785.7	3,810
N-Butane	4,301.3	3,984.7	3,662.5
I-Pentane	8,180	—	11,170.6
N-Pentane	5,560	—	5,186.9
Propylene	3,148	5,658.4	2,752.2
Cis-2-Butene	4,540	5,967.9	3,665.2
Trans-2-Butene	4,475	5,940.3	3,657.3
I-Butene	4,555.7	5,962	3,659.6
Tr-2-Pentene	5,600	—	3,976.6
Heptene	13,340	—	12,882

" – " indicates that corresponding components are never present in the stream 20.

For this simulation, we used the modules developed by Friedman and Pinder (1972) and Gaines and Gaddy (1976) within the general process simulator CHESS (Motard et al. 1968). The costing routines given by the system PROPS (Gaines and Gaddy 1974) are also employed.

Classification of the Disturbances and Decomposition of the Control Tasks

Within the context of multilayer control we will use the criteria developed earlier. The "slow" disturbances as they are characterized by the frequency of their change are:

1. ambient reactor temperature,
2. cooling water temperature in the depropanizer,
3. cooling water temperature in the debutanizer,
4. feed flowrate,
5. feed composition (propane to propylene ratio taken as the characteristic paraffin to olefin ratio), and
6. propane recovery in the depropanizer.

From previous plant experience, these slow disturbances are the most important, and create serious control and optimization problems. The last disturbance (#6) is a result of a production management division and is introduced intentionally as a part of the operational policy.

For given nominal values of the above disturbances, the optimization design specifications are given in Table 1. We classify the disturbances and the control tasks around this point. From the stationarity conditions (10), we estimate the linear sensitivity π_i for each disturbance. A reasonable estimate of the optimal values for the Lagrange multipliers λ_i, corresponding to the interconnection constraints, are obtained from the adjoint set of equations.

This set is derived from the stationarity conditions of the Lagrangian, with respect to the interconnection inputs (see Westerberg 1972, Brosilow and Nunez 1968). The values of the Lagrange multipliers for the critical streams #19, 20 and 26 (Figure 7) are given in Table 2. The values of the λ_i's for the rest of the streams can be found through a sequential computation and are omitted here, but can be found in Arkun (1979). The values of the $(\partial \Phi_i/\partial d_i)_{f_i=0}$ and $(\partial y_i/\partial d_i)_{f_i=0}$ are computed by a simple numerical perturbation on the corresponding subsystem i only. Thus, the computation of the π_i's was completed and their values are given in Table 3, together with the distribution of their economic impact on the various parts of the plant. Based on the absolute values of the π_i's from Table 3, we have the following classification:

Disturbances belonging to the optimizing control tasks:

i) feed flowrate $|\pi| =$ 1,730
ii) feed composition $|\pi| =$ 94,328
iii) propane recovery in the depropanizer $|\pi| =$ 504,500

Disturbances belonging to the regulatory control task:

i) ambient reactor temperature $|\pi| =$ 160
ii) cooling water temperature in the debutanizer $|\pi| =$ 244
iii) cooling water temperature in the depropanizer $|\pi| =$ 304

Process Decomposition

Alternative decomposition schemes will now be generated and evaluated for the three slow disturbances with a serious economic impact (allocated to the optimizing control task.) The decomposition schemes considered here are shown in Table 4. They are appealing from an operator's point of view for the functional unity of the processing units in each resulting subsystem.

Evaluation of the Decomposition Schemes

Earlier, we discussed techniques to evaluate various decompositions when the disturbances are considered deterministic or stochastic. In this section, for illustration purposes, we present an exhaustive and detailed evaluation of the various decomposition alternatives for each disturbance, separately.

Feed composition disturbance: This disturbance is characterized by the propane to propylene ratio as a measure of the paraffins to olefins ratio in the feed. For a standard deviation of 0.014 in the propane/propylene ratio, we have the following results

Decomposition A: (Subsystem S_1 only optimized)

$$\underset{m_1}{\text{Max}}\ l_1 = \Phi_1 + \lambda_{19}y_{19} - \lambda_{20}y_{20}$$
$$\text{s.t.} \quad g_1 \leq b_1$$

where

$m_1^T = [s_1, s_2, s_3]$ the three quench splits.

TABLE 3. ECONOMIC SENSITIVITY ANALYSIS RESULTS WITH RESPECT TO THE EXTERNAL DISTURBANCES

Disturbance d_i	π_i	$\partial\phi_i/\partial d_i$	$\sum_j \lambda_j Q_{ji} \partial y_i/\partial d_i$	Subsystem S_i	Torn Interconnection
Ambient Reactor T	160	0	160	Reactors	19,20
Cool Water T in Debutanizer	−244	−244	0	Debutanizer	26
Cool Water T in Depropanizer	−304	−304	0	Depropanizer	19, 20, 26
Feed Flowrate	1,730	−62	1,793	Reactors	19, 20
Propane/Propylene in the Feed	−94,328	38,048	−132,376	Reactors and Depropanizer	26
Propane Recovery in Depropanizer	−504,500	−418,150	−86,350	Depropanizer	17, 19, 26

Subsystem S_i together with the corresponding torn streams indicates the units where local numerical perturbations were carried out.

TABLE 4. ALTERNATIVE DECOMPOSITION SCHEMES FOR THE GASOLINE POLYMERIZATION PLANT

Decomposition A:	Torn streams #19 and 20, two subsystems
Subsystem S_1:	Reactors with feed preparation units
Subsystem S_2:	Sequence of the depropanizer and debutanizer
Decomposition B:	Torn stream #26, two subsystems
Subsystem S_1:	Reactors, feed preparation units and the depropanizer
Subsystem S_2:	Debutanizer
Decomposition C:	Torn streams #17, 19, two subsystems
Subsystem S_1:	Reactors, feed preparation units, depropanizer recycle, storage units
Subsystem S_2:	Depropanizer and debutanizer
Decomposition D:	Torn streams, #17, 19, 26, three subsystems
Subsystem S_1:	Reactors, feed preparation units, depropanizer recycle, storage units
Subsystem S_2:	Depropanizer
Subsystem S_3:	Debutanizer

$$g_1 = \begin{bmatrix} 760 \leq T_i \leq 945 & i = 3, 5, 7, 19 \text{ streams} \\ s_4 = 1 - s_1 - s_2 - s_3 & \end{bmatrix}$$

T_i's are the reactor bed temperatures. At the decentralized optimum $\tilde{m}_1^T = [0, 0, 0.755]$ and $\delta\Phi(\delta d, \delta\tilde{m}) = 111.6$

Decomposition B: (Subsystem S_1 only optimized)

$$\underset{m_1}{\text{Max}}\ l_1 = \Phi_1 + \lambda_{26}y_{26}$$
$$\text{s.t.} \quad g_1' \leq b_1'$$

where

$$g_1' = \begin{bmatrix} g_1 \text{ (same as above)} \\ \text{Flooding in depropanizer} \leq 95\% \end{bmatrix}$$

$m_1 = [s_1, s_2, s_3, s_r$ = recycle split,

p_p = depropanizer pressure]

At the decentralized optimum: $s_1 = 0$, $s_2 = 0$, $s_3 = 0.656$, $s_r = 0.4685$ and $p_p = 363$ psia (2.5×10^6 Pa) with $\delta\Phi = 835.51$

Decomposition C: (Subsystem S_1 only optimized)

$$\underset{m_1}{\text{Max}}\ l_1 = \delta_1 + \lambda_{19}y_{19} - \lambda_{17}u_{17}$$
$$\text{s.t.} \quad g_1 \leq b_1 \quad \text{(same as above)}$$
$$m_1 = [s_1, s_2, s_3, s_r]$$

At the optimum $m_1 = [0, 0, 0.675, 0.47]$ with $\delta\Phi = 715.62$

Decomposition D: as for decomposition C, $\delta\Phi = 715.62$ For the integrated plant a centralized optimization (no decomposition) gave the following results:

TABLE 5. EVALUATION OF THE DECOMPOSITION SCHEMES IN THE PRESENCE OF THE THREE ECONOMICALLY IMPORTANT DISTURBANCES

	Disturbance		
Decomposition Scheme	Feed Composition Δ	Feed Flowrate Δ	Propane Recovery Δ
A	0.8673	0.0619	n.a.
B	0.0068	0.0001	0.003
C	0.1493	0.0171	0.0363
D	0.1493	0.0171	0.0363

$$s_1 = 0 \quad s_2 = 0 \quad s_3 = 0.655 \quad s_4 = 0.344$$
$$p_p = 365 \text{ psi} \quad p_b = \text{pressure in the debutanizer} = 110 \text{ psi } (0.77 \times 10^6 Pa)$$

with a $\delta\Phi(\delta d, \delta m^*) = 841.26$.

In Table 5 we summarize the effects of the feed disturbance on the plant economics for the four decomposition schemes. As a measure, we used the quantity Δ defined by (19). Clearly as Δ decreases, the decomposition scheme becomes more attractive for decentralized control. From Table 5 we conclude that scheme *A* is unacceptable, as it leads to 86.7% deterioration compared to centralized optimizing control.

Feed flowrate disturbance: We considered a standard deviation of 1 mole/hr. The formulation of the subproblems remains the same as for the case of the feed composition disturbance, and the results are shown in Table 5 (for details, see Arkun 1979).

Disturbance in the propane recovery of the depropanizer: Around the design optimum of 99% recovery we considered a deviation of 0.1%. The results are tabulated in Table 5. For numerical details, see Arkun (1979).

For all three disturbances with significant economic impact, the decomposition scheme A causes the largest deterioration compared to the performance of centralized control. The other three alternatives are acceptable, with scheme D preferred because of its operational advantages (three distinct subsystems, well defined function for each subsystem, better regulation of each subsystem, etc.)

Selection of Secondary Control Objectives and the Feedback Optimizing Control Structure

Here, we examine feedback alternatives to the open-loop feedforward optimizing control schemes discussed earlier. The objective is to select process outputs c regulated at given levels $c = c_d$ so that $c = c_d \Rightarrow \Phi$(with feedback regulation on c) $\approx \Phi^*$ (open-loop optimum).

For the reactor beds, the decentralized optimal results above indicate that the temperature T_7 of the output stream from the third bed being near its upper bound, could be regulated at 945° (upper bound). This requirement will reduce by one the manipulated variables. It will determine uniquely the s_3 for known values of the disturbances. For the nominal operating point of the plant, we found, $s_3 = 0.652$, $s_1 = 0$, $s_2 = 0$, $s_r = 0.465$ and T_{19} (temperature at the exit of fourth bed) = 945°R(525°K).

For the depropanizer subsystem, the tray load in the stripping section will also be regulated at its current optimal value of 95% flooding by adjusting the cooling water flowrate. This simple feedback loop will determine uniquely the column pressure drop, and eliminate the need for optimal feedforward adjustments of the pressure. The third process variable to regulate is the steam pressure in the reboiler of the debutanizer. We found that the optimal operation of the debutanizer is limited by the reboiler's rate of heat transfer. Keeping the steam pressure at its highest available value determines uniquely the column pressure for different throughputs, eliminating the feedforward optimum adjustment on the column pressure.

Now, we examine the economic impact of the three main disturbances on the economic performance of the plant with the three newly created feedback regulatory controls.

Changing the propane/propylene ratio from the design value of 1.35 to the new value of 1.22 (feed richer in olefin) produces $\delta\Phi(\delta d, \delta\bar{m}) = 6{,}174$. The T_7 is regulated at $T_7 = 945°R(525°K)$ yielding $s_r = 1.504$, $s_1 = s_2 = 0$ and $s_3 = 0.675$. The flooding constraint for the depropanizer yields $p_p = 365$ psi (2.512×10^6 Pa) and the reboiler constraint for the debutanizer determines $p_b = 106$ psi (0.74×10^6 Pa). The feedforward optimizing scheme adjusting optimally all available manipulated variables yields $\delta\Phi(\delta d, \delta m^*) = 6174$ and $\Delta = 0$.

Now, change the nominal design value of the flowrate (250 moles/hr) by 10 moles/hr, then $\delta\Phi(\delta d, \delta\bar{m}) = 16605$ under the additional regulatory control, while the feedforward optimum policy yields $\delta\Phi(\delta d, \delta m^*) = 17414$. Deterioration caused by the feedback regulation is $\Delta = 0.046$ or 4.6%, considered acceptable. The values of the dependent manipulated variables under feedback control now become: $s_3 = 0.598$, $p_p = 358$ psia (2.2×10^6 Pa), and $p_b = 108$ psia (0.756×10^6 Pa).

A 1% reduction in the recovery of propane changes the pressure in the depropanizer to $p_p = 380$ psia (2.6×10^6 Pa) by keeping the flooding constraint active. For the debutanizer, the reboiler constraint yields $p_b = 112$ psia (0.784×10^6 Pa) while the control of T_7 at 945°R(525°K) results in $s_3 = 0.652$ and $s_r = 0.469$. Then, $\delta\Phi(\delta d, \delta\overline{m}) = 3769$ while the corresponding value for the feedforward optimizing control is $\delta\Phi(\delta d, \delta m^*) = 3769$ and $\Delta = 0$.

Conclusions

Within the context of multilayer decomposition, we classified disturbances in terms of their economic impacts and decomposed control into regulatory and optimizing tasks, for different set of disturbances.

There are three different satisfactory decomposition schemes for the gasoline plant. Scheme A, where the recycle quench split is not available as a manipulated variable to the reactors subsystem, was unacceptable.

Decomposition schemes result in two or three interconnected subsystems such as reactor, depropanizer and debutanizer subsystems. The decentralized controller for each subsystem has its own manipulated and controlled variables. For example, according to the decomposition schemes, reactor subsystem's manipulated variables are the recycle and quench splits to satisfy reactor temperature constraints as controlled objectives.

For a feedback optimizing control structure as an alternative to feedforward optimization, controlled variables for each subsystem given by decomposition criteria were selected. The controlled variables were chosen to be the current active constraints at optimum for each subsystem (i.e., T_7, flooding constraint, reboiler constraint). For feed composition and propane recovery disturbances, the proposed feedback optimizing control results in no deterioration when compared with the feedforward optimizing control. For the feed flowrate disturbance, the feedback optimizing control brought 4.6% deterioration in the objective function. The deterioration results because for this specific disturbance, the optimal plant operation dictates the control of T_{19} (last reactor bed temperature) at its upper bound, which we found to be active at the new optimum corresponding to δd. Control of T_{19} instead of T_7 at the design optimum did not constitute a feasible alternative, since T_7 would be violated, i.e., $T_7 > 945$. The decision between feedback and feedforward optimizing strategies then depends on the tradeoff between economic incentive and additional optimizing control effort required.

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Financial support from the National Science Foundation through the Grant ENG75-11165 is gratefully acknowledged.

NOTATION

C = matrix defined by $\partial f/\partial m^T$
$\overline{C}$ = matrix defined by $\partial \overline{f}/\partial m^T$
c = output process variables selected as secondary control objectives
c_d = the set point of the regulated process variables c
D = matrix defined by $\partial f/\partial d^T$
$\overline{D}$ = matrix defined by $\partial \overline{f}/\partial d^T$
d = disturbances
d_1 = slow disturbances
d_2 = fast disturbances
f = composite vector of equality constraints; $f^T = [g'^T, g_1''^T]$
$\overline{f}$ = augmented composite vector of equality constraints under feedback optimizing control
g' = vector of transformation equations
g'' = vector of general inequality constraints
g_1'' = subset of constraints g'' which are active equality constraints
g_2'' = subset of constraints g'' which remain inequality constraints
J = square matrix defined by $\partial f/\partial x^T$
$\overline{J}$ = square matrix defined by $\partial \overline{f}/\partial x^T$
m = vector of manipulated (independent) variables
$\tilde{m}$ = vector of optimum values of the independent variables under decentralized optimizing control
$\overline{m}$ = vector of optimum values of the independent variables under feedback i optimizing control
p = pressure
Q = incidence matrix denoting the interconnection among units
s = number of subsystems resulting from multiechelon decomposition
s_1, s_2, s_3, s_4 = quench splits for the 1st, 2nd, 3rd, 4th beds of the reactor system
s_r = recycle split
u = vector of inputs into a unit coming from other units of the plant
W_1, W_2 = weighting matrices
x = vector of state (dependent) variables
y = vector of output variables

Greek Letters

λ = vector of Lagrange multipliers associated with interconnection units
π = vector of Lagrange multipliers associated with the disturbance specification constraints
Φ = objective function of the optimization problem (operating cost or operating profit)

Subscripts

i = variable or a function associated with the ith subsystem or unit
19 or 20 etc. = process variable associated with stream 19 or 20 etc.
p = depropanizer
b = debutanizer

Superscripts

$*$ = optimum value of a variable under open-loop feedforward control

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Part II: Structural Aspects and the Synthesis of Alternative Feasible Control Schemes

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The classification of control objectives and external disturbances in a chemical plant determines the extent of the optimizing and regulatory control structures (see Part I). In this article we discuss the structural design of alternative regulatory control schemes to satisfy the posed objective. Within the framework of hierarchical control, criteria are developed for the further decomposition of the process subsystems, reducing the combinatorial problem while not eliminating feasible control structures. We use structural models to describe the interactions among the units of a plant and the physicochemical phenomena occurring in the various units. The relevance of controllability and observability in the synthesis of control structures is discussed, and modified versions are used to develop all the alternative feasible regulatory structures in an algorithmic fashion. Various examples illustrate the developed concepts and strategies, including the application of the overall synthesis method to an integrated chemical plant.

SCOPE

In Part I, the control tasks were divided into those of the regulatory and of the optimizing type. The first can always be expressed in the form of functions of operating variables, which have to be kept at desired levels through the use manipulated variables. The same is possible for the second, if certain conditions derived in Part I are satisfied. The structure of the feedback controllers used for that purpose is developed here on a sound theoretical basis. The following problems are addressed:

1. Development of a suitable type of system representation (model), requiring a minimal amount of information.

2. Formulation of mathematical criteria to be satisfied by every feasible control structure.

3. Development of guidelines for decomposing the overall problem into manageable subproblems.

4. Algorithmic procedure to develop alternative control structures.

The approach adopted in this work is based on the structural characteristics describing (a) the interactions among the units of a chemical process and (b) the logical dependence (of the Boolean type) among the variables used to model the dynamic behavior of the various units. Thus, detailed dynamic modelling at an early stage is avoided. The mathematical feasibility criteria for the generated alternative control structures are

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