

ONSTREAM COMPUTERS -
AN EXAMPLE AND SOME GENERALITIES

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There are many excellent articles (1,2,3,4,5,6,8) giving the general reasons for and the philosophy behind the use of digital computers in the controlling of production processes. Some of the pioneering efforts by Stout and Laspe (1,2,3), as early as 1957, formed the basis for many of the digital control systems in use today. Subsequent papers by Roberts (6), Stout (6), Brandon (5), Madigan (12,13,14), Freilich (19), and Laspe (15) presenting the results of actual case studies have bolstered the technical literature on computer control systems. It is not the intent of the present paper to dwell heavily upon the objectives of computer systems, nor upon their design, for these aspects of the problem have received adequate attention in the afore-mentioned papers.

It is the purpose of this paper to present the broad aspects of on-stream computer control and especially as these aspects affect the curricula of chemical engineering. In attempting to accomplish this objective, I would like to present a few generalizations, followed by a survey of the extent to which computers are used in on-line control. Next, as an example, the computer control of an ammonia plant will be discussed to illustrate the various branches of engineering and science required in its design. Finally, the most important point, as touching upon this present session, will be a discussion of those fundamental things which a student in an engineering school should learn to understand the use of on-line control computers.

In order to orient our thinking along the lines of on-stream control computers, a few generalities should be considered. What are the ingredients that go into making up a computer controlled process? Once these individual ingredients are recognized, then we are in a better position to determine the engineering talents required for the design, construction and operation of such a system.

Let us briefly review a few fundamentals. All manufacturing processes are designed and intended to be operated to produce a profit. This profit results from the creation, by a combination of physical and chemical transformations, of a product or products whose value exceeds the cost of the raw materials and their processing. A major goal of management in plant operation is the maximization of this profit. This statement may be considered as the process objective. Therefore, the purpose of computer control is to provide the latest and the most efficient means of reaching this process objective. It is realized that, since physical and chemical transformation are involved, many variables influence the realization of the process objective. When one or more of these variables are beyond the control of the operator, such variables are classed as disturbance variables. Compensation for these disturbances is the prime justification for any control scheme. For without disturbances, control would not be required.

When there is but a single disturbance variable involved in the operation of a plant, then it is possible to derive a unique solution to the control problem. In other words, for any given value of the disturbance variable, there is only one set of control variables which will meet the desired objective. In this instance, simple relationships may be found which will relate the manipulated variables to the disturbance variables then in effect. On the other hand, when two or more variables are beyond the control of the operator an interesting situation arises. In this case there are generally two or more feasible solutions. Of these feasible solutions, one will probably yield the greatest economic return and, therefore, is the desired optimum solution. It is in these areas where computer control may be justified. Recently, an excellent article by Elliott and Longmire (21) gives the dollar incentives for computer control. The results of their studies on six different production processes is presented.

The March issue of Control Engineering presented a survey of on-stream control computers. At that time the score card showed 35 closed loop computing control installations, either on-line or scheduled to be on-line by early 1962. Of these 35 installations, nearly half were to be used in either chemical or petroleum processes. In September of 1961 Freilich (19) presented another survey of process control computers in use. Freilich shows a total of 63 process control computers, of which 20 are used in the chemical and petroleum industries. The latest figures available from the May 1962 issue of Control Engineering (20) show a total of 159 control computer sales, of which 43 are installed in the chemical and petroleum fields.

Although the preceding statistics are both encouraging and interesting, they do not tell the complete story. Table I summarizes the known installations of digital computers in process control or those units known to be on order. In the petroleum field, several installations have been reported on catalytic cracking plants and on crude distillation units. Single installations have been reported for catalytic polymerization, alkylation, and thermal cracking. In the chemical field ethylene and ammonia appear to be good candidates for computer control by reporting several installations on each. In addition other computer controlled chemical processes include vinyl chloride, styrene, acrylonitrile, acetaldehyde, ethylene oxide, and the exotic "alfol" plant of the Continental Oil Company. As can be seen from a study of this list, the gamut of applicable processes is limited only by economic necessity and the imagination of the system designer.

From the above list we have chosen as the working example to be discussed here today, the computer controlled ammonia plant of Monsanto Chemical Company at Luling, Louisiana. A fairly complete description of this particular installation has already been given by Eisenhardt and Williams (17) in the November 1960 issue of Control Engineering.

For purposes of description, the ammonia process can be conveniently divided into three separate operations. The first of these is concerned chiefly with the preparation of raw synthesis gas. The second section is concerned with purification and compression, and the third and final section is the synthesis unit itself. In the gas preparation area three chemical reaction stages are involved. The primary reformer, the secondary reformer, and the CO converter. The feed to the primary reformer consists of natural gas and steam which in the presence of a catalyst reacts to produce hydrogen, carbon monoxide, and some carbon dioxide. External heat is applied to this unit from a reformer furnace burning natural gas. Essentially 90% of the incoming gas is converted. Steam reforming is the principal reaction involved, although the water gas or CO conversion reaction accounts for some of the hydrogen produced. The variables over which control can be exercised are the flow rates of the natural gas, the fuel gas and the process steam.

The secondary reformer serves two specific functions. Firstly, to provide additional reaction volume for continuation of the reforming and CO conversion reactions initiated in the primary, secondarily, to serve as the injection point at which nitrogen is introduced into the system. Atmospheric air is used as the source of nitrogen. In the secondary reformer the oxygen from the air which has been introduced reacts with some of the methane and hydrogen in the feed to form water plus CO and CO₂. The only independent variable over which control can be exercised is the flow of process air. Note that at this particular point in the process, essentially all of the natural gas has been converted into product gases. The residual methane content is in the order of 0.3 of one percent. There is also an appreciable amount of carbon monoxide. The effluent from the secondary reformer flows directly to the CO converter.

The sole purpose of the CO converter is to produce additional hydrogen from the incoming carbon monoxide by means of the water gas reaction. Additional water is injected at this point in the form of low pressure steam. Because of fundamental thermodynamic and kinetic considerations, the carbon monoxide is not completely consumed. The exit concentration is in the order of three percent. At this point in the process the hydrogen to nitrogen ratio is fixed and remains constant throughout the remainder of the operations. At this particular point in the process, carbon dioxide represents approximately 15% of the entire raw synthesis gas. This along with the carbon monoxide must be removed before the synthesis gas can be charged to the final ammonia synthesis reaction stage.

Carbon dioxide is removed from this raw gas stream by passing it through a standard Girbotol unit. Mono-ethanol amine is used as the absorbent.

A compression plant consists of several parallel reciprocating compressors. Each compressor is equipped with five stages of compression. The gas pressure is boosted from approximately 20 pounds per square inch at the inlet to 5,500 pounds per square inch gage at the outlet. The entire gas stream, however, does not pass through all five stages. At the outlet of the fourth stage, the process gas is diverted to the high pressure purification unit. The main function of this unit is to remove carbon monoxide, plus any residual carbon dioxide. Copper formate is used as the absorbent for CO. The residual CO₂ is removed by a final caustic wash. After removal of impurities, the purified synthesis gas is then directed to the last stage of compression from whence the gas flows to the synthesis unit. An analysis of the exit gas shows an essentially pure hydrogen, nitrogen mixture in the ratio of approximately 3 to 1.

Table 1
SURVEY OF PROCESS COMPUTER APPLICATIONS

<u>Company-Location</u>	<u>Computer</u>	<u>Delivery</u>	<u>Process</u>
1. Allied Chemical Corp. South Point, Ohio	RW-300	1961	Ammonia
2. American Oil Company Whiting, Indiana	IBM-1710	1961	Crude distillation
3. B.A.S.F. Ludwigshafen, Germany	RW-300	1961	Chemical process
4. B.F. Goodrich Chemical Calvert City, Kentucky	RW-300	1959	Vinyl chloride and acrylonitrile
5. Celanese Corporation Bay City, Texas	H-290	1962	2-Ethly hexanol
Bishop, Texas	RW-300	1962	Vapor phase oxidation
6. Continental Oil Company Lake Charles, La.	RW-300	1961	Alfol process
7. Dow Chemical Company Midland, Michigan	GE-312		Styrene
8. Dupont Beaumont, Texas (2)	ISI-609	1960	Chemical process
Florence, S.C.	ISI-609	1960	Chemical process
Circleville, Ohio	ISI-609	1961	Chemical Process
Gibbstown, N.J.	IBM-1710	1961	Acrylonitrile pilot plant
9. DX-Sunray Tulsa, Oklahoma	RW-300	1961	Crude distillation
10. Gulf Oil Company Philadelphia, Pa.	RW-300	1961	Catalytic cracking
11. Imperial Chemical Ind. England	Ferranti		Soda Ash
12. Monsanto Chemical Co. Luling, Louisiana	RW-300	1959	Ammonia
Chocolate Bayou, Texas(4)	H-290	1962	Chemical process
13. Owens-Corning Fiberglass Aiken, S. Carolina	ISI-609	1960	Logger
14. Petroleum Chemicals, Inc. Lake Charles, La.	RW-330	1963	Ethylene
15. Phillips Chemical Co. Borger, Texas	Recomp II	1959	Portable Logger
Bartlesville, Oklahoma	TRW-330	1962	Portable logger
16. Shell Development Company Emeryville, Calif.	PB-250		Logger
17. Sun Oil Company Marcus Hook, Pa.	IBM-1710		Catalytic cracking logger
18. Standard Oil Co.(N.J.) Linden, N.J.	LGP-30		Pilot plant logger
Baton Rouge, La.	LGP-30		Catalytic cracking logger
19. Standard Oil Co.(Calif.) El Segundo, Calif.	IBM-1710	1961	Catalytic cracking
Richmond, Calif.	Recomp	1959	Product run calculations
20. Tennessee Eastman Kingsport, Tennessee	GE-312	1961	Chemical process
21. Texaco Port Arthur, Texas	RW-300	1959	Catalytic polymerization
22. Tidewater Oil Company Delaware City, Delaware	ISI-609		Naphthalene
23. Union Carbide Corp. Charleston, W. Va.	RW-300		Pilot plant logger
Seadrift, Texas	RW-300	1960	Chemical process
Seadrift, Texas	Daystrom	1961	Ethylene
24. Universal Oil Products Des Plaines, Illinois	Daystrom	1958	Pilot plant logger

Table II
CRITERIA FOR JUSTIFYING MONSANTO'S
COMPUTER CONTROL SYSTEM

1. Maintain maximum gas flow in spite of changing weather and process conditions.
2. Maintain an optimum hydrogen-to-nitrogen ratio.
3. Maintain an optimum methane concentration at the shift converter exit unless in conflict with 1 or 2.
4. Maintain maximum shift efficiency if not in conflict with objectives 1, 2, or 3.
5. Maintain objectives 2, 3, and 4 under reduced flow conditions.
6. Reduce raw materials flow immediately and safely to compensate for any loss of compression.
7. Log out all important process variables.
8. Provide the plant operator with messages in case of abnormal process or instrument conditions.
9. Provide failsafe features such that instrument or computer malfunctions are detected, alarmed, and prevented from affecting the process.
10. Control the fuel and air to the reformer furnace.
11. Maintain a specified steam-to-dry gas ratio at the exits of the secondary reformer and the CO converter.

The synthesis plant feed is combined with a recycle stream to form the feed to the synthesis reactors. Because of the low conversion per pass, (approximately 12%) a high recycle ratio is required. Ammonia is recovered in the reactor effluent gases by condensation. In order to prevent excessive build-up of inerts in the system, purging or venting is required.

Now let us turn our attention to some of the factors involved in making this particular plant a good candidate for computer control. As has been pointed out by Eisenhardt and Williams (17).

"While there may be a tendency to overdesign some plant equipment an engine-compressor system is usually conservatively sized because it represents a major fraction of the capital cost of an ammonia plant. The engine compressor system is thus likely to be one of the first units to bottleneck the plant as production increases. At Luling the highest possible production rate and therefore the maximum economic return is obtained by operating the compressor system at maximum possible capacity."

Due to the very definite influence of ambient conditions, particularly temperature, upon internal combustion engine compressor efficiencies, the allowable horsepower to be expended by the compressor is not a fixed or arbitrary constant. In fact the compressor capacity varies not only as the ambient temperature changes, but also as the mechanical condition of the compressors themselves are changed. In the case of a production limited plant, such as the one we are now discussing, it can readily be seen that the maximum plant throughput is never fixed, but varies in accordance with compression capacities. The purpose of the computer control system now becomes apparent. Its main function is to keep the plant running at maximum capacity by determining the maximum as limited by the capacity in the compression section. Once knowing the maximum allowable flow of purified synthesis gas, the computer can then go about its business of setting the many flow controllers in the reforming section. It is not enough that the compressors be fully loaded at all times. The synthesis gas must also have the proper quality as measured by the hydrogen and nitrogen ratio. Since each of the processes in the reforming area, namely, the primary reformer, the secondary reformer, and the shift converter involve chemical conversions, complicated kinetic and thermodynamic equations must be solved in arriving at the proper flow settings. To keep the plant properly balanced as well as keeping the compression section fully loaded then becomes the major job of the control computer. Table II lists the criteria for justifying Monsanto's computer control system. This table was taken directly from Eisenhardt's and Williams' article.

A question which immediately comes to mind is whether or not the predicted economic gains have been fully realized. Of course, basic economic figures are considered as proprietary information. However, in a qualitative way we can answer in the affirmative as Mr. Eisenhardt and Williams have said

"Immediately after placing the computer on control, the gains in control-ability became evident. When the process is not on computer control, the operator makes minor changes in controller setpoints trying to hold process temperatures within limits and maintain gas composition as required by the synthesis loop. Superimposed on top of these minor changes are larger step changes in throughput which are required to compensate for those uncontrolled variables affecting the plant capacity. At best these larger changes are made only several times a shift. Under computer control, however, the plant throughput is adjusted every eight minutes to obtain maximum possible production as uncontrolled variables changed. Qualitatively, one can observe from the computer log sheet the steadying of gas compositions and temperatures under computer control as compared with the irregular control obtained by even the best operator."

This now brings us to a consideration of the topic of engineering fundamentals as related to an understanding of computer control processes. The design of a computer controlled process requires the systems engineering approach. This means that the person in charge of the over-all project must view the project in its entirety. He should not be burdened with the many small details that go into the system design. But on the other hand, he should be fully aware of the many fundamental engineering sciences which are involved in such a project. In this sense the system engineering approach may be synonymous with the common core approach in chemical engineering education. In Table III are listed some of the fundamentals required of chemical engineering students for understanding of digital computer control processes.

Topping the list of required fundamentals is an understanding of economics. Since computer control is a tool to assist management in meeting the process objectives, which is normally the maximization of operating profit, the importance of a thorough understanding of economics can hardly be overemphasized. Methods for pricing intermediate products, an analysis of profit from incremental production, and a working knowledge of payout criteria for capital investment are especially important.

The basic curricula of chemical engineering will permit a reasonable understanding of the workings of most of chemical processes. However, in the computer control design area perhaps a little more emphasis should be placed upon chemical thermodynamics, chemical kinetics, and stoichiometry. For these are the basic sciences involved in deriving the predictive mathematical models used in the control computer.

Mechanical engineering enters into the design of computer control systems firstly, in the determination of the operating characteristics of the mechanical equipment involved. For example, in the ammonia plant system previously discussed, compressor capacity calculations were made. In addition to these, certain mechanical equipment limitations had to be evaluated. These limitations, which in computer parlance are called constraints, oftentimes determine or limit the area in which the process variables may be operated.

In the field of electrical engineering, as applied to the design of computer control systems, a main consideration is the communication between the computer proper and the process itself. A working knowledge of the basic AC/DC theory, transmission lines, impedance matching, and the filtering of electrical noise will go a long way in the understanding of the electrical requirements of computer control systems. It is not necessary to become too deeply involved in the computer circuitry itself. However, to deepen the appreciation for the entire control system, some instruction in this area would be profitable.

The ultimate success of any computer control system depends very heavily upon the ingenuity and mathematical ability of the process analysts. Most computer control systems operate on the basis of mathematical models which simulate or represent the operation of the existing plant. These models may be derived from fundamental theoretical considerations or possibly from regression analyses of plant data. In either event, considerable mathematical skill must be exercised in obtaining an accurate and representative set of equations. Once the mathematical model has been developed, the job is only half done. From here various optimizing techniques must be explored in order that the model may be used most efficiently in reaching the process objective.

Table III

FUNDAMENTALS REQUIRED OF CHEMICAL ENGINEERS FOR
UNDERSTANDING OF DIGITAL COMPUTER CONTROLLED PROCESSES

I. Economics

- A. Process objectives
- B. Investment and payout criteria
- C. General knowledge of market prices
- D. Methods for pricing intermediate products
- E. Analysis of incremental profit
- F. General knowledge of utility costs, etc.

II. Chemical Engineering

- A. Unit operations
- B. Chemical thermodynamics
- C. Chemical Kinetics
- D. Stoichiometry

III. Mechanical Engineering

- A. Operating characteristics of mechanical equipment
- B. Constraints imposed thereupon

IV. Electrical Engineering

- A. Basic AC & DC theory
- B. Transmission lines
- C. Impedance matching
- D. Filtering of noise

V. Mathematics

- A. Methods of correlation analysis
 - 1. Regression techniques
 - 2. Curve fitting
- B. Optimizing techniques
 - 1. Maximization by calculus
 - 2. Gradient methods
 - 3. Linear programming
 - 4. Nonlinear programming
 - 5. Dynamic programming
 - 6. Calculus of variations

VI. Control System Theory

- A. Linear Feedback systems
- B. Nonlinear feedback systems
- C. Sampled data systems
- D. Laplace transforms
- E. Z- transforms

VII. Instrumentation

- A. Hardware
 - 1. Types
 - a. Pneumatic
 - b. Electric
 - c. Hydraulic
 - d. Other
 - 2. Measurement equipment
 - a. Temperature
 - b. Pressure
 - c. Flow
 - d. etc.
 - 3. Analytical instruments
 - a. Chromatographs
 - b. Infrared
 - c. Physical properties
 - d. etc.
 - 4. Controllers
 - a. Proportional
 - b. Derivative
 - c. Integral
 - d. Other
- B. Methods of interconnection
- C. Reliability and accuracy

VIII Computer Fundamentals

- A. Types and characteristics
 - 1. Digital
 - 2. Analog
 - 3. DDA
- B. Applicability of computers
- C. Basic understanding theory of operation
- D. Programming
 - a. Flow charting
 - b. Coding
 - c. Machine language
 - d. Instructions
 - e. Routines and sub-routines

As a part of the applied mathematics curricula, considerable attention should be paid to control system theory. Here such subjects as linear feedback systems, nonlinear feedback systems, sampled data systems, Laplace transforms, and Z transforms should be studied. Since the on-stream computer is connected, as it were, to a live process, attention must be paid to the process dynamics. All computer systems must recognize these dynamics. Obviously, control actions must not be taken too frequently that the plant is always in a state of jitters, nor must they be taken too infrequently or else the full benefit of computer control will not be realized.

The study of instrumentation is essential for a complete understanding of the computer control process. By instrumentation we think of the hardware involved - the sensing elements, the transducers, and the control equipment. It is these items that allows the computer to recognize or sense the state of the process. It is also these items that allows the computer to take corrective action upon the process. In a sense the primary measuring elements represent the sensors of a living organism. The transmission lines are the nerves. The control valves and controllers are the muscles, while the computer controlled systems possess the same attribute via the local feedback control loops.

Finally, some instruction should be given in computer fundamentals. The differences between the characteristics of digital, analog and the DDA computers should be carefully noted. A basic understanding of the theory of operation of these computers is profitable, though not essential. Some programming instruction should also be given with exercises in flow charting, coding, and in the use of routines and sub-routines.

In closing I might say that it is impossible for any single man to understand completely all the workings of a digital computer control system. The design of such a system is the work of a team of experts. And yet, this complexity does not preclude its use as an effective and efficient production tool. Let me give you an example. There are not many people that completely understand the entire working of a television set or even, for that matter, of the automobile in which we drive to and from work. And yet, there are millions of these machines in everyday use. By the same token the digital computer controlled process, though its design is complex, its operation can be made simple enough for a single operator to comprehend. The efficiency of this production tool, this man-machine-process combination will be increased in the future through continued research efforts in all the areas that have gone into its design.

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