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MEASUREMENT AND CONTROL IN CHEMICAL AND ENVIRONMENTAL ENGINEERING.

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MEASUREMENT AND CONTROL IN CHEMICAL AND ENVIRONMENTAL ENGINEERING.

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Applications of automatic control methods and associated measurement techniques on chemical and environmental processes are surveyed. The main applications considered are distillation columns and other mass transfer processes, reactors and wastewater treatment plants. It is shown that advanced control theory has been applied to several systems. Due to the complexity of many plants and to inadequate instrumentation there is, however, still a large field for new control applications.

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1. INTRODUCTION

If the title of this paper should be strictly followed the result would be a thick book. The literature on the subject is overwhelming and it is truly most difficult to see the significant contributions among those published. This survey will just cover some highlights in the area of chemical and environmental process control during recent years and mainly after 1970.

In order to limit the number of possible applications, areas like paper and pulp industry, glass and mineral industry, metallurgical industry are excluded. Mainly three areas of chemical processing will be considered in some more detail, viz. mass transfer processes (mostly distillation), reactors and wastewater treatment plants.

The word "application" has many different meanings in different papers. Here we will restrict the concept of an application only to the case where real industrial data have been used or pilot plants or full scale processes have been controlled.

In the text several other surveys of special areas will be mentioned. There are several surveys given especially in the fields of instrumentation and model building and identification.

The paper is organized as follows. After the introduction some special dynamical features of chemical processes are summarized. The instrumentation problems are of major interest in process control and therefore some emphasis here is also put on these problems. Some recent developments in pollution monitoring and chemical engineering are mentioned. Computers are now being incorporated in analyzing instruments thus giving new areas for feedback control.

Model building is certainly a central task in all control system design. Several surveys of identification of chemical processes are listed and the essential problems are mentioned. The control synthesis task is by no means a standard one; one reason is that the system structure plays an important role in chemical processes. There are several theories available for handling multivariable systems as well as nonlinear systems, but the control of complex processes still lacks a coherent theory.

The computer development during the last few years will probably cause a tremendous development in both instrumentation technology and control tasks. Microcomputers and minicomputers can change the whole way of thinking in terms of computer control.

In three chapters a review is made of the developments of control and instrumentation methods in the fields of distillation, reactors and wastewater treatment control. Some major features of the contributions are listed, but the survey is by no means exhaustive; rather it illustrates some typical features of the development in the different areas.

As observed in the final chapter it is not only that the practitioners should learn the new theories but there are still several problems for the theoreticians to solve. The latter should also direct their research to the real needs of chemical process control.

2. SOME TYPICAL PROBLEMS IN CHEMICAL PROCESS CONTROL

General control theory does not, in itself, pay any special attention to the system's physical or chemical nature; the plant is just a set of differential equations or transfer functions.

In designing control systems for chemical processes there are, however, several special features which must be considered and some of those problems will be considered here. All of them are not unique for chemical process control, but added together they define the special type of approach which it might be necessary to assume for the control of a chemical plant.

(a) Disturbances

Usually the word "regulation" means that certain states or perhaps time-averages of states should be kept constant. Disturbances may consist of slow drifts, such as feed changes in a distillation column or slow diurnal variations of the flow rate in the influent to a wastewater treatment plant or the decay of a catalyst activity. In the first case the amplitude might be quite small while in the second case the amplitude variation might be very large. Sometimes disturbances are similar to explosions as in some catalyst reactors, at other times they consist of persistent random upsets or they may result from a purposeful change in the level of operation. In some of these cases it is easy to measure the disturbance, such as the flow rate in a feed. However, a shock load, consisting of heavy metals entering a wastewater treatment plant is difficult to observe before the process output has already responded. Frequently stochastic disturbances are not measureable at all but can be observed through the plant outputs. In all these cases, the plant regulation should work satisfactorily and safely.

(b) Time constants

There is an immense difference between the smallest and the largest time modes in many chemical plants. Some reactions in a catalytic reactor may last for a fraction of a second, other dynamical features in the same plant last for several minutes or hours. A control system must be defined in the proper frequency domain to work adequately. The long time constants are not always easy to handle, where oscillations can occur in recycling processes which last from one labour shift to the next. It may prove very difficult to control these slow oscillations manually.

(c) Nonlinearities

Nonlinear behaviour is the rule and not the exception in chemical plant dynamics, particularly in reaction systems;the nonlinearities are so significant that linearizations are seldom adequate for analysis and control system synthesis.

(d) Couplings

The coupling between many variables plays perhaps the largest role in making chemical processes so complex and in addition many variables are coupled in a nonlinear fashion. Conventional control strategies are therefore often inadequate, and e.g. multivariable control has to be applied. See also (i).

(e) Transportation lags

It is common that transport lags are present in chemical processes, thus causing stability problems. Lags can also be created by measurement techniques, e.g. by semi-continuous analysis instruments. The analysis is time-consuming and the control action is consequently delayed.

(f) Spatial distributions

Most chemical processes need to be described by partial differential equations. This is not only a theoretical problem but many practical problems arise too, such as where to place the instruments, how many instruments are needed to measure a distributed variable and the best location at which to manipulate the process.

(g) Measurement problems

Measurement can only be made of a very small fraction of the variables and for some it is practically impossible and for others very costly. All measurements are subject to various random and systematic errors and can be misinterpreted or obscured by unaccountable effects. And as we have mentioned before the receipt of information is often delayed, e.g. in analyzers.

(h) Control objectives

Regulation of certain process variables at desired levels is by far the most common objective in continuous chemical processes. All measured variables need not be regulated, however. E.g. in the case of the control of internal reflux and feed enthalpy of distillation columns, regulation is applied to functions of the state variables. In systems like complex chemical plants one single criterion for control is usually insufficient. A whole spectrum of control objectives is often required. Probably a whole performance vector is needed and the control designer will have to decide how to weight the various criteria included in that vector.

(i) Control system structure

It is by no means obvious how to achieve the best control. There is a crucial step in the control system configuration and structural formation which is seldom discussed in a systematic manner. A good example is the multitude of different control schemes suggested for a distillation column. There are many questions concerning which variables should be measured, and which inputs should be manipulated, before the feedback control law can even be formulated. This problem might be the most important control problem and it is certainly extremely difficult. Mostly it has been tackled in a virtually qualitative way with no quantitative analysis.

(j) Process design and control design

There is - I believe - a largely ignored area where substantial progress is possible, the integration of process design with control design. Processes are most often designed from a steady-state point of view with insufficient attention to dynamic behaviour and controllability. There a control engineer should have a responsibility which extends to the process design. Major contributions to effective control systems often are due to clever modifications of the process itself.

3. INSTRUMENTATION AND MEASUREMENTS

A key factor to implement automatic control in many chemical and environmental processes is the availability of on-line instruments. Even if there is much development being done on new instruments there is certainly still a need of reliable, sensitive continuous on-line instruments at reasonable costs.

This problem is particularly difficult in wastewater treatment plants because of the hostile environment which is typical for such processes. Instruments for several physico-chemical variables have existed for many years, but their reliability in a bad environment may be so poor, that their function will fail in some few minutes or hours.

Many of the pollution instruments which are described are initially developed in other chemical industries. Therefore similar trends can be observed in both chemical and environmental engineering instrument development.

3.1 Pollution instrumentation.

In recent years there has been a rapid increase in the pollution control activities. This development is strongly coupled with the development of new instruments and measurement principles, which are now being used in laboratories and in processes for control or monitoring. A good survey of available instrumentation principles in air and water pollution is made by Garrod (1971). New articles and surveys appear constantly in periodicals such as Chemical Engineering, Measurement and Control, and Environmental Science and Technology. The Environmental Protection Agency in USA and many other national agencies are supporting a lot of instrumentation research activities.

3.2 Air pollution characteristics.

The clean air acts recently stated in many countries are by no means any new phenomena. In England, the first smoke abatement act was passed in 1273. This was necessary because of the use of cheap cole in London and concern on the effect of coal smoke on the health. In 1306 the problem was so large in London, that coal burning was forbidden by a royal proclamation, and wood had to be used instead. It is told that a man was hanged for disobeying the royal command. Modern environmental laws seem to be somewhat more liberal.

Research on air pollution monitoring instruments has been going on for several years. The recent clean air acts, however, have significantly amplified this development, and a large number of commercial instruments, made for continuous monitoring air quality are now available in the market.

There is a lot of literature on pollution monitoring. The three books by Stern (1968) as well as reviews appearing in Analytical Chemistry ("Air pollution," 1967, 1969, 1971) are good general references. Several meetings on air pollution have been arranged, and the AIChE meetings reported by Coughlin et al (1972) and Butt et al (1971) should be mentioned. A large number of sources for the methodology of measurements are available, such as American Soc. for Testing and Materials (1971), Cooper et al (1970), and Morrow et al (1972). Three different types of air pollution will be emphasized here: particulates, sulphur dioxide and carbon monoxide. Other important pollutants are nitrogen oxides and hydrocarbons coming e.g. from motor vehicles.

Particulates means finely divided dusts of all sorts which are emitted in the athmosphere. The particulates may be classified as grit (1000-75 μ), dust (75-10 μ) and fume or smoke ($\leq$10 μ). ($1\mu = 10^{-6}$m). Technology now exists for capture and separation of up to 98% by weight of the solid matter emitted. Cyclones, bag filters and electrostatic precipitators will take up everything from lumps down to particles with a diameter of some 50-80 μ.

Most of the sulphur dioxide comes from operations associated with either oil fired power plants or with pyrometallurgical processes for metals, such as copper, nickel, lead and zinc from sulphide ores. The gas is oxidized by the atmosphere into sulphur trioxide which then forms particles of sulphuric acid. These particles may fall down as an acidic rain.

About three quarters of the carbon monoxide produced comes from gasoline powered motor vehicles. About half of the carbon dioxide produced by combustion processes finally ends up in the sea and the remainder is added to the atmosphere. If the concentration should be doubled from today's value it has been calculated that the earth temperature should increase by about 1.3^{o}C, because of the "greenhouse" effect. Consequently carbon monoxide formation in the first place should be prevented at a reasonable cost, the real challenge of the seventies.

3.3 Air pollution monitoring.

There is a great number of standard methods in use today for on-line continuous sampling of air pollutants. To monitor fine particulates measurements of light absorption, scattered light, or electric charge carried by dust can be used. For coarse particles standard dust monitors are available.

The Kem-Tek paper by Eckhoff (1974) describes another most important aspect of dust pollution, viz. the potential hazard of dust explosibility in many industrial plants or mines. The characterization of dust properties is mandatory and considerable work is going on to tackle these problems.

Also in the next paper, that by Bjørseth (1974) the problem of dust characterization is emphasized. A Lundgren impactor has been experimentally tested particularly in an aluminum melting plant to measure exhaust gases. The particle sizes vary mainly between about 0.4 μm and 10μm. As both Bjørseth and the next contributor Kolderup (1974) remark it is essential to perform continuous dust measurements. The latter author has reported test experiences with another type of dustmeter, viz. a radiometric β-meter. Also this device has been tried out in an aluminum plant.

Some of the standard techniques which are used for gas monitoring include infrared absorption (carbon monoxide, carbon dioxide, sulphur dioxide, hydrocarbons), flame ionization (hydrocarbons), flame photometry (sulphur dioxide), colorimetry (carbon monoxide, sulphur dioxide, nitrogen oxides, lead, hydrogen sulphide, fluroides, ammonia), coulometry (sulphur dioxide), conductometry (sulphur dioxide, hydrogen sulphide), as well as gas chromatography and radioisotopes.

All these measurement principles are used in continuous instruments, and are commercially available. The principles can also be used in non-continuous sampling if desired.

In the last few years the development of air pollution analyzers has grown rapidly. Hochheiser et al (1971) have surveyed the parameters continuously monitored in the air and the availability of on-line instruments. Already in 1971 they found 25 companies offering sulphur dioxide analyzers based on five different methods.

The application of computerized multichromatographic systems has become quite common, especially in the petroleum industry. An estimate of more than 20 such systems in North America is reported in the literature (source: Chem Engr vol 79, No 20 September 1972).

The National Air Control Administration in USA has a continuing program for the development of instruments for pollution. Some of this development is described by Maley (1972) and some developments can be mentioned. A flame luminescent method to measure sulphur is being developed.

Sulphur dioxide can also be measured simultaneously with carbon monoxide and nitrogen dioxide in a triple system. The sensors in this system are based upon the fuel cell principle and they time-share the circuitry.

Chromatographs for new applications are being developed, such as an automated chromatograph for the simultaneous determination of carbon monoxide, methane and total hydrocarbons. Another one is aimed for hydrogen sulphide and certain organic sulphides.

The principles of chemiluminescence is used in a couple of instruments, one for determining ozone and the other for measuring oxides of nitrogen. Ozone is titrated in the gas phase with a reactive gas and the reaction produces light by chemiluminescense.

The continuous measurements of particulates in the atmosphere can be made by a couple of different principles. In one development there is a special adaptation of lidar (light detection and ranging). In the other one a piezoelectric instrument is used.

Specific ion-selective electrodes are also under constant improvement, both for air and for water applications.

Researchers at EPA in USA are experimenting with solid sorbants instead of cumbersome wet impingers for collecting materials, such as fluorides, chlorides, carbon monoxides and sulfates.

3.4 Wastewater Monitoring.

Wastewater coming from domestic or industrial sewers can be characterized by a large number of parameters or quality variables. Such parameters are biochemical oxygen demand, chemical oxygen demand, total oxygen demand, content of phosphates, nitrogen, heavy metals, suspended solids, turbidity, dissolved oxygen, organic carbon, trace organics, pesticides, viruses and pH etc.

Flow measurements are of basic importance in most chemical processes and wastewater treatment plants. A large number of techniques are in use, and depending on the type of fluid, viscosity, flow velocity, flow rate, harmful environment etc. different methods are suitable. In the Kem-Tek paper by Thorsen (1974) a survey is given on flow measurement methods.

Measurement of wastewater characteristics is needed for several purposes. Quality control in rivers and lakes is desirable to check the standard of cleaning. Measurement for control of wastewater treatment plants is a necessary condition for an adequate treatment.

There are two principal types of instruments for aquiring process information,

- o in-stream probes or sensors
- o automated analytical procedures (or automated wet chemistry)

Several commercial probes and instruments work satisfactorily in laboratory type analysis, but are usually not suitable for long term unattended use.

Instruments e.g. for dissolved oxygen, suspended solids (turbidity meters) and pH need careful maintenance in order to work adequately, as slime often accumulates on the probes. Methods therefore have been developed to clean the sensor element. Water jets have been, and are being used and ultrasonic cleaning is being carefully examined.

There is a tendency to avoid the wet chemical analytical techniques and much efforts are paid instead on the development of electrode type sensors; ion selecting type probes.

Ghosh (1973) reviews the literature on water characteristics measurements during the period 1972/73 and has listed 72 references. Some interesting developments from a wastewater plant control point of view may be mentioned. A new method for the determination of suspended solids concentration is described by Liskowitz (1971, 1972). The method is based on the depolarization of scattered light and should be used for the continuous determination of the concentration of particles in suspensions. According to Liskowitz the range is from less than 100 mg/l up to about 5000 mg/l. The measurements were unaffected by size distribution of particles, density variations, sources of samples, or color variations.

Summs (1972) and Talley et al (1972) have reviewed the state-of-the-art of turbidity measurements for process monitoring and control purposes in industry.

Reviews of the basic chemistry of the analyses of water in quality control are made by Taylor (1971), Meredith (1972) and by Lumb (1972). A survey of instrumentation for control in wastewater treatment plants is given in Olsson et al (1973)

A promising sludge density meter, based on cross correlation techniques has been developed, see Wormald et al (1973). The method is based on the measurement of conductivity fluctuations within a turbulent flowing stream. The meter is claimed to be useful in the range 1 - 8 % solids concentration.

A survey of ion-selective electrodes for process control is found in a paper by Cornish (1973). On line process analyzers are also surveyed in two papers by Kehoe (1969, 1972) and by Lipták (1973).

Ultrasonic has been introduced as a competitive technology for control applications in process industry. In its simplest form it is used for level control of liquids and solids. In the field of liquid flow metering the ultrasonic flow meter is utilizing the Doppler principle, so that the measurements depend on the value of the velocity of the sound in the fluid.

3.5 Automation of analyzing instruments.

Many instruments in chemical industry are used for the determination of quite complex variables, such as composition in streams or tanks. Previously most process analysis from chromatographs, spectrometers and autotitrators was only possible to perform off-line in the laboratory. With the introduction of cheap computation facilities it is getting possible to introduce those instruments for on-line purposes in feedback control systems. Process analyzers can very well be automated, and fast processing of the instrument data makes it possible to use the signal for control purposes.

The table below gives a flavour of the tremendous forecasting of the use of analytical instruments only on the American market. (source: Control Engineering, July 1973). Of the total sales 47 % are for scientific research, 24 % for medical R & D, 29 % for all industries which includes 11 % for the chemical process industry. For comparison the total investment in the chemical process industry in 1970 was estimated to be $ 12 - 15 billion (=10^9).

TABLE: Analytical instruments market forecast

	Millions of dollars		
Product Group	1970	1973	1978
Computers for analysis	85	130	260
Spectrophotometers (UV, IR, Visible)	75	90	115
All types of chromatographs (20 % in chemical process industry)	60	75	100
Spectrophotometer, atomic absorption type	16	33	68
Total analyzer sales	400	550	880

There are, however, some essential difficulties in using these instruments for control, i.e.

- the process analysis instrument is not continuous in general, i.e. each analysis might require several minutes just to collect data before the result can be interpreted.
- the time delay due to the analysis can cause stability problems as well as practical programming problems.

In his Kem-Tek contribution Kirkov (1974) describes a device which in many senses satisfies the needs of a multipurpose analytical instrument in chemical industry. The component, a tin oxide semiconductor electrode is used as a selective electrode for several different reactions. It is claimed to be useful in instruments for measuring optical, photochemical and suspension characteristics etc.

In some cases, e.g. for mass spectrometers, the time constants may be made quite small. They may well be in the order of seconds or less, depending on the desired accuracy, see e.g. Damoth et al (1972).

Because of cost and reliability problems, process analysers are seldom used alone in feedback loops. Instead continuously measured variables such as temperature, pressure, flow etc. are used indirectly to control the plant and the analyzers are used to observe the trend of a plant variable. One example, of this philosophy is described by Shah et al (1969), who describe the control of an ammonia plant.

The possibilities for reconstruction of state variables should be carefully examined in several cases, both dynamically and statically. One example from distillation control demonstrates the idea. There it is common to reconstruct compositions from temperature and pressure measurements. Those possibilities are by no means exhausted in situations where measurements are needed and no sensors are available.

By increasing information processing capabilities connected to the instruments the sensors can be checked out as well. Outliers or instrumentation errors can be tested, and the calibration can be adjusted periodically.

4. METHODS FOR PROCESS MODELING AND CONTROL SYSTEM DESIGN

In this chapter a short review will be given on different methods which are relevant for chemical process control. The modeling problem is first treated. After that different synthesis methods are commented on. Especially in multivariable systems there is a large number of approaches available, and different methods applied to chemical process control are considered. For a basic description of multivariable systems, we refer to e.g. Schultz(1967),Rosenbrock (1970).

4.1 Modeling and parameter estimation.

Process modeling is a central task both for system design and control design. In a large complex system like a chemical plant modeling becomes a major task, and one of the main questions is how to simplify the model in an adequate fashion.

Needless to say the purpose of the model should be the primary question. If the goal is to understand the dynamical behaviour, the model should be quite detailed. On the other hand, if the model should be used for control system design, it is most often sufficient to use quite less complex models. It is, however, important to model not only the input - output relationships but also the character of the disturbances in order to handle them adequately.

Due to the complexity of chemical processes modeling has to be complemented with parameter adjustments to measurements. The areas of identification and parameter estimation have proven to be quite successful tools in finding models for control purposes. A lot of applications of identification techniques in the chemical field have been reported.

The problem of identification is to estimate a number of unknown parameters in a model of known structure. The available information is a number of sequences of measured values of the different input and output variables of the process under consideration.

The model structure can be of many different forms. The simplest form is a so-called black-box approach. Then a canonical structure or transfer function is assumed with unknown coefficients. These coefficients then do not have any special physical interpretation. Linear, stochastic systems with many inputs and one output can be treated completely by standard methods today. In the multi-output case one has to be more careful because of the interaction problem.

The structure can also be much more fixed both in the single variable and in the multivariable cases. The model can be given in terms of a number of first-order - linear or nonlinear - differential equations with unknown parameters. Depending on the noise assumptions and the linearity of the system different methods are available for identification.

Methods like the least squares, the generalized least squares, the instrumental variable and the maximum likelihood method can be used. Which method to apply depends on the complexity of the dynamics and noise, on available computer facilities and on the desire for accuracy.

There are several good surveys of the field, and Åström et al (1971) give a comprehensive presentation of available methods. In another survey Gustavsson (1973) has summarized identification applications in chemical and physical processes. These surveys contain a large number of references which are not listed in this paper. Identification methods are also presented in Nieman et.al. (1971).

Some papers have presented comparisons of identification methods on industrial data, and those by Gustavsson (1972) and Clarke (1973) should be mentioned.

4.2 Control of single variables.

There is certainly no single method that can solve all different types of control problems arising in a chemical plant. Neither is it possible to give a comprehensive list of all possible approaches in a survey like this. A flavor of the available possibilities, however, will be given and references to other works will be made.

The majority of process control systems of today still contain mostly local control loops and sometimes nested loops or cascaded systems. Linear design technique from the servo - mechanism theory is still in use for analysis and synthesis. The classical PID controller is certainly satisfactory in many cases, and there is no need to try more sophisticated control methods. The gain in using more advanced theory would perhaps be too little.

Single loops methods are, however, inadequate in systems with significant interactions. There has been presented several approaches to handle such systems. Methods for multivariable control have to be applied. An excellent survey of such methods is given by MacFarlane (1972). Here we will comment on some of the theories relevant for chemical process control. In 4.3 the so-called non-interacting control is briefly mentioned. Reduction of model complexity can be achieved by e.g. modal control, which is considered in 4.4. Multivariable control is more generally regarded in 4.5. Reconstruction is mentioned as a tool in 4.6, and the chapter is finished with some remarks on adaptive control.

4.3 Non-interacting control.

Non-interacting control has been tried as the solution for typically coupled systems. An often cited example is the control of both top and bottom compositions in a distillation column. In this method a control is sought, such that a change in set point of one variable influences only one output.

To achieve this goal, a network can be introduced between the controllers and the plant, creating a decoupling of the interactions. Single loop theory is then used to design the controllers. A control system with non-interacting properties may, however, be most undesirable for chemical processes. The reason is, that such servo performance should not be imposed,when it is the diminution of the disturbances that is important. A non-interacting control system may also create other difficulties. Many chemical engineers claim that interaction instead should be used in order to achieve a better control. The decoupling in a non-interacting system restricts the compensations that can be applied. There is also a non-minimum phase problem ("wrong-way") involved, as pointed out by Rosenbrock (1966) and MacFarlane (1972). If the determinant of the transfer function matrix has right-half plane zeros, as in many multivariable chemical processes, the technique yields a poor performance. Non-interaction control therefore should be used with great care, and in many cases there are competing methods.

4.4 Model reduction.

The size of the number of states in models is often prohibitive. In order to reduce the complexity of chemical process models several techniques have been used. The modal control theory was introduced by Rosenbrock (1962 b).

The central theme in all work on modal control is that the transient behaviour of a process is predominantly determined by the modes associated with the slowest eigenvalues of the state matrix (i.e. the slowest poles). If it is possible to approximate a high-order system by a low-order system whose slow modes are the same as those of the original system, then one can concentrate upon altering the slow eigenvalues in order to control out a disturbance. It is very important to note, that different disturbances can excite different modes of the system. In Rosenbrock's approach it is possible to alter each eigenvalue separately so that the resulting control system can be considered a non-interacting control scheme.

There are serious drawbacks of the modal techniques, however. Modal control theory exploits the interactions among the variables, but those ideal conditions do not occur always in chemical processes. All the states cannot be measured in practice and control cannot be applied to all states.

Nevertheless modal control has been applied in chemical process control by Gould (1969), to a diffusive distributed process, by Davisson (1967), (1972) to the control of a distillation column and a 41-variable chemical plant model. Some of the disadvantages of the modal control theory are also discussed by MacFarlane (1970, 1972). The method gives attention only to the poles, while the closed loop zeros are left unattended.

Bengtsson (1973) has developed quite a different approach to the problem of approximative controllers. The control system is first synthesized to an "optimal" controller which is made suboptimal by imposing constraints in the control structure. To start with state feedback control is used. Then this control is fit in a rational way into another "similar" control with a predefined structure. The method has been successfully applied to a three machine power system. The method is well designed for the high-dimensional problems that often occur in chemical plants.

4.5 Multivariable control theory.

In classical design technique there is a large amount of different criteria that can be used for synthesis. In optimal control theory there has been a systematic approach to define one single scalar function, that reflects the performance of the closed loop system. This performance index is a function of all states and control variables of the system and in the general case it can be formulated quite arbitrarily. The optimal control theory then states systematic ways to synthesize controllers, both for linear and nonlinear multivariable systems.

The word "optimal" has been misunderstood by many. A controller is not optimal in any other sense, than it has minimized the performance index. In a real plant, probably a large number of criteria must be tried out before the most adequate criterion can be found, that can give a satisfactory behaviour of the system also in other respects, not formulated in the criterion.

For nonlinear systems open loop solutions can be achieved, for example to get input histories that minimize the time required to bring the process to a new operating point. In case of linear dynamics, where the control criterion can be expressed as a scalar function, quadratic in the state and control variables, the control system can always be formulated as a feedback (closed loop) system. Application of linear quadratic theory for feedback and feedforward control of chemical processes have been reported extensively.

There is a great amount of literature on the subject, such as the standard texts by Bryson et al (1969) and Anderson et al (1971). Optimal control theory has been applied to a number of chemical processes, e.g. stirred tank and tubular reactors, distillation columns, extraction columns, absorption columns as well as to the "standard chemical process", the second-order-plus-delay-system.

4.6 Reconstruction of state variables.

In too many application studies it is assumed that all state variables of a plant are measureable only because the linear quadratic theory assumes such a fact. It is not only unrealistic to assume all states known - in many cases it is also unnecessary. There are good methods to find the states by different sorts of reconstruction, if the states are not measured directly.

The most famous method for reconstruction of state variables in linear stochastic systems is the so called Kalman filter, which has been developed both for continuous and for time-discrete systems. A comprehensive treatment is found in e.g. Åström (1970).

Measurement and process noise can be taken into account in a direct way, but the filter has to assume that the process model as well as noise statistics are known, which might be prohibitive. There are, however, identification methods available, see Åström et al (1973) in which a steady-state Kalman filter can be identified directly out of measurements of a process.

The reconstructed state variable can now be used in a multivariable linear-quadratic controller. The statistical problem of getting the reconstructed variable and the deterministic problem of calculating a control law can be separated into two different tasks. This is the content of the so called separation principle, see Åström (1970).

4.7 Adaptive control.

In many chemical processes some parameters may vary slowly as a function of time, such as a catalyst activity. These parameters can vary in such a way that the overall dynamics gets adversely affected, if the controller is not properly adjusted.

Adaptive controllers are most desirable in such control systems. Such a controller can adjust its parameters on-line and consequently maintain a good performance in spite of uncontrolled and unmeasurable process parameter changes.

A successful approach to solve this problem - a self-tuning regulator - has been presented by Åström et al (1972) and Wittenmark (1973). The regulator consists of two parts, one identifier and one controller. It is useful not only when parameters are slowly varying but also for tuning of regulators, which might be a time-consuming and difficult task. The self-tuning regulator has been applied to two different full-scale processes, an ore crusher (see Borisson et al (1973)) and a paper machine (see Borisson et al (1974)). The same type of controller has also been implemented on another paper machine for moisture and basis weight control, see Cegrell et al (1973).

In a feasibility study van Aarle (1973) has examined, if adaptive controllers are desirable in distillation control. In the special case studied some process parameters varied by a factor of 2-3. For the process studied, however, van Aarle hesitates, if adaptive control is attractive.

There are also multivariable counterparts to the self-tuning regulators as described by Peterka-Åström (1973).

5. THE ROLE OF COMPUTERS IN CHEMICAL PROCESS CONTROL

Digital computers and associated information processing capacities for monitoring and control are among the most significant technological advances in the past decades. A few aspects of this development will be considered.

5.1 Review of the present status.

It is more than 14 years ago, almost half a generation since the first application of computer control was announced in Port Arthur, Texas in 1959. Now the great pioneering period is over, and computer control is a standard routine.

The annual increase of process computers between 1959 and 1966 was about 50 % and after that about 20 %. Minicomputers constitute the greatest part of the increase. The computing capacity/computer price ratio has increased dramatically in the last ten years.

Hardware reliability has increased so that DDC is considered quite realistic in most applications. Software development has also made a lot of standard solutions possible, so that few installations today are tailor-made. Rather standard process oriented program packages are offered. Depending on the application they may be of either a fill-in-the-blank type or some extension of Fortran type languages. A status report on DDC applications can be found in Bailey (1972).

The traditional differences between medium size and mini computers are getting more and more obscured. In the following paragraphs we define a midi computer as having 16 to 24 bit word length, or alternatively with a price more than $ 10 000 (such as IBM 1800, CDC 1700, GE 4000). A mini computer then may have a word length less than or equal 16 bit.

In Ferrar (1971) a summary of new computer installations in petrochemical industry is made for the period 1967-1971. It is shown that the use of medium size computers in new projects has been quite constant in this period, see fig. 1. Except for 1970 the number of new projects was between 66 and 82 for the USA and 95 and 150 for the whole world. For 1970 the figures were 105 and 190 respectively. The minicomputers constitute the largest increase with 12 new projects in 1967 and 56 in 1971 in USA. The number of new major DDC projects does not, however, increase significantly any longer; only 4 in 1967 and 6 in 1971 in the USA.

In the tables below the type of applications of computers in the petrochemical industry in shown (valid at the end of 1971). The percent figures are based upon the number of projects and not on the number of computers. The classification indicates the primary function of the computer; then there is often some additional information processing task. The computers in "process control" almost always are used for local control of some process variables.

TABLE 1: Midicomputers in petrochemical industry

Process control: supervisory and operator information	60 %
Process control: DDC	7 %
Information systems	12 %
Oil movements: loading terminals, tankage, planning	11 %
Analyzers and laboratory control	5 %
Others	5 %

TABLE 2: Minicomputers in petrochemical industry

Process control	52 %
Process control: DDC	4 %
Information systems	4 %
Oil movements	4 %
Analyzers and laboratory control	30 %
Others	6 %

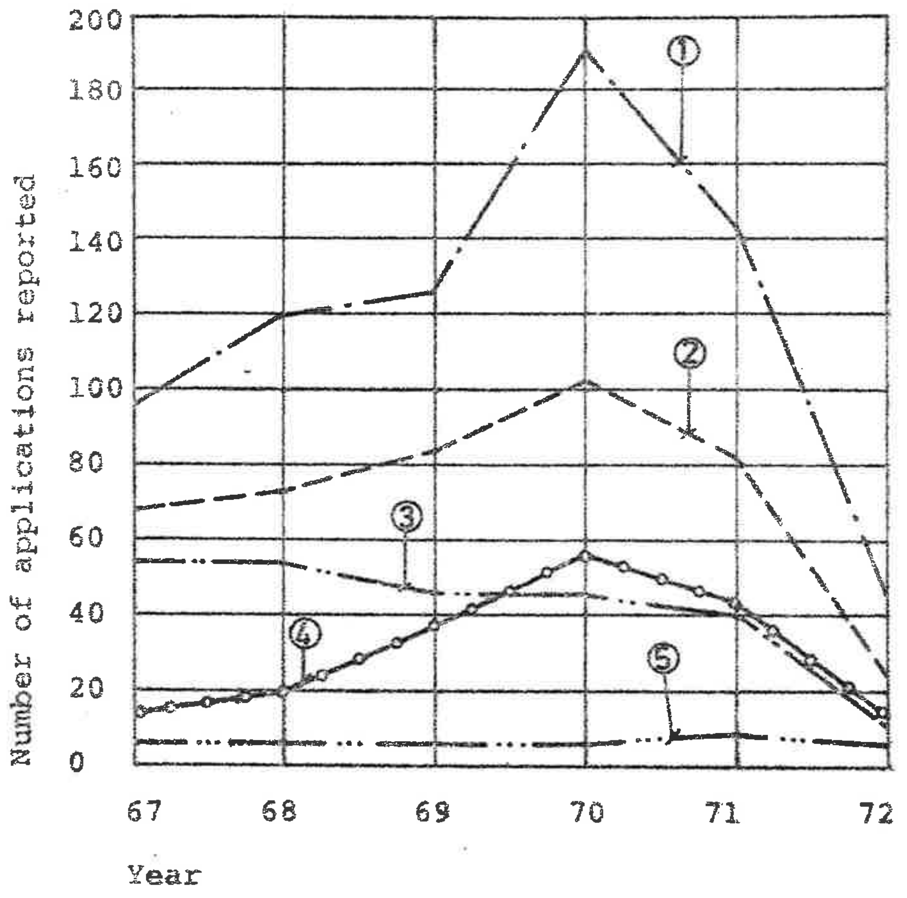

Figure 1 - Computer applications in petroleum and petrochemical plants.

1 Worldwide total applications.
2 U.S. total applications.
3 U.S. medium size computer applications.
4 U.S. mini computer applications.
5 U.S. major DDC projects.

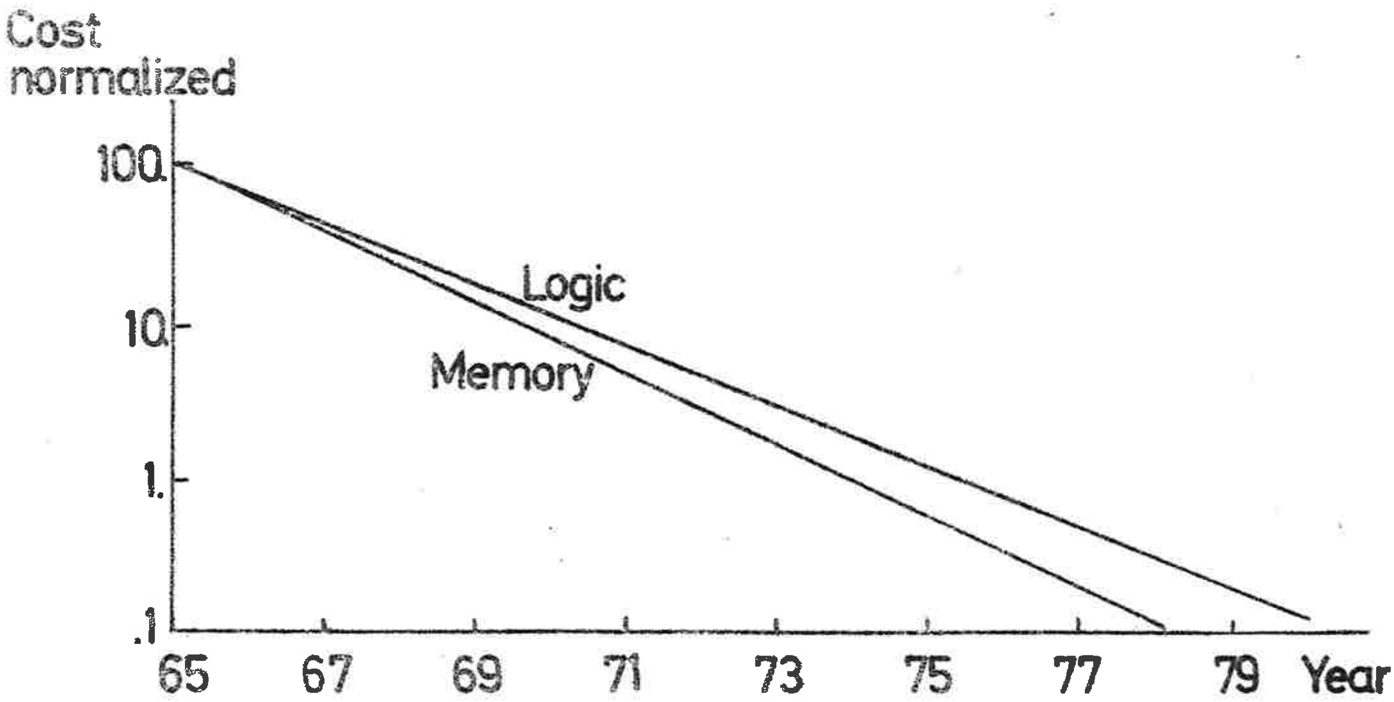

Figure 2 - Expected cost development of LSI circuits.

5.2 Some trends in computer control.

With the introduction of the microcomputer or the "computer on a chip" it has been possible to think in terms of completely new concepts in computer control. The increasing number of functions that are being built in a single LSI (large scale integration) circuit is phenomenal. Just look at a desk calculator or a digital watch. The prices per function is therefore getting down constantly, see fig. 2.

Digital/analog and analog/digital converters are also getting cheaper, thus making it more favourable to use remote multiplexing and data highway systems. Today there is much talk about dedicated computers with fixed programs in read-only memories (ROM) for standard tasks in instruments, simple process loops, transmission units or displays.

The idea of decentralized systems is getting applied. The trend toward local on-line control instead of just one central computer is noticeable today. This control with its digital flavour has a lot of interesting features. It gives a flexibility and modularity which is not possible with a centralized system. It is not necessary to make excessive investments from the beginning.

There are several reasons to decentralize. Cable costs are excessive, and the programming costs for a central computer should by no means be neglected. Cable costs can be drastically reduced by remote station multiplexing. This may be interesting already for more than about 50 loops and average distances from the CPU to the plant of more than 60 - 70 m.

Advanced instruments can be supported by their own little computer, and certain process units can be controlled by a minicomputer. Not all, but part of, the information is interesting to transfer to a central computer. With this type of arrangement the plant reliability can be increased.

To sum up,the interesting features of this trend may be:

- increased reliability
- both serial and parallel digital data transmissions
- compatibility and communication with higher level computers
- ability to handle advanced control algorithms
- capability of handling a large variety of measurements and control signals
- favourable economy
- flexibility
- no drift problems
- modularity

Software standard for microcomputers is still an unsolved problem. No highlevel languages (maybe not even assemblers) are available, why programming may be time-consuming. There is, however, a trend toward macro level languages, where typical process oriented features should be easily programmable. It should also be possible to compile programs for a microcomputer in a bigger machine, thus making high level languages available.

The compatibility between the small and the big computers is therefore important, if a decentralized computer system should be successfully connected by a central computer.

6. APPLICATIONS TO MASS TRANSFER PROCESSES.

Mass transfer processes make up an essential part of many chemical process plants. There are several processes where mass transfer in some form is used, such as absorption, distillation, extraction, adsorption, humidification and membrane operations.

As distillation is so important as an object for process control, we will concentrate the text on distillation columns. Some other applications are also mentioned, such as gas absorbers and evaporators.

6.1 Distillation columns.

Distillation columns serve numerous purposes. Let us just mention the fractionation of such a complex mixture as crude oil, (superfractionating operation) or the complete elimination of an impurity in a product. In a modern refinery plant, distillation columns make up about 50 - 55 % of the capital investment. There is a vast literature on the dynamics of distillation columns, but still new contributions should be expected in the control field, especially the application of multivariable control and dynamical optimization.

Conventional approaches to distillation control are well described in standard books such as Buckley (1964) and Harriot (1964). A good description of the dynamics of distillation processes for control purposes is also found in Gould (1969). Several other surveys on distillation columns operations can be found, and only some highlights will be mentioned here. Bolles et al (1968, 1969, 1970) cover in an annual review the literature published on distillation columns for the preceeding year ending up with June 1970. In each review there is a section on system dynamics and column control, where several adequate references are cited.

A case study has been reported by Foulard et al (1973), where emphasis is put on parameter estimation and identification of columns. A survey on applications of identification methods to chemical processes is also made in the previously cited paper by Gustavsson (1973)

The modeling problem is intimately connected to the purpose of the model. In a paper van der Grinten et al (1969) review several methods for the construction of mathematical models for distillation columns. Both the modeling of each tray on one hand and the black box approach on the other hand are considered with their respective advantages and drawbacks from a control point of view. The problem to choose the adequate model complexity for control purpose is also emphasized by Gustavsson (1973).

6.2 Distillation column dynamics.

A typical distillation column is shown schematically in fig. 3.

If all the detailed dynamical behaviour of a column should be represented in à mathematical model, this one would certainly be very complex. It includes overall and component mass balances, energy balances, hydraulic flows and vapor dynamics. The most important part of the dynamics is the concentration dynamics of the different components in both liquid and vapor phases as well as overall balances. Those equations are mostly linear, and the dynamics for each tray is coupled to its neighbouring trays. There are also nonlinear relations, such as the equilibrium curve and the liquid flow as a function of the hold-up on a tray. Also the pressure drop for vapor through the liquid is a nonlinear function of the vapor flow.

If the number of trays is getting large, the number of coupled ordinary differential equations describing the balances may be approximated by partial differential equations. This approach is made in many theoretical investigations in order to get more generalized tools for analysis and synthesis. This situation is equivalent to the continuous operation of a packed column, which alternatively can be considered consisting of a large number of fictitious trays.

A distillation column can be manipulated by a number of different variables. The most important ones belong to the flow rates of feeds and products, reflux ratio, heating and cooling capacities. The main disturbances may be influenced by other processes and are related to the feed flow rate, composition and enthalpy.

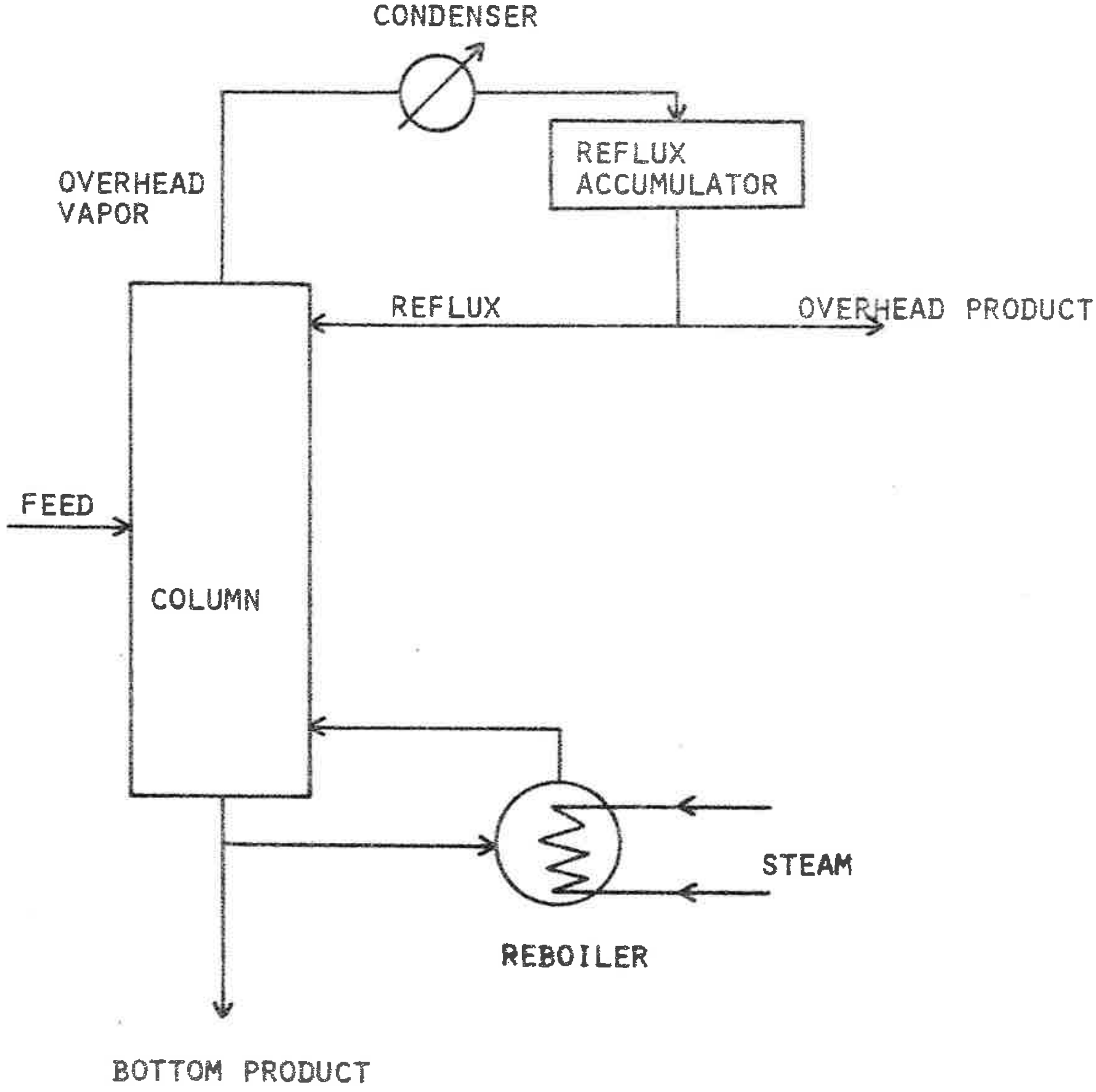

Figure 3 - Typical distillation column.

The most important outputs are

- o the pressure at the column top
- o differential pressure between some plates
- o levels in the reflux and bottom tanks
- o temperature on certain trays
- o concentration of the different drawing-offs

Then there are other state variables describing the internal behaviour in the column, such as

- o pressure
- o internal flow rates of both phases
- o tray concentrations, temperature and enthalpies
- o liquid-vapor equilibrium relationships
- o various tray efficiency coefficients

The measurements which are generally the most required ones are flow rates, temperatures, pressures and concentrations. The three first entities are generally quite reasonable and easy to measure, while concentration is often the weak point. The accuracy might be increased by using a chromatograph or a mass-spectrograph, but the costs are in many cases prohibitive. See further chapter 3.5.

For control purposes there is always a difficult compromize to choose the right system complexity. It is certainly too complex to take the dynamics of each single tray into consideration for control purposes. On the other hand, significant interactions and nonlinearities may cause a conventional control system to be too rough an approach to the control.

It is typical for a distillation column, that a major problem in designing a control system is to choose a suitable structure, rather than to determine the actual values of the control parameters. This means that it is not at all clear à priori which variables to manipulate and which outputs to measure. This is both a matter of operational convenience, equipment costs, safety, dynamical behaviour and plant yield and economy.

There is a large amount of different structures suggested in the literature for different columns. It is interesting to compare the different control philosophies taken by e.g. Buckley (1964), Harriot (1964) chapter 14, and Rosenbrock (1962a) Other approaches are also shown e.g. in Gould (1969), Sieler (1970) and Anderson et al (1969).

Few systematic efforts are made to compare and evaluate different structures. It is quite clear that experience must guide the designer to a large extent in order to limit the number of possible combinations. There are, however, so many different processes with their specific construction, that experiences from one column plant might be of little value for another one. It should be a great challenge for the theoreticians to find more general methods for a systematic control structure approach.

6.3 Feed-forward control.

As mentioned, the most important disturbances have to do with the feed to the column. Those disturbances are in general measurable. This makes it possible to take advantage of feed-forward techniques to control the column. In general the disturbances in the feed variables are quite small in amplitude or might be slow gradual changes. Because of this, the transient behaviour of the column is seldom of a major interest. Rather the feedforward control is made quasi-stationary, as will be shown in a couple of references.

Buckley (1964) has given quite a systematic approach to the idea of using feed-forward control in distillation columns. The inlet disturbances were fed directly to the reflux ratio and heat capacity controls, thus creating a high speed loop. The model for this feed-forward control has seldom to be accurate, partly because of the size of the disturbances and partly because feedback control from the product variables should always be used as a complement to the feed-forward control. This is also discussed by Shinskey (1967) p. 307 and Wardle et al (1969).

Several applications of feedforward control have recently been published. Miller et al (1969) discuss feedforward control and provide a survey of 42 references on the subject. They note that only 5 of the references describe applications in commercial equipment. There is also remarked by Nisenfeld et al (1973) a tremendous gap between the number of applications and the number of publications of them. Only in the USA and Canada more than 150 full scale columns are operating under feedforward control. Only four of these have been described in the literature before 1969.

Three different applications have been reported by Nisenfeld et al (1973). The case histories are documented "before" and "after" the feedforward installations. The authors discuss how to gain an adequate complexity of the model necessary for the feedforward control. The models are primarily steady state models. Of course, such models give transient errors which are not desirable. Now, it has been possible to gain satisfactory dynamic behaviour just by adding first order dynamic systems to the steady state models. Typically the measurable disturbances, the feed flow and column temperature, are used to feed signals to the distillate flow and to the pressure set points. This was made for a debutanizer in a Fluid Catalytic Cracker unit and for a gasoline depropanizer.

For a superfractionator (crude oil distillation) the first step was to provide a fast corrective action for upsets in energy balances, which can be reconstructed (by static relations) from differential pressure and reflux accumulator level. The flow rate of only one of the side streams, viz. the propylene product was manipulated by the feedforward system.

Another paper by Wood et al (1972) deals with comparisons between feedforward, feedback and combinations of these for a binary column having a diameter of 0.23 m and containing 8 trays. Typically first order models with time delays were used. The models were achieved by pulse testing.

6.4 Regulation and steady state optimization.

Two levels of control are often discussed in distillation control papers. The first level may be conventional set-point control, where a number of local variables should be kept within certain limits. On the second level the operating point of the columns should be at an optimum. Under assumptions of steady state behaviour, a profit function is formulated, and this function should be maximized during the operation.

Sawaragi et al (1971) have considered a quasi-dynamic operation of a pilot distillation plant. The plant is to be operated at a maximum profit rate under the condition that the overhead product composition is maintained constant. A binary mixture of methanol and water is processed in a sieve tray distillation column. The control variables are the feed flow rate and the heating duty in the reboiler. The profit is a nonlinear scalar function of the two control variables and of five state variables (flow rates and compositions), under the condition of steady-state operation.

Maarleveld and Rijnsdorp (1969) studied a constrained static optimization problem, where the purity of both streams should be considered. Thus both the feed preheating and the column pressure should have optimum values in a refinery column - a deisopentanizer. No quantitative models were given in the paper. Similar approaches, a combination of feedforward control, feedback control and steady state optimizing control have also been applied by Bornard et al (1969) on a superfractionating column. Duyfjes et al.(1973) discuss the similar problems for a general binary column or a pseudo binary state column. The transients are not taken into consideration at optimizing control. Also these authors claim that little is gained by dynamic optimal control.

Shunta et al (1972) have developed a control scheme that compensates for both set point changes and load disturbances. Two separate algorithms are implemented simultaneously. One is receiving its input signal from the setpoint and the other from the measurement variable. This control is shown to be better than conventional PI controller.

6.5 Multivariable control of distillation columns.

The control of distillation columns should in many cases be multivariable because of the significant interactions present. One example is the so called two point control problem, i.e. both exit compositions are to be maintained within prescribed limits simultaneously. Rosenbrock (1962a) was one of the first ones to point out the interaction problem in distillation columns.

One approach to solve the two point control problem is by decoupling. Different approximations of the decoupling scheme have been suggested. Rijnsdorp et al (1966) have described a non-interacting control scheme for the simultaneous control of both end compositions. This study has been taken up by Wood et al (1973) in an experimental evaluation of the same non-interacting control scheme.

The two point control problem has also been taken up by Toijala (Waller) (1972, 1974). A truly multivariable control law, such as linear quadratic control has been suggested and applied to the control of columns, e.g. by Brosilow et al (1968), King (1969), Hu et al (1972) and Toijala (Waller) (1972).

The linear quadratic control law (see section 4.5) is however unsuitable without some important modifications. Still feed-forward control should be taken into consideration as counteraction of the disturbances should be made as fast as possible. The output regulation problem is considered also by Bengtsson (1973, ch. 6). He shows that the multivariable feedback and feed-forward problems for linear systems can be treated with similar computations.

The linear quadratic control strategy should also be complemented with some "integral action" corresponding to a classical PI controller. Thereby the outputs can be returned to the desired levels after slow or steady state disturbances. There are several approaches to this problem. A survey is given in Bengtsson (1973), where also new methods are presented. Waller (Toijala) (1974) have used another approach, which also means a sort of integration of the output. Waller et al (1974) have also adopted the idea of modal control, discussed in chapter 4, in order to reduce the complexity of the controller. This control is tried out on a binary distillation column model and is found to be better than the decoupling control, previously used.

The same modal analysis approach has also been used by Davisson et al (1972), for a complete chemical plant, described by 41 differential equations. The processes consist of tank reactor, a heat exchanger, a decanter and a distillation column.

6.6 Other control algorithms.

The distillation column contribution by Roffel (1974), describes models for heavily loaded trays. These models are then verified by experiments on a sieve tray column with the components air and water. For the high loading that the author considers, flooding of a tray is a real threat to the operation of the plant, hence it is important to better know the conditions for flooding to occur and how to avoid it by control methods. A slight modification of a PI controller was found to be successful. The proportional part of it has the structure

$$K\, e \cdot |e|$$

Another type of control algorithm has been proposed by Merluzzi et al (1972). It is a type of on-off control strategy, which has been applied to a full distillation column separating a binary mixture. The controller uses a linear combination of temperature measurements to adjust the reflux ratio in order to maintain a desired overhead product composition. By using some simple relationships between the control coefficients the authors have reduced the tuning of the controller to the adjustment of one single parameter, corresponding to a very simple model of the column.

6.7 Reconstruction of process variables.

A linear control law must generally know the whole state vector (See chapter 4). This is seldom the case, and therefore it has to be reconstructed e.g. by a Kalman filter. Hamilton et al (1973) describe how they have applied a time-discrete Kalman filter to estimate the state of a pilot plant evaporator. The filter was a part of a multivariable computer control system. Although the noise and process noise levels were at about 10 %, the filter caused good control. The results were significantly better than those achieved with conventional exponential filters. In this application the standard Kalman filter was reasonably insensitive to incorrect estimates of initial conditions and also for noise characteristics as well as for model parameters.

6.8 Other mass transfer processes.

An experimental and theoretical investigation of the unsteady-state operation of a pilot scale packed gas absorption column has been made by Bradley et al (1972). Carbon dioxide was removed from an air - carbon dioxide mixture into an aqueous monoethanolamine (MEA) solution by absorption accompanied by chemical reaction. The mathematical model describes the mass transfer in a packed bed counter current absorber and the conservation equation for the gas and liquid phases are partial differential equations. In order to verify the model, a step change in gas feed composition was effected by manually changing the setpoint of the CO_2/air flow ratio controller. For changes in the MEA flow rate the setpoint of the feed flow controller was stepped.

A similar application with step responses analysis is also presented by Malpani et al (1973). The partial differential equations, describing the absorber, were reduced to ordinary differential equations by the method of characteristics. Afterwards the two unknown parameters in the system were determined by step response analysis.

An example of optimal control of a pilot plant evaporator is shown by Newell et al (1971). In order to make up for deterministic disturbances, the authors have extended the state equations by the integral of the output thus getting an "integral control action" (cf 6.5 and 4). By taking the interactions of the system into consideration, Newell shows that a considerable improvement is achieved. There is, however, no comparison made between the optimal control technique and other multivariable synthesis methods.

The question on the integral action should be commented on. Newell et al have used the classical approach to integrate the whole output vector. This is the only solution if the disturbance sources are unknown. Bengtsson (1973) has derived another approach where he shows that the number of integrators can be decreased, especially if there are fewer disturbance sources than controlled variables. As the author remarks, this is not merely an academic question, since each introduced integrator will cause a phase redardation. The system is then harder to stabilize or it might even be unstabilizable.

7. APPLICATIONS TO CHEMICAL REACTORS

A chemical reactor is usually the very heart of a chemical process plant and embodies a major source of its economic gain. Therefore questions on optimization play a central role in the design, operation and control of a reactor. This is sometimes in contrast with some physical processes, where optimization is important in design and steady-state operation but is of less significance in dynamic control.

7.1 Classification of reactors.

Chemical reactors may appear in many different forms, depending on type of reactions, arrangement of flows, presence of a catalyst or not, thermal conditions and number of physical phases involved. Some major types according to the flow pattern are the batch, the stirred-tank and the tubular type reactors. Many industrial reactors may have a design between the extremes of a stirred tank and a plug flow reactor. It is also differed between adiabatic and isothermic reactors. Of course, the thermal conditions are also affected if the reactions are endothermic or exothermic.

It is much easier to describe a homogeneous reactor, where the reactions take place in one single phase than a heterogeneous reaction, where several phases are present. There the problem of mass and heat transfer between the phases is added on top of the reaction complexity.

Catalytic reactions are characterized by the presence of materials in the reacting mixture, that do not take part of the reaction rates. Usually catalysts are used in liquid or solid phases and are associated with heterogeneous systems. The catalytic reactor is one of the most important units of the typical chemical or petroleum industry. Approximately 70 % of the total output of chemical industry is processed at some stage with a solid catalyst material, usually in a tubular or fluidized bed reactor. All catalysts are also deactivating with time, which makes the optimization of those reactors most interesting from an economic point of view. The basic facts on the dynamics of chemical reactors are found in standard text books, such as Aris (1961, 1965), Gould (1969), Harriot (1964), while the basic facts on kinetics can be found e.g. in Walas (1959) and Levenspiel (1962), Couganowr - Koppel (1965) and Asbjørnsen (1971). The book by Kunii - Levenspiel (1969) gives a comprehensive description of the knowledge about fluidized beds, both theories and practical applications. The high complexity of the reactor equations, both in the stirred case and in the tubular case, is one reason that it is difficult to find sophisticated applications of advanced control theory on reactors.

There is an overwhelming list of contributions, where reactor models have been derived from à priori knowledge. Analysis has been made or simulations of the system behaviour are performed and different control strategies have been calculated. Very little, however, is described about real measurements, experimental identification or applied optimal control of reactors. The contribution by Lowry et al (1967) is, however, an interesting exception. A large amount of measurements and steady-state calculations have been performed.

7.2 Stirred tank reactor dynamics and control.

The dominating feature of the dynamics of chemical reactors has to do with the significantly nonlinear behaviour. The range of linearized models is in general very small, why mostly a more elaborate description of the dynamics is required. In contrast to this a distillation column is almost linear, even if its dynamics might be complex of other reasons, see 6.2.

The dynamical behaviour of a stirred tank reactor is derived out of material and energy balances for the components which take part in the reactions. The stochiometric relationships serve to restrict the behaviour of the system and decrease the dimensionality of the state space. A discussion of these phenomena can be found in e.g. Aris (1965). It is, however, much disputet in the literature how to apply this constraint in general terms, and further contributions are found in Gould (1969) and Asbjørnsen et al (1970).

The differential equations describing a chemical reactor are often stiff, i.e. the ratio between the fastest and the slowest time modes of the system is very large. This means that there are real numerical problems to simulate such systems. Edsberg (1972) has made a program package for the simulation of ordinary differential equations, describing stirred tank reactors, where the stiffness is taken into acount.

Because of the nonlinearities, mainly introduced by the Arrhenius law, it is possible to get several operation points for the reactor. Both the heat production and consumption in the vessel must be matched in steady state. In an exothermic reaction there may be up to three solutions, some of which are steady state unstable and some others are stable. If more reactions occur there are of course more operating points. In an endothermic reaction, however, there is just one operating steady-state point.

If an operating point is found to be steady-state stable, it is not sure, that the same point is dynamically stable for small disturbances. Further conditions then must be imposed to ensure dynamical stability. A linearization of the equations does not give any information about the size of the region where the linear equations are valid. Therefore in most cases, stability properties have to be determined by more sophisticated methods, either by nonlinear simulation or by analytical methods such as the Liapunov method. To find an adequate Liapunov function is, however, only possible in the simplest cases. Therefore simulation is the dominating tool for reactor analysis.

Control of stirred tank reactors can mostly be managed with conventional methods, as soon as the steady state point is stable and the disturbances are small. If an optimal control is desired, then the nonlinear model has to be taken into consideration. Even if the control system synthesis might be straight forward, the effect of disturbances might be confusing. It is possible that non-minimum phase effects from feed rate changes to the temperature response appear. A control system that does not take this effect into consideration may overreact and cause severe errors.

It is a non-standard task to determine possible operating points in steady-state. For systems or networks of reactors one must add further equations in addition to the basic heat and mass balance equations. These are needed when there is heat or material re-cycling or when separations are present. To find the "best" operating point in such a system is certainly a major calculation. One has to define clearly what is meant by "best" at that time. Such calculations include optimum residence time, optimum temperature to maximize yield in tank reactors, determination of optimum temperature profiles in tubular reactors as well as selection of the best transfer means for tubular and stirred tank reactors. Tazaki et al (1972) present one approach to apply a decentralized theory to the steady state optimization of a complex chemical plant. The large scale problem is subdivided into a number of optimization subproblems, which are coordinated in a certain manner.

Stephens et al (1973) have performed a steady-state and dynamical analysis of an ammonia plant. Some of the concepts of stability for simple reactors have been transferred to the big plant and they have been proven to be useful. The reaction taking place is exothermic, and therefore several operating points can appear. A simple control scheme has been used for disturbance stabilization.

Dynamical optimization is much less used because the problem is so difficult to solve. For stirred tank reactors or lumped parameter approximations of tubular reactors, optimal control theory has been applied, but to a very limited extent. Mostly the applications are simulation studies. The author is not aware of one single full scale application of dynamical optimal control theory to chemical reactors. There are several reasons, not only that optimal control should be difficult to handle. The kinetic behaviour as well as other dynamical features of the reactors are often poorly known. These facts are a real challenge to both modeling and control people.

Allen et al (1971) have reported a digital computer control application of a batch reactor, used for the production of unsaturated polyester resins. The objective of the control system is to maintain uniform temperature and pressure and to improve uniformity. The reactor is connected to a packed column distillation column and a variable surface partial condenser. The control strategies are fairly simple but apparently successful for the purpose.

An interesting numerical study of applied optimal control has been performed by Mårtensson et al (1973). They have considered the optimal control of a batch acid sulphite digester. The main contribution of this paper is that this is the first time that numerical optimization methods have been applied to such a complex system, where constraints are prescribed to the state variables, to the inputs and to the final state. Moreover, the differential equations are highly nonlinear and discontinuous. Five state variables and two control variables describe the process. The optimal control task then consists of the problem to reduce lignin content in the cellulose below a predetermined level in such a way that the hemicellulose reduction is minimized at the terminal time, which is fixed à priori.

Javinsky et al (1970) have applied optimal control theory to a jacket cooled continuous flow stirred tank reactor with a homogeneous liquid phase exothermic irreversible chemical reaction. The reaction is of the form A + B → C + D. The optimal control problem is the following: using the heat transfer coefficient between the reaction mixture and the coolant as the control variable, what is the control law which drives the reactor system from the given initial state to a specified final state in minimum time. Three practical applications are considered

- o reactor start-up
- o changing from one steady state to another
- o regulating specified final state conditions.

A pilot plant reactor has been compared to analog studies.

Kalman filtering has been used both for state estimation and parameter estimation in tank reactors by Wells (1971) and Seinfeld (1969, 1970).

7.3 Tubular and fixed bed reactors.

In a sense the distributed variable reactor may be considered a logical extension of the stirred tank approach. Still the mass and heat balance equations have to be calculated, but their form is getting more complex than in the stirred reactor case. The mass balance equation for each component is now a diffusion equation. The energy balances will result in partial differential equations of first order in time and space. Consequently the dynamical behaviour is getting more complex compared to the tank reactor case.

For a fixed catalyst reactor there are even more complications. Thus the basic dynamical behaviour in a fixed bed reactor can be described by the mass balance equations for every compoment and energy balance equations for the wall, catalyst and reaction gas. In addition to these equations, the mechanisms that determine reaction rates tend to be much more complex since the presence of a solid catalyst implies that the reaction is heterogeneous. The more sophisticated models of those reactors therefore should include inter and intra particle heat and mass transfer equations. The dynamics then results in coupled nonlinear partial differential equations. To handle such a complex system for optimal control by any general techniques is far beyond what has been applied in any full scale plant. Major dynamical effects in a tubular reactor result from the highly nonlinear coupling between the temperature and composition distributions.

To explain hot spots in the tube or "blow-outs" or "blow-downs" linear analysis is seldom fruitful.

If the axial diffusion can be ignored, i.e. if the Peclet number is large enough, then an idealized plug flow can be assumed. Then the reactor equations in steady-state are completely similar to the stirred tank case if the spatial variable is replaced by time. It is possible to do some steady-state analysis with ordinary differential equation calculus. This calculus, however, does not show, how instability evolves in time for the tubular reactor.

There is a large number of papers, articles and books about the theoretical derivations of catalyst reactors of different configurations. Except the previously mentioned books some articles will be reported.

Hoiberg et al (1971) have developed dynamic models of a fixed bed catalytic reactor as a result of identification. The experiments were using the platinum catalyzed reaction between hydrogen and oxygen because the coupling between the temperature and concentration of this reaction system is large. Frequency analysis identification was applied and measurements were made of the gas temperature and concentration along the centre line of the catalyst bed.

It is wellknown that partial differential equation descriptions are not well suited for control synthesis. Therefore it is natural to look for approximations in terms of spatial differences, lumped systems or some sort of stirred reactor approximation of the tubular reactor. Michelsen et al (1973) have given an interesting contribution in this context. Instead of approximating the partial differential equation with straight forward spatial differences the method of orthogonal collocation has been used, thus creating ordinary differential equations in the so called state space form. The new state variables are then weighted sums of the states at certain points of the reactor, those points being calculated out of a Legendre polynomial. It is shown by numerical examples that a plug flow reactor can be satisfactorily approximated by only 6 or 8 points, which is remarkable.

The Kem-Tek contribution by El Rifai et al (1974) is mainly devoted to the optimal design problem of reactors, both lumped and distributed. The dynamics of gas-particle heat transfer in both fluid and fixed beds is derived in terms of ordinary and partial differential equations respectively. The models are then used to find optimal equipment size, temperature operating conditions as well as duration of each of the two actual regenerator cycles in two regenerator models.
Kalman filtering techniques have been applied to simplified models of tubular and packed bed reactors, as in Gavalas et al (1969), Joffe et al (1972), McGreavy et al (1972) and Vakil et al (1972).

Generally the control purpose in tubular reactors is to keep the reactor stable. Conventional control is used. It is, however, worth mentioning, that the problem to keep the reactor stable might not be more difficult than in the tank reactor case. Some reactions may well be even easier to control in a distributed flow pattern than in a vessel like a stirred tank. The problem to dynamically optimize is, however, a different question. It is quite common to practice a similar control philosophy as in the distillation case. On top of the conventional control there is a steady-state or quasi- steady-state optimization. One example of this type is found in a full scale methanol plant, described by Shah et al (1970).

There are several simulation studies of optimal dynamical control reported in the literature and a couple of examples will be given. Gould et al (1970) have investigated the dynamic optimization of a simplified model of the fluid catalytic cracking process. A linearized version of the nonlinear control laws appeared to yield a better result than conventional control. The plant and study was not implemented. Ray (1971) has derived optimal control schemes for a tubular reactor with catalyst decay. Still much work remains to do before the control laws can be implemented on-line.

8. APPLICATIONS TO WASTEWATER TREATMENT

The present chapter is a summary of a more comprehensive report written by the author (Olsson et.al. (1973)). The report contains almost 100 references. Here it is not referred to any of those references but to standard books and to a few essential articles and recent papers.

8.1 Why control?

Wastewater treatment is quite a new field for automatic control applications. Not until recently much interest has been paid to the problems of automation and on-line control. There are several reasons for this, and some facts may be considered.

The quality of the effluent water has to satisfy quite strict regulations today. In order to keep the quality at a smooth level, advanced techniques are necessary. The operation of wastewater treatment plants is getting more expensive, and if it is possible to save money, control equipment is certainly of interest.

There are significant energy costs for pumps and compressors, as well as for chemicals, and there are potential possibilities to save some of these costs by clever control methods. On the other hand, it is difficult to give satisfying overall profit measures for a wastewater treatment plant, as the output product cannot be sold. The value of improvements of water quality is therefore difficult to estimate.

The development of new instruments during recent years is also making automatic control of wastewater treatment plants meaningful. In the conference proceedings, edited by Bennett (1973) there are several discussions on problems in automation of wastewater treatment plants.

8.2 Wastewater composition.

Contrary to popular belief, sewage is only slightly contaminated water. In fact, usual domestic wastewater is 99.95% water. For most uses, however, the water must contain much lower levels of contaminants. This shows that, even if waste treatment technology need only extract small quantities of contaminants from wastewater, they must be reduced to very low levels.

The diversity of contaminants has already been mentioned in chapter 3. In fact, the diversity is so great and the concentrations are so low that only a few substances exist at a measurable level. This makes much of the instrumentation a major problem.

The water quality, both for the influent and for the effluent water, can be characterized by a large number of parameters. The most common ones are biochemical oxygen demand (BOD), chemical oxygen demand (COD), total phosphorus, nitrogen and suspended solids contents. In addition there are several more relevant parameters, such as heavy metals, trace organics, pesticides and viruses.

The problem for the control engineer is to find the most relevant variables to measurefor control purposes. In a biological process the control purpose should be to keep the biological activity at a certain level so as to maximize the organics consumption, but biological activity cannot be measured directly. Other physico - chemical variables have to be monitored instead. In a chemical precipitation stage one would like to optimize the condition for flocculation, but there are extremely complex conditions that determine the rate of flocculation, not only the pH and the phosphorus or phosphate content.

A major problem is also to characterize the influent water in such a way that proper control actions can be taken according to the water composition. Even if the long term characterization of the wastewater at a certain plant can be calculated, it is almost impossible to get the momentary characterization of the "raw material" coming in for processing.

The literature review by Ghosh (1973) is referred to for further studies.

8.3 Some basic features of wastewater treatment plants.

A wastewater treatment plant consists of a large number of complicated unit processes. Here two of them will be emphasized, viz. the activated sludge process and the chemical precipitation stage. Those units will probably be the most important parts of wastewater treatment plants for a long time.

8.3.1 The activated sludge process.

This process is a biological process, which has been specifically developed to remove suspended solids, biodegradable organics and microorganisms from the wastewater. A flow sheet is shown in fig. 4.

In the process a biological oxidation of soluble organic material by microorganisms takes place. The microorganisms consume the organics, thus producing cell mass, carbon dioxide and water. This reaction takes place in the aeration basin. Air is blown into the tank to keep the dissolved oxygen content over a certain level in order to maintain the biological activity.

In the secondary sedimentation tank the active microorganisms are separated from the flow. Some of the settled material, which is mainly organic material, is recycled to the aeration tank (return activated sludge) in order to maintain an adequate population of the microorganisms. The excess sludge is pumped to the sludge treatment part of the plant. That problem will not be considered here.

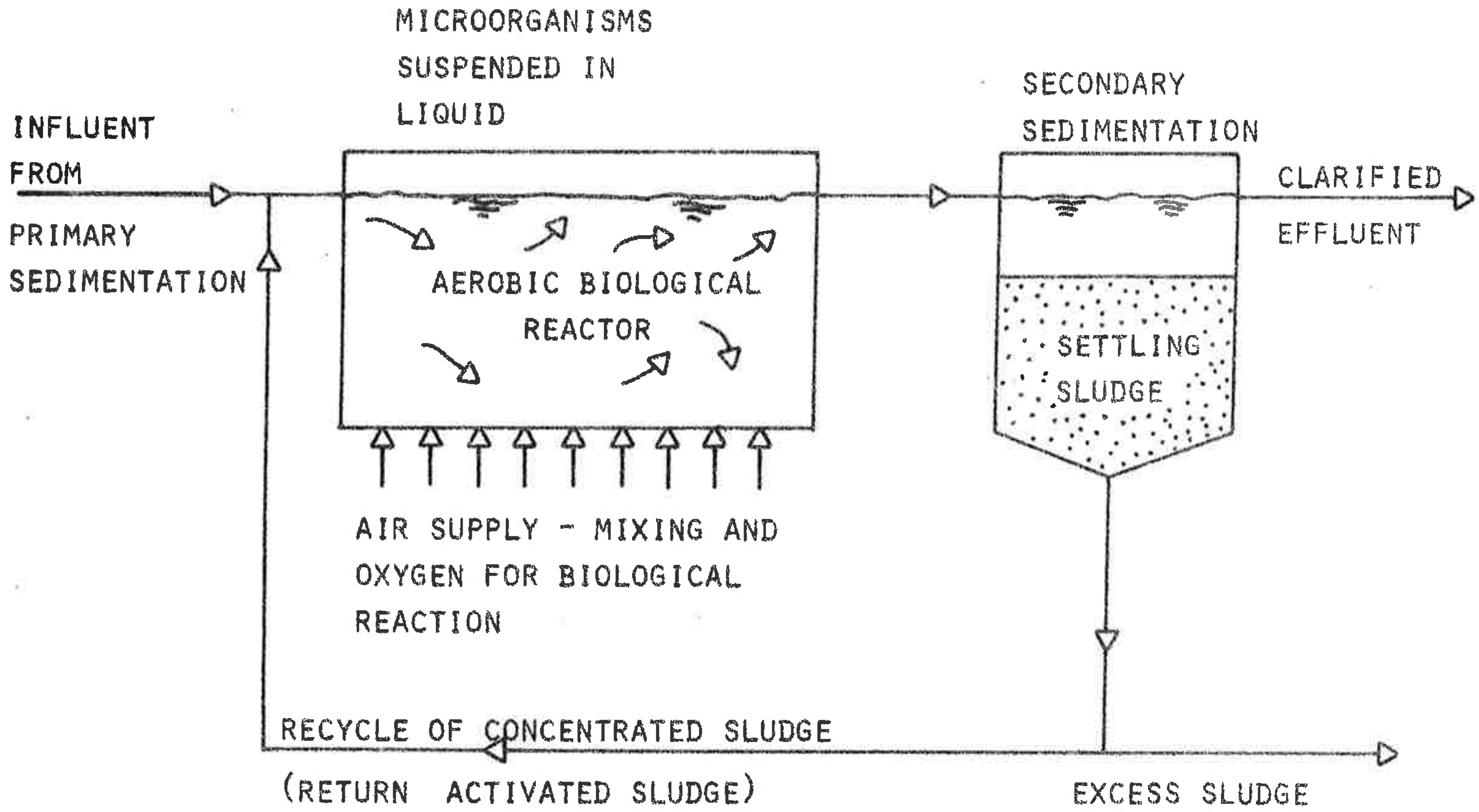

Figure 4 - The activated sludge process.

For further studies of the process description we refer to some of the books by Metcalf et al (1972), Eckenfelder (1966) or Culp (1971). The literature review by Azad et al (1973) gives more recent references.

8.3.2 Phosphorus removal.

The essential removal of phosphorus must be realized by chemical precipitation. Phosphorus forms essentially insoluble precipitates with a number of substances. High rate of phosphorus removal thus can be obtained when the right chemicals are added in proper doses. The use of salts of aluminum and iron or lime as chemicals is dominating mainly because of economical reasons.

Both metal salt and lime precipitation are very complex reactions. It is beyond the scope of this paper to describe any details of these. Here we merely consider in what way the dosage of chemicals can be controlled. The pH basicly determines which types of phosphates that will be dominating. The precipitation is strongly dependent on the pH.

A control law for chemical dosage should consequently at least be based on flow rate and pH measurements. The phosphorus or phosphate content is also a most desirable information, but that information is not enough either. There are a lot of other factors decisive for the chemical dosage, and the average dosage therefore has to be determined experimentally for each plant with its special wastewater composition.

The chemicals can be added in different parts of a wastewater treatment plant, as illustrated by fig. 5. In Swedish plants post-precipitation is common (80-85% of the chemical plants) but direct, simultaneous or pre-precipitation is also possible to use.

There is a vast literature on chemical precipitation. Let us here just mention the books by Weber (1972) and Culp (1971) and the literature review by Cohen el al (1973). Some Swedish experiences are reported in Ulmgren (1973).

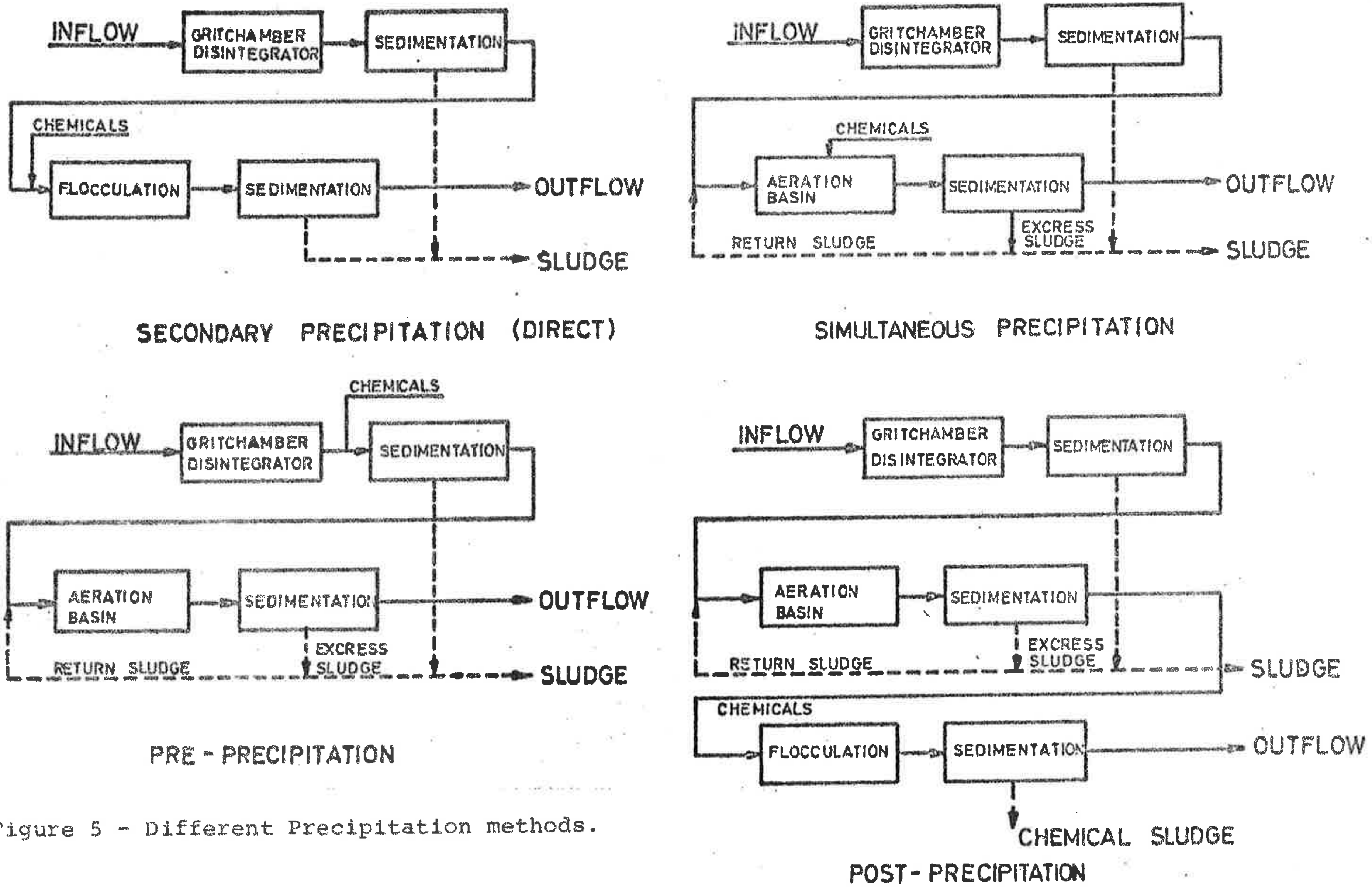

Figure 5 - Different Precipitation methods.

8.4 Typical disturbances on the processes.

The most interesting disturbances are related to the influent, either to the flow rate or to the composition. In contrast to feed disturbances in chemical processes these disturbances are really significant both in terms of flow rate and concentrations. The diurnal variations of the influent flow might be 30-50 % of the average flow for a big plant with a large system of sewers. For another type of plants the possible variations may well be 5-10 times the average flow. Consequently, the disturbances are of major interest, and the dynamical behaviour is of much greater importance than in many chemical processes. In the design of new plants, few attempts are made to take these variations into consideration. Parallel basins, tubes and pumps, however, may be installed. The plant is mainly designed to operate at a steady state flow, but such a steady state flow does never occur. That fact explains why so many wastewater treatment plants are operating poorly.

Not only the predictable diurnal variations have to be considered. Sudden chock loads of industrial waste might enter the process. A rain storm can cause a rapid increase of the influent flow rate, while at the same time the concentrations are going down. A decrease in concentration is not desirable, because the biological activity might be diminished due to too little food for the microorganisms, and consequently the removal of organics is getting poor.

When the flow rate changes the sedimentation properties also vary with time, as the hydraulic time constants of the basins depend on the flow rate.

Changes in pH will directly affect the chemical precipitation, and the chemical dosage must be properly adjusted. Disturbances in phosphorus content or other composition variables of course also influence the chemical precipitation.

Depending on the amplitude of the disturbances, different types of actions are needed.Linear, conventional control schemes may often be sufficient for small disturbances. For large amplitudes, however, the whole dynamical behaviour of the process is affected, and much more refined techniques are required to handle such a situation adequately.

8.5 Control variables.

A wastewater treatment plant is a highly complex system like many other chemical processes. Therefore it is not at all clear which variables to manipulate, where to locate the sensors and which variables to measure. Here an attempt is made to list some parameters, possible to use as control variables.

In some plants it is possible to regulate the influent flow gates. If the sewer is large enough, it can serve as an equalization basin. Thus the influent flow can be partially controlled and the peaks can be attenuated.

In any sedimentation tank it is important to know when to remove the sludge on the bottom. The sludge pumping cycle should therefore be considered.

For the activated sludge process the most important control variables are the air blower speed influencing the dissolved oxygen content and the flow rate of the return activated sludge. With those two variables both the biological activity and the ratio between substrate and living microorganisms can be controlled

It is clear that the rate of chemical dosage is the major control variable for the chemical precipitation.

8.6 Some important control loops.

The unit processes are very complex systems. Considerable research has been performed on biological kinetics under laboratory conditions, but very little is known about the biological activity in an activated sludge process in a real plant.

Before any complex multivariable control or optimal control can be applied simple regulation must be tried out carefully. The choice of suitable control algorithm is not the first major question. Rather it is mandatory to get the proper instrumentation and the adequate locations for the instruments.

The control of dissolved oxygen is of great interest. The blower speed or mechanical aerator power is used to control the dissolved oxygen level in the aerator. This type of control has been succesfully installed in some plants. The most advanced application is supposed to be the one in Palo Alto, California, as reported by Stepner et al. (1973). The cost savings of such a loop can be significant, because the oxygen content need not be higher than a certain level (1 - 2 mg/l). Therefore power can be saved. It is calculated that a 20% saving of the power costs is achieved in the Palo Alto plant due to the control.

It is also essential to maintain a certain ratio between the amounts of food and microorganisms. The return activated sludge flow rate can be used for the control of this variable. As the biological activity cannot be measured directly, indirect physico-chemical variables, like turbidity, dissolved oxygen content and respiration, have to be measured instead.

Control of chemical precipitation was mentioned in 8.3.2. In most plants today the chemical dosage is manual, and in some few plants it is made proportional to the influent flow rate or depending on pH. It is important to consider the potentials of using a feed-forward - feedback control scheme. Incoming disturbances from the influent can be directly fed to the dosage control. Effluent quality variables can then be fed back to maintain a smooth quality.

There are great potentials to save a lot of chemicals with a dosage control system.

In Olsson et al. (1973) some dynamical models of the activated sludge process have been reviewed. These models may be used for control system synthesis, but no application of such a control law has been made hitherto. In a recent article Fan et al. (1973) have made simulation studies of advanced control of an activated sludge process. The models presented in Smith et al (1970) are currently being improved at EPA in USA.

9. TOPICS FOR RESEARCH IN CHEMICAL PROCESS CONTROL

In the survey it has been demonstrated that advanced control theory has been applied to some extent in chemical processes. There are, however, many systems which would be interesting control objects if adequate methods were at hand and if instruments were available.

The problem of control system structure is important. The solution of that problem would be one of the really essential steps forward.

It is recognized by some researchers (see Åström et al. (1971) that a practical method of state and parameter estimation is one of the keys to progress. There is also a clear trend to re-examine and extend the classical methods of frequency analysis, which is reflected in e.g. MacFarlane (1972).

It is not true that the linear, quadratic theory has solved the structural problem of linear systems, even if it is a most significant contribution. The real problem is more difficult than that. The distillation process is one example, where it is not clear what to measure and what to manipulate.

In other processes, such as the activated sludge stage in a waste-water treatment plant, there is also the problem of which variables to measure. How can the state best be characterized? Where should the oxygen and suspended solids monitor be placed? Should the process be a step-aerated process or one which approximates plug flow? And how do we know if we are receiving representative samples of the stream? Such are the questions that need answers, and it is the burden of new theories to invent ways both of asking and answering the questions.

The representation of the process dynamics alone is a major task, and much work has been done in the identification field although nonlinear and distributed systems require much more attention. Furthermore, the parameters determined by these identification methods should preferably be of a physico - chemical nature and not those parameters resulting from numerical transformations into canonical structures.

The adaptive control of complex processes is still a new field for applications and there is certainly a need for this type of advanced control. Some promising approaches need to be tested more in full-scale industrial processes.

It is important to look for more elaborate methods to formulate objective functions for process plants. This choice is crucial for the success of optimal control theory. It is not clear which attribute of the controlled system these indices should reflect.

The status of instrumentation is rapidly improving. For the next few years this development will hopefully continue, because there is still a strong need to get reliable and sensitive on-line instruments for several process variables. Without an adequate instrumentation even the most advanced control method will fail.

In a quite recent article Foss (1973) critisizes chemical process control theory. I am ready to agree with this author that the gap between theory and practice today has also to be filled by the theoreticians. Because of the complexity of many chemical processes, the theory still lacks some essential concepts. Suffice it to say that the existing theory should be examined practically in those cases where it is relevant.

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