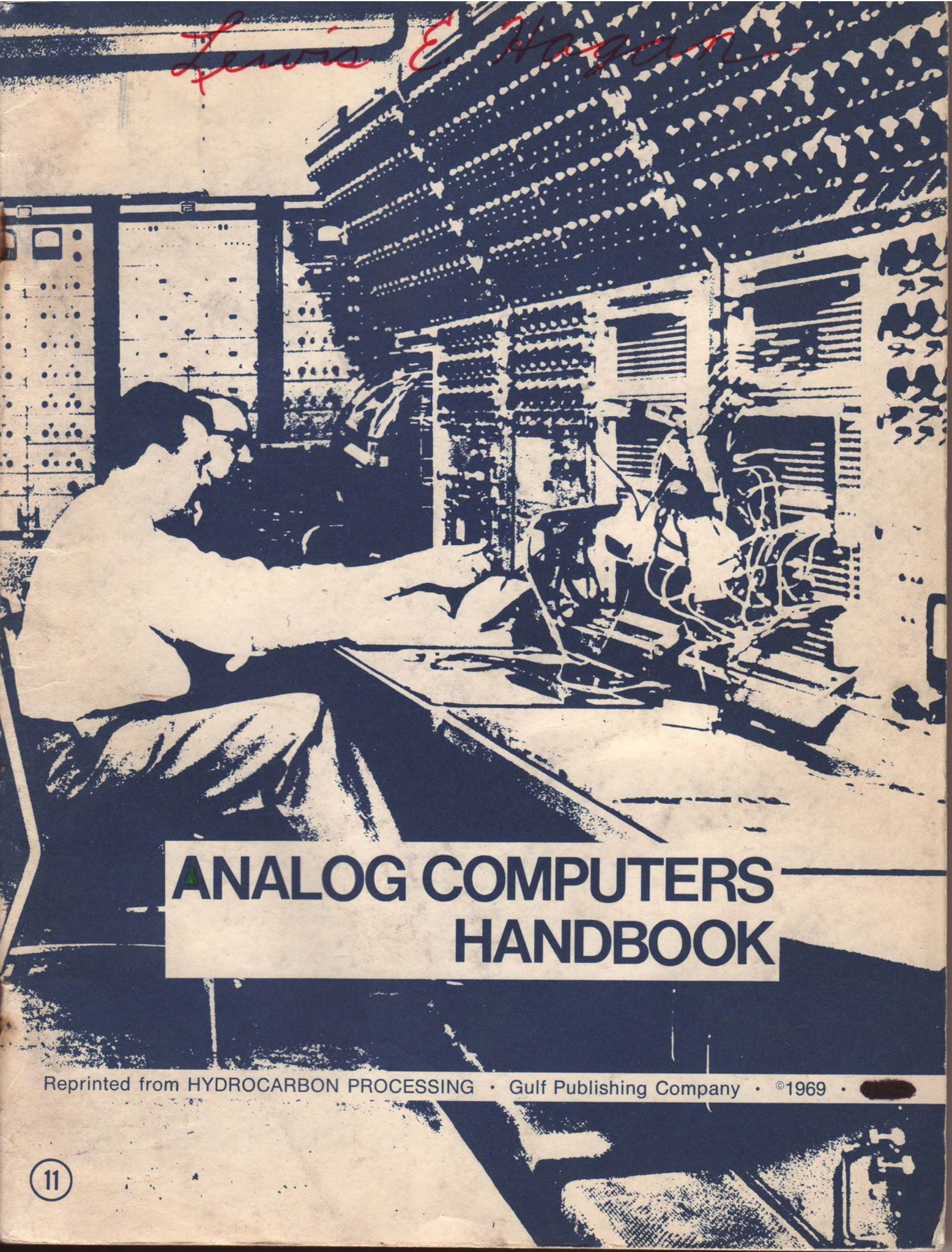
Lewis E. Hogan



ANALOG COMPUTERS HANDBOOK

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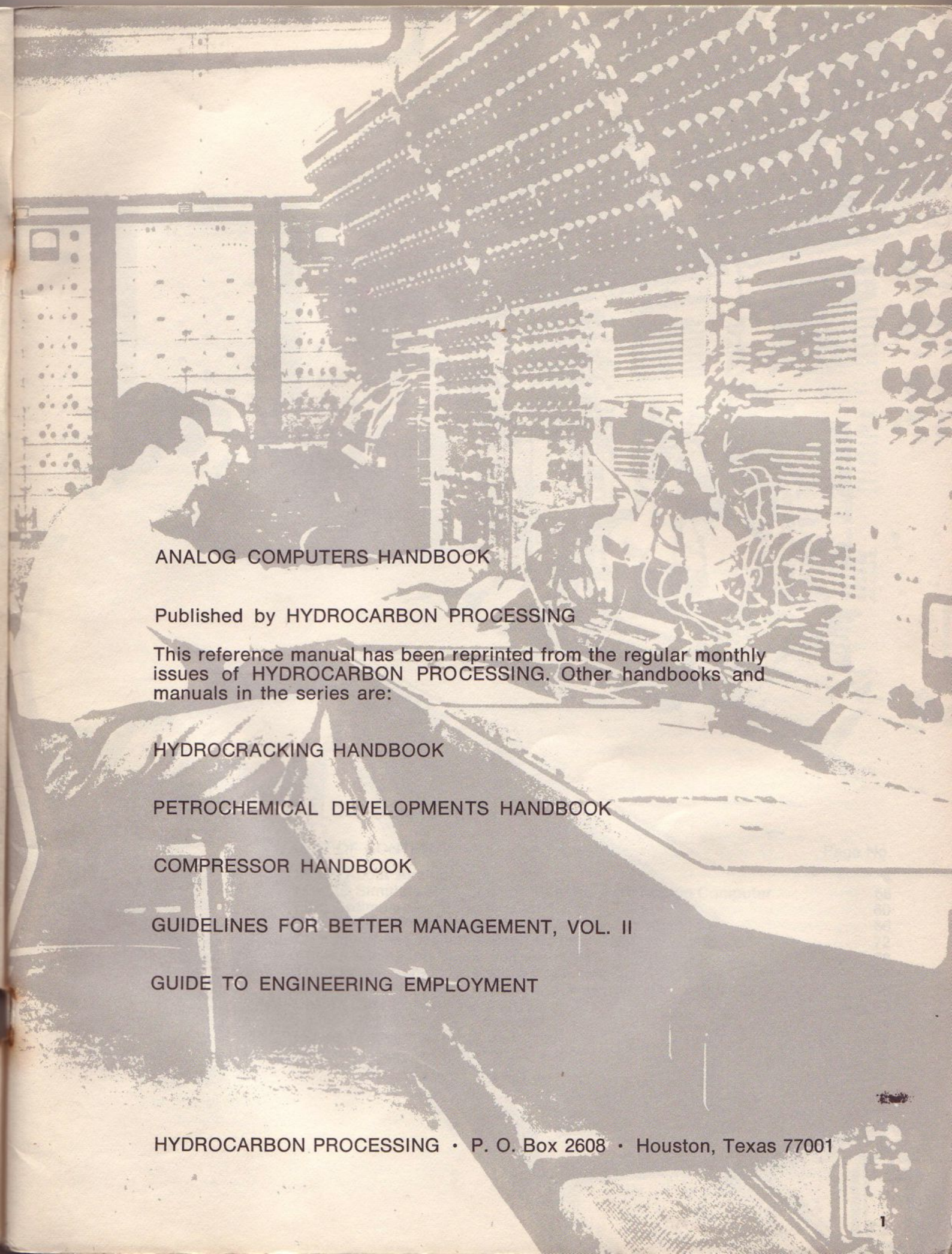

ANALOG COMPUTERS HANDBOOK

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ANALOG COMPUTERS

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Learn About

PART 1: INTRODUCTION–The role analog computers can play in engineering is discussed for the practicing engineer. Computer components are identified

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

CALCULATIONS, previously done by hand, can now be completed using computers with a great reduction in calculation time and a marked increase in computation precision. While such incentives are frequently sufficient to justify the widespread interest in computers, the application of computers to the solution of engineering problems has had a much more fundamental effect on chemical and petroleum engineering. When the speed and precision of modern computers are coupled with their variety, versatility, and large capacity, the reasons soon become apparent.

The practicing engineer now has at his disposal computational devices which enables him to handle economically problems of a complexity which he could not have handled 10 years ago. As a result, the class of problems which the engineer can be expected to handle has been greatly extended. This extension has resulted in a re-evaluation of what can be classed engineering calculations. The re-evaluation is still in progress, but it appears clear that the engineer of today, and certainly of tomorrow, will be constantly associated with problems once considered too complex, time consuming, or precision oriented to be amicable of solution. Consequently, computers have not only proven to be useful computational tools for the engineer, they have also provided a means for extending the scope of engineering calculations and, in so doing, have extended the scope of engineering itself.

The increasing complexity of engineering problems is recognized by universities so that engineers today are being routinely trained in the use of computers, as they in the past were trained in the use of slide rules and hand calculating machines. While the degree of computer competence which is required of a practicing engineer varies with his position, some knowledge of computers must be considered an integral part of his already varied skills.

For the practicing engineer who is directly associated with the programing and operation of computers, a high degree of competence on the computer is required. A common situation found in many companies is that in which a group of experts, highly trained in the use of computers, is available for consultation with the practicing engineer. In this case, the practicing engineer can rely on these experts for assistance in programing and operation. In many cases, these experts will handle all of the details of obtaining a solution once the engineer has properly defined his problem.

If experts are available, the degree of competence required by an engineer to solve a specific problem on a specific computer is inversely related to the degree of help he can obtain from the experts. However, frequently the engineer's problems are vaguely defined. Assumptions of varying degree must frequently be made, the reliability of the data examined, and, if several computers are available, the choice of which to use must be made. Consequently, the engineer is seldom concerned only with the solution of a specific problem on a specific computer, and, even when computer experts are available, knowledge of the use of computers can significantly aid the practicing engineer.

A background of computer knowledge:

- Enables the engineer to communicate more effectively with the expert. It permits him to state his problem more clearly to the expert and to anticipate the potential pitfalls which the expert may encounter during the details of solution.

- Makes the engineer aware of the limitations of the available computers. This aids the engineer in making the choice of computer to use to solve his current problem and enables him to gear his method of solution so as to minimize the importance of the limitations. The engineer will also be aware of the versatility of the chosen computer and be able to decide the feasibility of relaxing some of his assumptions on an individual program.

- Perhaps most important, stimulates the engineer to attack problems which he could not previously consider. By being aware of the speed, precision, variety, versatility,

Analog Computers

and capacity of computers as well as of the techniques of application, the engineer will not lightly brush off a unique problem because of its complexity. Indeed, he will be stimulated to examine new approaches to problems and new solution techniques as they may arise in his day-to-day activities.

Comparison of Computers. Modern computers may be classified as either digital, analog, or hybrid computer:

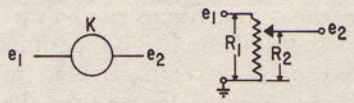
The digital computer has the characteristic that the arithmetic operations of addition, subtraction, multiplication and division of only discrete values can be accomplished very rapidly. Digital computers can be equipped with a large memory capacity which permits the storage of and the operation of an almost limitless number of discrete values. Moreover, the arithmetic operations can be performed to a high degree of precision which is generally fixed by the manufacturer on any particular machine. Thus the digital computer is in a sense the equivalent of a very reliable and extremely rapid desk calculator.

In addition to arithmetic operations the digital computer can be used to make logical decisions by comparing two discrete values and deciding whether one is equal to, less than or greater than the other. The result of the digital's facilities is a most versatile computational tool which when coupled with the numerical techniques for trial-and-error, integration, etc. permits the handling of a very wide class of problems. However, since only discrete values are used and calculations are done sequentially, considerable time may be required for problems in which a large number of discrete values must be used. Programing a digital computer is a very precise operation. Detailed instructions, generally in a very specialized language, must be given for every calculation. Digital computers find widespread application in data reduction, statistics, solution of algebraic equations, steady-state calculations, etc., where discrete values occur. Numerical technique and the accompanying versatility of the digital computer further extend its range of application.

The analog computer, in sharp contrast to the digital performs computations in parallel and continuously. The computations which can be performed include the arithmetic operations as well as continuous arbitrary function operations, such as squaring, taking the logarithm, exponentiation, etc. The most significant feature of the analog, however, is the capability of performing integration on a continuous basis. The analog computer excels

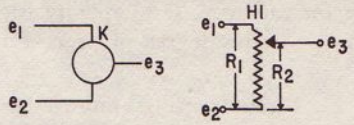
TABLE 1—Analog Computer Components

ATTENUATOR (GROUNDED)



$e_2 = Ke_1$
$K = R_2/R_1$
$K \leq 1$

ATTENUATOR (UNGROUNDED)

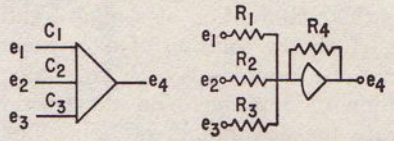


$e_3 = K(e_1 - e_2) + e_2$
$K = R_2/R_1$
$K \leq 1$

HIGH GAIN AMPLIFIER

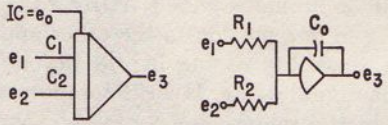
$e_2 = Ce_1$
$C \cong 10^8$

SUMMER



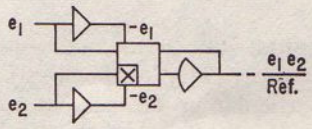
$C_1 = \frac{R_4}{R_1}, C_2 = \frac{R_4}{R_2}, C_3 = \frac{R_4}{R_3}$
$e_4 = -(C_1e_1 + C_2e_2 + C_3e_3)$

INTEGRATION

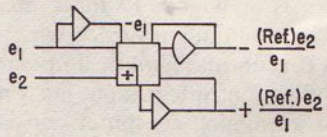


$e_3 = -\int\left[\frac{e_1}{R_1C_o} + \frac{e_2}{R_2C_o}\right]dt - IC$
$e_3 = -\int\left[C_1e_1 + C_2e_2\right]dt - e_o$

MULTIPLICATION

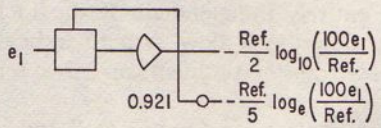


DIVISION

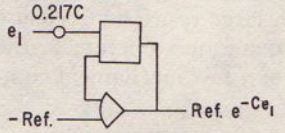


$e_1 \geq e_2$
$e_1 \neq o$

LOGARITHM



EXPONENTIAL FUNCTION



$o \leq e_1 \leq Ref.$

in the solution of differential equations regardless of whether they are linear or nonlinear. The solution from an analog computer is presented in continuous form which is analogous to the exact solution rather than in

terms of discrete values which can only approximate the exact solution. Furthermore, the computations can be carried out at practically any speed desired. This permits the rapid examination of a wide range of parameters in a space of time that can be significantly shorter than the fixed time of calculation on the digital. Analogs do not, however, have the capacity for memory, the capacity for a large number of operations, nor the degree of precision of the digital.

Programing an analog does not require knowledge of a highly specialized language as does the digital. The details of programing are generally quite similar to classical methods of solution with which the engineer is familiar. Analog computers find their greatest application in the solution of differential equations, such as occur in the dynamic analysis of processing systems, in which the amount of algebraic and logical operations required is rather limited.

A hybrid computer is the combination of a digital and an analog computer in which the solution of a problem is shared between the two. By containing both an analog and a digital, the solution of a problem on the hybrid computer can incorporate the advantages of both. The digital computer portion provides a large memory capacity and permits rapid logical and algebraic operations while the analog permits continuous integration. The transfer of information from one portion to the other and back again extends the versatility of the hybrid beyond that of the analog or the digital alone. Hybrid computers are finding application in the solution of complex problems where the time required for a digital solution is excessive and where analogs do not possess the capacity or the precision required for a solution.

Analog Computer Components. The term analog in analog computer is really a misnomer. That is, the electrical circuitry used to solve a particular problem is not an electrical analog in the conventional sense that electrical current is analogous to fluid flow, voltage is analogous to pressure, electrical capacitance is analogous to mass, etc. The electrical analog computer is actually a device which has been designed to perform certain mathematical operations, such as addition, multiplication, integration, etc. on specified voltages. The use of an analog computer consequently involves the specification and completion of the mathematical operations required to solve a particular set of equations and is entirely independent of the fact that the equations may describe a flow system, a heat exchange problem, a mass transfer problem, or a reactor system.

Since most of the analog computers being used today are transistorized, this discussion is restricted to this type of analog computer. This is not a large restriction because most of the older vacuum tube computers operate in the same fashion with the exception of a few mechanical components.

A list of the components found in a modern electronic analog computer is given in Table 1. The first column in Table 1 contains a symbolic representation of each component, the second column contains an electrical representation of each component and the third column shows the mathematical operation that each component performs. Although it is not shown in Table 1, one of the most important components of the computer is the constant voltage DC power supply. Depending upon the design of the computer, the power supply is usually either 100 or 10 volts. This DC voltage is called the reference or machine voltage and its stability will determine to a large degree the accuracy of the solution that one obtains.

The first element in Table 1 is an attenuator commonly called a pot—an abbreviation for potentiometer. Two types of pots are commonly found in an analog computer. One is referred to as a grounded pot and the other an ungrounded pot. The grounded pot enables the operator to obtain an output voltage which is some fraction between 0 and 1 of the input voltage. The ungrounded pot performs the function shown in Table 1 and is generally used in the construction of special function circuits. Attenuators are usually adjusted manually to set the value of a constant K. This value is determined by measuring the output voltage from an attenuator with the voltage measuring device built into the computer.

The next component listed in Table 1 is the high gain amplifier. The function of the high gain amplifier is to multiply an input voltage by a large constant, generally of the order of 10^8. The high gain amplifier is seldom used by itself, but usually forms an integral part of other common analog components. The high gain amplifier is generally designed so that it provides very stable operation if the magnitude of the output voltage does not exceed the computer reference voltage. If the output voltage of the high gain amplifier exceeds the machine voltage the operation of the computer will be non-linear. For this reason, the output of a high gain amplifier during operation should not exceed that of the computer reference voltage. Most computers have a built in alarm system which warns the operator when the output of an amplifier exceeds machine voltage. This restriction on the output voltage holds for every component in which a high gain amplifier appears.

The next component of interest in Table 1 is the summing circuit. As its name implies, the summing circuit adds two or more voltages and gives the resulting sum. The summing circuit consists of a high gain amplifier with a feedback resistor and three or more input resistors. The input resistors and the feedback resistor, in a summing circuit, are usually fixed not variable resistors. The input voltage to a summing circuit is multiplied by the negative ratio of the resistance of the feedback resistor to the resistance of the input resistor. For most computers the value of this ratio is usually 0.1, 1 or 10. Since a summer contains a high gain amplifier, the output from a summing circuit must not exceed the reference voltage.

One of the most important components of an analog computer is the integrator. The circuit for an integrator is essentially a high gain amplifier equipped with a capacitor in the feedback line and two or more input resistors. The output from an integrator is the negative sum of the initial condition and the integral with respect to computer operating time of fixed ratios of the input voltages as indicated in Table 1. Since the output of the integrator is time varying, there is a possibility that this value may be greater than machine voltage at sometime during the problem. Therefore, special precautions must be taken to insure that this does not happen. These precautions will be discussed later in the series.

The components discussed to this point are commonly

called linear components and the principle of superposition holds. The next group of components to be discussed are commonly called non-linear components.

Nonlinear mathematical operations, including multiplication, division, exponentiation, etc., are achieved through the use of specially designed components. Generally a particular component can be used to obtain both the designed operation and its inverse depending on the particular patching used. Thus, what is termed a multiplier can be used to achieve either multiplication or division. The details of patching and the electronic circuitry varies from one type of analog to another. The usually acceptable programing symbols are in Table 1.

A discussion of the internal construction of the nonlinear components will be covered in a later part. The purpose here is to present some of the more common nonlinear components and to examine their limitations and the precautions which must be exercised in their use.

When it is desired to generate a function such as $y = x^2$, where x is the input and y is the output, a nonlinear component is used to achieve this operation. Transistorized nonlinear components can be used to produce an output which is a series of straight-line approximations as indicated by the dotted lines in Fig. 1.

Generally, for economic reasons, sufficient line segments are not used to closely approximate the desired function over the entire input range. The best response is usually obtained when the input is near its maximum magnitude (that is, the machine reference voltage).

A high gain amplifier is an integral part of nonlinear components. Because of this, the output from a nonlinear component can not exceed the reference voltage. Numerical factors are included in nonlinear components so that when the input is near its maximum magnitude the output is also.

Because certain nonlinear operations such as squaring may be more easily obtained than other operations, mathematical relationships such as Equation (1) may form an integral part of a nonlinear component. Perhaps the most common of these is the relationship used in the quarter-square multiplier

$$xy = \frac{(x+y)^2 - (x-y)^2}{4} \qquad (1)$$

which is used to obtain a product because squaring is fairly easily achieved.

Due to the internal construction of nonlinear components, they will draw a varying amount of current depending on the value of the input. It is, therefore, very important that the output from a pot never be used as an input to a nonlinear device since a varying current produces a varying voltage distribution from the pot. Inputs to nonlinear components should always be outputs from high gain amplifiers contained in other analog components.

The size of an analog computer is usually gaged by the number of high gain amplifiers that it contains. Most commercial computers normally run from ten to several hundred high gain amplifiers, most of these high gain amplifiers are normally summers. A somewhat smaller number are integrators, which may also be used as summers. The remainder of the high gain amplifiers are usually integral parts of specialized nonlinear components.

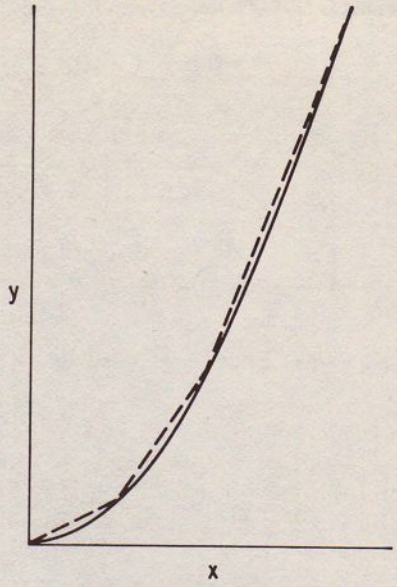


Fig. 1—The nonlinear relation shown by the solid line can be approximated by a series of linear relations.

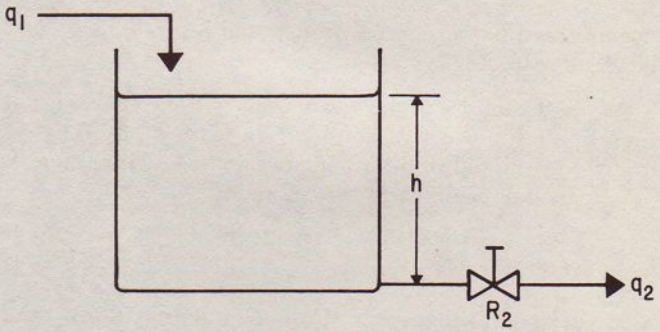


Fig. 2—An analog computer circuit is developed to compute the height of liquid in this tank.

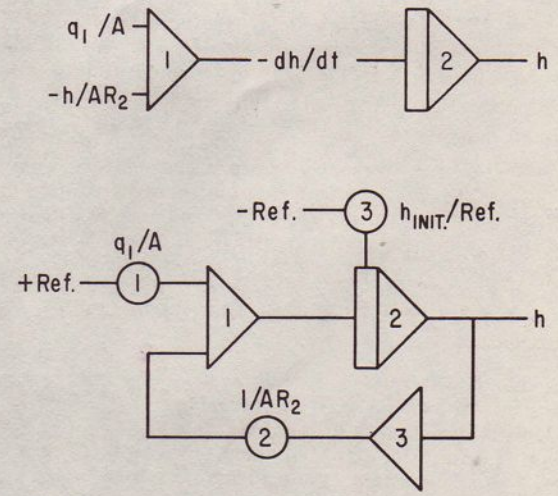


Fig. 3—Steps are combined to give the finished circuit.

The complexity of the problem which may be solved is very closely related to the number of high gain amplifiers available on the computer. A problem is usually solved on an analog computer by connecting the various com-

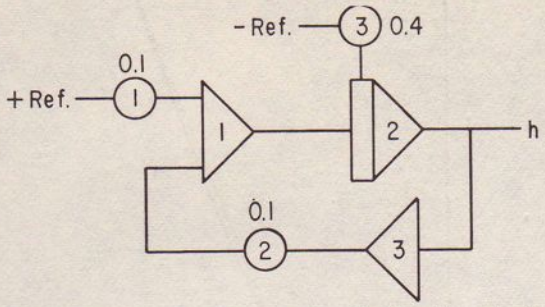


Fig. 4—Numerical values are added to the circuit.

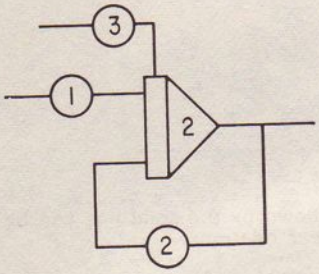


Fig. 5—The analog circuit is simplified.

ponents on a patch panel with external leads. This process is called patching.

As an example of how an analog computer circuit may be set up we will consider the case of the change in height of liquid in a tank having a cross-section area A.

A mass balance on this system yields:

$$\text{Accumulation} = \text{Input} - \text{Output} \tag{2}$$

$$A\,(dh/dt) = q_1 - q_2 \tag{3}$$

We will assume that q_1 is constant and that the rate of flow out of the tank is linearly related to the height of fluid in the tank through the flow line resistance R_2.

$$q_2 = h/R_2 \tag{4}$$

Then our relation becomes upon substitution and rearrangement

$$dh/dt = (q_1/A) - (h/AR_2) \tag{5}$$

The analog diagram may be constructed from the differential equation by applying the following steps:

Step 1. Write the differential equation with the highest ordered derivative by itself on the left side of the equation.

Step 2. Begin a diagram by showing the highest ordered derivative at the output of a summing amplifier.

Step 3. Perform as many integrations as are necessary to form all of the variables on the right side of the equation.

Step 4. Use the generated variables to form the original highest ordered derivative.

Step 5. Insert any forcing functions.

The sequential construction of the program is shown in Fig. 3.

The pot settings can be determined when the values of parameters in the problem are known. Assume that

$h_{initial} = 4$ ft. — Pot 1 $= q_1/10A = 0.1$
$A = 10$ sq. ft. — Pot 2 $= 1/AR_2 = 0.1$
$q_1 = 10$ cu. ft./min. — Pot 3 $= h_{initial}/10 = 0.4$
$R_2 = 1$ min./sq. ft.

The final diagram with pot settings is given in Fig. 4. Although the analog diagram appears satisfactory, it may indeed be unsatisfactory for one or both of two reasons.

- The output from a high gain amplifier may exceed the reference voltage and hence yield a faulty solution.
- The output from a high gain amplifier may be so small that inherent limitations of the analog results in a faulty solution or difficulty is encountered in monitoring the value.

From a knowledge of the nature of the numerical solution, the output, h, from amplifier 2 has an initial value of 4 v., a final value of 10 v., and asymptotically approaches the final value in an exponential fashion. Hence for a 100 v. or a 10 v. machine, amplifier 2 will not be overloaded. Similarly amplifier 1 with the output dh/dt will not be overloaded because it has an initial value of 0.6 and decreases montonically to 0. However, for a 100 v. machine, the values of h and dh/dt are quite small and for a 10 v. machine dh/dt is quite small. Since the circuit uses no nonlinear components, the solution will probably be satisfactory although monitoring may be difficult.

It should be noted that, if the value of the highest derivative does not need to be available for monitoring, step 2 above may be eliminated. In this case, the diagram shown in Fig. 5 is obtained for the chosen example with a net reduction in the number of analog components required for a solution.

In the next article of this series, techniques will be presented which permit an analog solution to be obtained when the aforementioned reasons prevent a direct solution. The process by which satisfactory computer variables are chosen so that the outputs from amplifiers are maintained near, but do not exceed the reference voltage, is termed amplitude scaling.

Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Electricity-10, Engineering-4, Programing-10, Simulation-4.

About the authors

THEODORE W. CADMAN is assistant professor *in the chemical engineering department of University of Maryland, College Park, Md. where he teaches graduate and undergraduate courses in process control, separation processes, mathematical modeling, and computer applications. Dr. Cadman also conducts research in process control, computer applications, and process modeling. Before receiving his Ph. D. degree in chemical engineering from Carnegie-Mellon University, he held short-term positions with St. Joseph Lead Co., Allied Chemical Corp., and Gulf Research and Development Co. He is a member of AAAS, ACS, ISA, AIChE, NSPE, Sigma Xi and Tau Beta Pi.*

THEODORE G. SMITH *is associate professor in the chemical engineering department of University of Maryland, College Park, Md. He conducts research and instructs undergraduate and graduate courses on polymer physics, reactor design, and mass transfer. Dr. Smith received B.S. and M.S. degrees in chemical engineering from Johns Hopkins University and a D.Sc. degree in chemical engineering from Washington University. He has worked in the plastics department of E. I. duPont de Nemours & Co. and is a member of ACS, AIChE, AAAS and Sigma XI.*

Learn About Analog Computers

PART 2: AMPLITUDE SCALING—The outputs from high gain amplifiers in an analog computer should be maintained near the machine's reference voltage, but not exceed it

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

FOR SATISFACTORY OPERATION, the output from a high gain amplifier contained in any analog component must not exceed the machine reference voltage. On the other hand, the outputs should be maintained near their maximum permissible values for the most satisfactory operation of most nonlinear components and for ease and precision of monitoring. Thus a method is needed to scale an analog problem so that the outputs from high gain amplifiers are maintained near, but do not exceed, the reference voltage. This process is termed amplitude scaling.

Amplitude Scaling. This is accomplished by expressing equations in a normalized form, wherein the normalized variables are to be the outputs from high gain amplifiers with magnitudes which approach, but do not exceed, the reference voltage. The analog solution is consequently the solution of the normalized form.

The process of amplitude scaling is perhaps most easily achieved if the reference voltage is considered to be $\pm$ 1 unit, even though it may be $\pm$ 10 volts or $\pm$ 100 volts. Scaling accomplished using this generalization is termed unity scaling and has several advantages over scaling in which the value of the reference voltage is implicitly used.

First, unity scaling permits an analog computer program to be obtained which can be used on any analog computer regardless of the value of the reference voltage. Second, the normalized variables which are outputs from

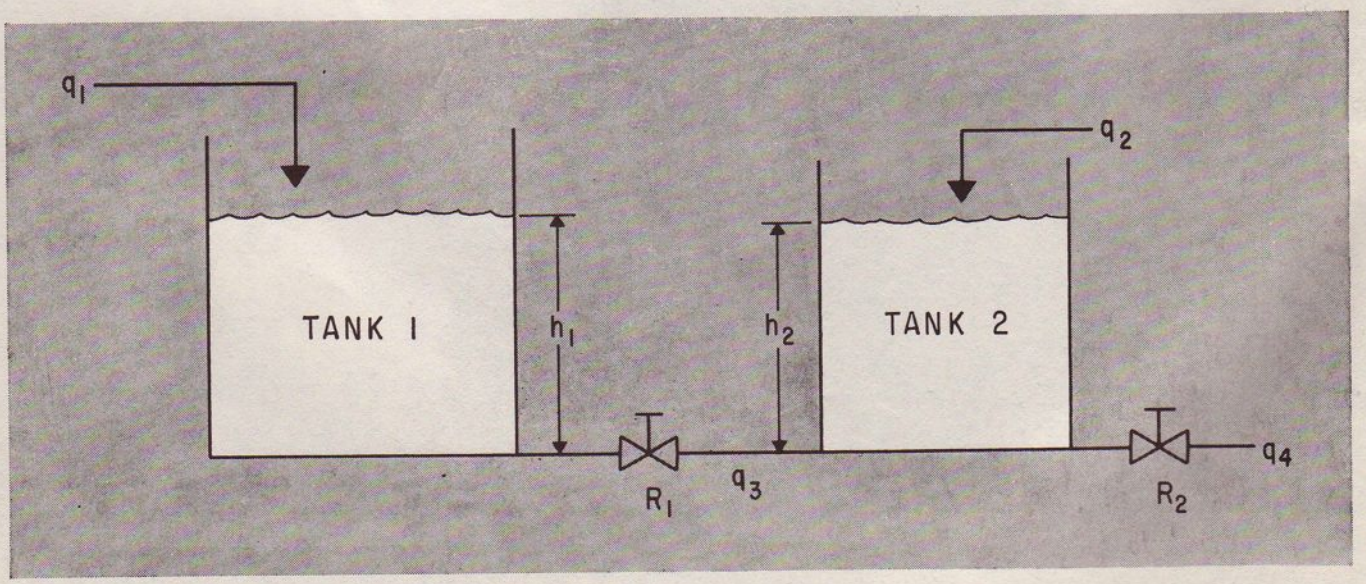


Fig. 6—Unity scaling is applied to an engineering problem before it is solved on the analog computer.

TABLE 2—Scaling Amplifier Outputs and Potentiometer Settings

Component	Output or Value	Estimated Maximum Value	Scaled Value
Amp 1	h_1	h_1^*	h_1/h_1^*
Amp 2	$-h_1$	h_1^*	$-h_1/h_1^*$
Amp 3	h_2	h_2^*	h_2/h_2^*
Amp 4	$-h_2$	h_2^*	$-h_2/h_2^*$
Pot 1	$h_1(0)$	—	$h_1(0)/h_1^*$
Pot 2	q_1/A_1	—	$q_1/A_1h_1^*$
Pot 3	$1/A_1R_1$	—	$1/A_1R_1$
Pot 4	$h_2(0)$	—	$h_2(0)/h_2^*$
Pot 5	q_2/A_2	—	$q_2/A_2h_2^*$
Pot 6	$\frac{1}{A_2}\left[\frac{1}{R_1}+\frac{1}{R_2}\right]$	—	$\frac{1}{A_2}\left[\frac{1}{R_1}+\frac{1}{R_2}\right]$
Pot 7	$\frac{1}{A_1R_1}$	—	$\left(\frac{1}{A_1R_1}\right)\left(\frac{h_2^*}{h_1^*}\right)$
Pot 8	$\frac{1}{A_2R_1}$	—	$\left(\frac{1}{A_2R_1}\right)\left(\frac{h_1^*}{h_2^*}\right)$

high gain amplifiers are simply the value of the original variable divided by the maximum magnitude of the original variable. Third, and perhaps most significant, the process of scaling non-linear components is greatly simplified.

For example, if x and y are the inputs to a multiplier, the output expressed in volts for a 10-volt machine is $xy/10$. For a 100-volt machine, the output is $xy/100$ expressed in volts. But in terms of unity scaling it is xy regardless of the machine reference voltage. The simplification encountered for other nonlinear components is similar.

Unity scaling can be achieved by mathematical manipulation of the original equations before any programing is attempted. However, scaling is frequently more easily achieved and more clearly visualized if it is done after some preliminary programing. In particular, the following seven steps have been found to be a most convenient method of achieving unity scaling.

Step 1. Write down the differential and/or algebraic equations which describe the problem to be solved.

Step 2. Sketch a preliminary analog diagram, neglecting the problem of scaling, which connects all of the required analog components together. Clearly mark the output from each amplifier and the value of each pot as it appears in the problem equations.

Step 3. Make a list of the variables that are outputs from amplifiers. These are the variables which must be amplitude scaled. Also list the values of the pots. These may be changed as a result of the amplitude scaling process.

Step 4. Estimate the maximum magnitude of each of the variables which are outputs from amplifiers.

Step 5. Form the normalized or computer variables for the outputs from the amplifiers by dividing the problem variable by its estimated maximum magnitude. Note these on the list made in Step 3.

Step 6. Insert additional pots in the amplifier input lines and/or modify the values of the pots which were needed to complete Step 2 so as to compensate for the change in scale from one amplifier to the next in series. Again modify the list completed in Step 3.

Step 7. Sketch the completed analog diagram using the normalized variables and the new pot settings. Note that this step is easily accomplished by referring to the preliminary sketch and to the list which has been completed.

If the programer closely follows these rules and systematically lists each variable and the pot settings during the scaling process, scaling can be readily achieved, errors easily detected, and any further scaling rapidly completed. In addition, a completely general analog computer program can be obtained by symbolically retaining the maximum magnitude of the problem variables rather than computing their numerical values. The following example illustrates the use of this seven-step procedure for achieving unity scaling.

An Example. Consider a hydraulic transient problem involving two tanks as illustrated in Fig. 6.

Assume that the cross-sectional area of tank 1 is A_1 and that of tank 2 is A_2. Further assume that the volumetric flow of fluid through the valves is linearly related to the difference in liquid level across the valves. Given initial values for h_1 and h_2, it is desired to determine the variation in these levels with time. The equations which describe this system are given as follows:

For tank 1

$$A_1\,(dh_1/dt) = q_1 - q_3 \tag{6}$$

For tank 2

$$A_2\,(dh_2/dt) = q_2 + q_3 - q_4 \tag{7}$$

For resistance 1

$$q_3 = (h_1 - h_2)/R_1 \tag{8}$$

For resistance 2

$$q_4 = h_2/R_2 \tag{9}$$

Or

$$\frac{dh_1}{dt} = \frac{q_1}{A_1} - \frac{h_1}{A_1R_1} + \frac{h_2}{A_1R_1} \tag{10}$$

And

$$\frac{dh_2}{dt} = \frac{q_2}{A_2} + \frac{h_1}{A_2R_1} - \frac{h_2}{A_2R_1} - \frac{h_2}{A_2R_2} \tag{11}$$

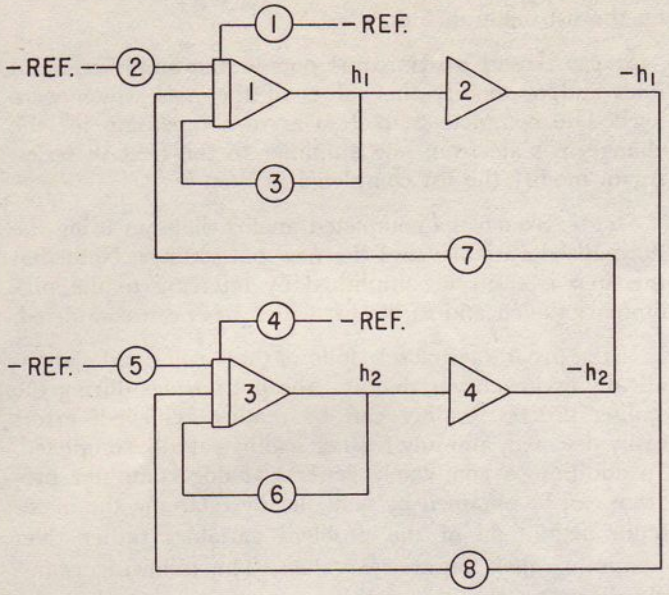


Fig. 7—This analog circuit represents the variables in the two-tank example problem.

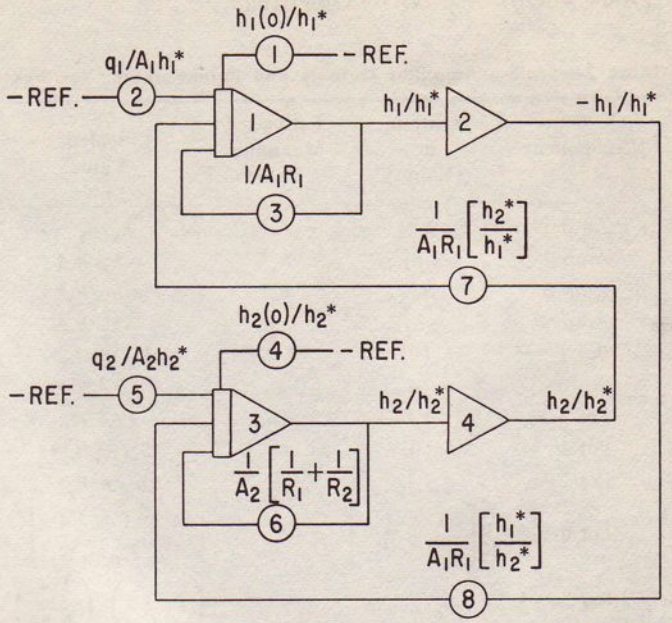


Fig. 8—Amplitude scaling determines the proper setting for the amplifiers and potentiometers.

with initial conditions of h_1 (0) and h_2 (0) respectively.

Assuming that q_1 and q_2 are positive constants, a preliminary analog diagram for solving Equations (10) and (11) for h_1 and h_2 versus time can be drawn. Prior to specification of numerical values, the diagram in Fig. 7 and the list of variables which are outputs from amplifiers and the pot settings in Table 2 are obtained.

Letting a superscript* indicate the maximum value of the output from the amplifiers as indicated in Table 2, the process of unity scaling can be symbolically carried to completion. The results obtained are given in the final column of Table 2. The output from each amplifier becomes the value of the problem variable divided by its maximum value and some of the values of the pots are changed to compensate in the change of scale from one amplifier to the next. The latter changes perhaps become more evident if the final analog diagram given in Fig. 8 is considered.

In readjusting pot values following the scaling of outputs from amplifiers, four cases arise:

Case 1. The pot value must be divided by a maximum expected value. Examples are pots 1, 2, 4 and 5 wherein the maximum value is included so that the inputs to the amplifier contain the same scale factor as do the outputs.

Case 2. The pot value remains unchanged. Examples are pots 3 and 6 which remain unchanged because the input to the pot contains the same scale factor as is desired in the output.

Case 3. The pot value is changed by a ratio of expected maximum values. An example is pot 7 which is changed by h_2^*/h_1^* because the input to the pot contains the factor $1/h_2^*$ whereas the output must contain the factor $1/h_1^*$. Pot 8 is another similar example.

Case 4. Additional pots must be incorporated into the circuit. This would arise, for example, had $h_1 - h_2$ been desired. In this case inputs of $-h_1/h_1^*$ and h_2/h_2^* would have been available and an output of $(h_1 - h_2)/(h_1 - h_2)^*$, where $(h_1 - h_2)^* \neq h_1^*$ or h_2^*, would have been the scaled output from the summer. Additional pots, not found necessary in drawing a preliminary diagram, would have been needed in the input lines to compensate for the change in scale factors.

Choosing the numerical values given in Table 3, a numerical solution can be obtained on the analog computer once h_1^* and h_2^* are estimated. These may be estimated by calculating the final values of h_1 and h_2 at equilibrium, noting that these values are larger than the initial conditions, and conservatively choosing maximums which are about twice the steady state values to account for the possibility of oscillation before the final values are attained. The numerical values of the variables and the pot settings for this numerical example are given in Table 4.

It should be noted that the analog diagram for the foregoing example does not include physical constraints which may be imposed on the actual situation. Consequently, for certain parameter values, the analog solu-

TABLE 3—Parameters Used for the Example Problem

Physical Parameter	Numerical Value
A_1	2 sq. ft.
A_2	4 sq. ft.
q_1	8 cu. ft./min.
q_2	6 cu. ft./min.
R_1	2 min./sq. ft.
R_2	1 min./sq. ft.
$h_1(0)$	15 ft.
$h_2(0)$	10 ft.
h_1 at equilibrium	30 ft.
$h_1^* \cong 60$ ft.	
h_2 at equilibrium	14 ft.
$h_2^* \cong 30$ ft.	

TABLE 4—Settings Used for the Example Problem

Component	Numerical Value
Amp 1	$h_1/60$
Amp 2	$-h_1/60$
Amp 3	$h_2/30$
Amp 4	$-h_2/30$
Pot 1	0.2500
Pot 2 (through gain of 0.1)	0.6667
Pot 3	0.2500
Pot 4	0.3333
Pot 5 (through gain of 0.1)	0.5000
Pot 6	0.3750
Pot 7	0.1250
Pot 8	0.2500

tion will predict negative values of h_1 and/or h_2. In a similar vein, values of h_1 and/or h_2 may be obtained which would represent an overflowing of the tanks. The manner in which such constraints can be built into an analog program will be discussed in a later article.

The maximum magnitudes for this example were estimated from a knowledge of the behavior of the physical situation. In other cases, one must resort to other techniques for estimating maximum and minimum values. One method is to obtain these values by a trial computer run. Another technique is that discussed by Jackson[1] which is called the equal-coefficient rule. For differential equations of second order or higher, this rule may frequently be used to estimate the maximum magnitude of the dependent variable and of its derivatives. Given an n-th order differential equation of the form

$$a_N \frac{d^N y}{dt^N} + a_{N-1} \frac{d^{N-1} y}{dt^{N-1}} + \ldots + a_1 \frac{dy}{dt} + a_o y = f(t) \qquad (12)$$

where $f(t)$ is the forcing function, the maximum magnitude of y,

$$\frac{dy}{dt}, \ldots, \frac{d^N y}{dt^N}$$

are estimated as follows:

Replace $f(t)$ by its maximum magnitude, denoted by A. The dependent variable and its derivatives are multiplied and divided by their maximum magnitudes to yield

$$a_N \left[\frac{d^N y}{dt^N}\right]^* \left[\frac{\frac{d^N y}{dt^N}}{\frac{d^N y^*}{dt^N}}\right] + \ldots + a_o [y]^* \left[\frac{y}{[y]^*}\right] = A \qquad (13)$$

Having numerical values for A, a_o, a_1, . . . , a_N, the maximum magnitudes are estimated by assuming

$$a_N \left[\frac{d^N y}{dt^N}\right]^* = a_{N-1} \left[\frac{d^{N-1} y}{dt^{N-1}}\right]^* = \ldots = a_1 \left[\frac{dy}{dt}\right]^* = A \qquad (14)$$

and

$$a_o [y]^* = 2A. \qquad (15)$$

Three precautions should be exercised when using this rule.

1. The estimated maximum magnitudes must either continually decrease or increase as the derivatives are considered in order. If this is not the case, the magnitudes should be estimated in another manner.

2. The rule assumes zero initial conditions. For a problem with non-zero initial conditions, the estimated magnitudes should be compared with the initial conditions and the larger of the two in each case used for scaling purposes.

3. The rule assumes that the problem has a stable solution. If the programer is doubtful of his problem's stability, the stability is easily examined by using the Routh criterion.

As an example of the equal-coefficient rule consider the hydraulic transient problem and the determination of h_1*. Combining Equations (10) and (11), eliminating the dependence of h_1 on h_2, the following equation is obtained.

$$\frac{d^2 h_1}{dt^2} + \left[\frac{1}{A_1 R_1} + \frac{1}{A_2 R_1} + \frac{1}{A_2 R_2}\right] \frac{dh_1}{dt} + \frac{1}{A_1 R_1 A_2 R_2} h_1 = \frac{1}{A_1 R_1 A_2} q_2 + \frac{1}{A_1 R_2} \left[\frac{1}{R_1} + \frac{1}{R_2}\right] q_1 \qquad (16)$$

Using the equal coefficient rule and evaluating using the numerical values in Table 3:

$$[h_1]^* = 2\,(q_2 R_2 + q_1 R_2 + q_1 R_1) = 60 \qquad (17)$$

$$\left[\frac{dh_1}{dt}\right]^* = \frac{\frac{q_2}{A_1 R_1 A_2} + \frac{q_1}{A_1 A_2 R_1} + \frac{q_1}{A_1 A_2 R_2}}{\left[\frac{1}{A_1 R_1} + \frac{1}{A_2 R_1} + \frac{1}{A_2 R_2}\right]} = 3 \qquad (18)$$

$$\left[\frac{d^2 h_1}{dt^2}\right]^* = \frac{q_2}{A_1 R_1 A_2} + \frac{q_1}{A_1 A_2 R_1} + \frac{q_1}{A_1 A_2 R_2} = 1.875 \qquad (19)$$

The magnitudes decrease as the order of the derivative increases, a check of the initial conditions indicate that they are less than the estimates, and the solution is known to be stable. Hence the indicated values may be used as estimates for the maximum magnitudes.

In many problems the computer operating time, in addition to the output voltage from amplifiers, must be scaled. If the physical problem takes hours or days for completion, the analog solution must be speeded up both for convenience and precision. Likewise if the physical problem is completed very rapidly, the analog solution must be slowed down. In the next article of this series, procedures which enable time scaling to be achieved will be presented.

LITERATURE CITED

[1] Jackson, A. S., Analog Computation, McGraw-Hill Book Co. Inc., New York, 1960, pp. 101.

Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Electricity-10, Engineering-4, Programing-10, Simulation-4.

Learn About Analog Computers

PART 3: TIME SCALING—When the actual time for a process change is very short or very long, time scaling is used to make it better suited to analog computer speed

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

THERE ARE A LARGE NUMBER of physical problems in which the variable of interest (the dependent variable) changes either very rapidly or very slowly. Reaction kinetics problems in which the concentrations of some of the components change in fractions of seconds are often found in the hydrocarbon processing industry. The combustion of a hydrocarbon is an example of a problem in which it may be very difficult to determine the reaction rate or follow concentration with time by using a computer running at the same speed as the problem (real time). For such a problem, voltage changes occurring in the computer may be so rapid that some of the computational elements may not accurately follow the changes because of the limited precision of analog components for high frequency voltage fluctuations.

Problems which require a great deal of time to exhibit the phenomena of interest are also important to practicing engineers. The study of the dynamics of large scale process equipment falls in this category. Because of the excessive amount of computer time which may be involved and the effect of noise and amplifier drift on a solution's validity, the analog simulation of such processes in real time may not be satisfactory. The ability to either speed up or slow down the solution of analog simulation is one of the important characteristics of analog computation. The process of scaling the independent variable is called time scaling.

Recording The Solution. Quite often it is desirable to record the results of an analog computation. The problem frequencies must then be adjusted by time scaling so that the recording device can follow the results. There are in general three types of recording devices commonly used to record analog results; cathode-ray oscilloscopes, galvanometer-type recorders, and servo-motor driven recorders. Cathode-ray oscilloscopes with ac and dc amplifiers can be used for the entire frequency range encountered in analog computations, while galvanometer-type recorders should not normally be used at frequencies greater than 60 cycles/sec., and servo-motor driven recorders, such as X-Y recorders, are restricted to frequencies less than about 2 cycles/sec.

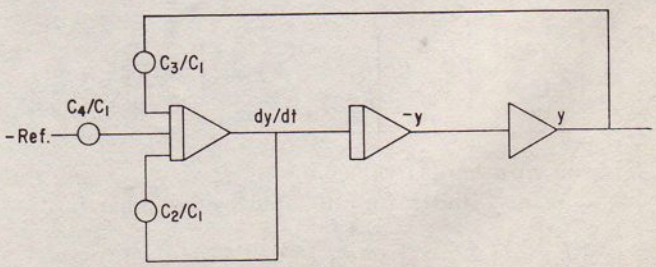


Fig. 9—The differential equation as depicted by an unscaled circuit.

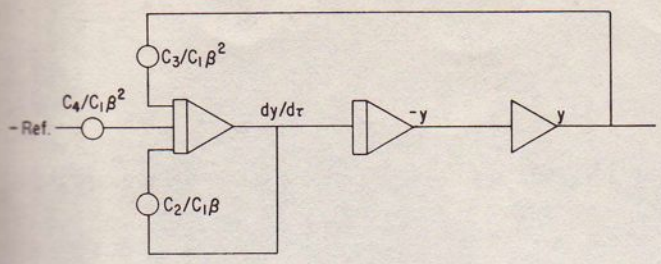


Fig. 10—The circuit after time scaling is considered.

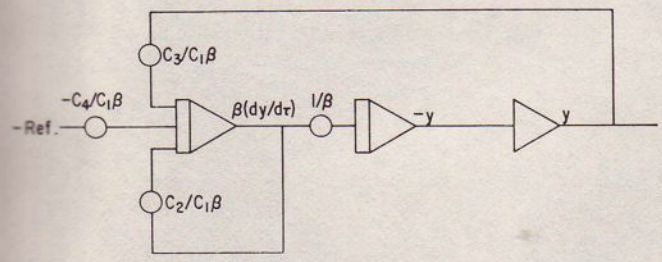


Fig. 11—The time-scaled circuit may be rearranged.

Solution Oscillation Frequency. It is often helpful before attempting to program a problem on the analog computer to make an estimate of the frequency of oscillation of the solution so that a decision can be made as to whether the problem will need time scaling. The frequency of oscillation of the solution of simple differential equations can be readily estimated. For a first-order differential equation the reciprocal of the time constant is a rough estimate of the problem frequency. For example for:

$$C_1\,(dy/d\Theta) + C_2 y = C_3 x$$

$$T = 1/\omega = C_1/C_2$$

For this type of equation the solution of the problem will have progressed to within 63 percent of its final value within a period of time equal to the time constant T.

TABLE 5—An Example Problem

Component	Output	Max Value	Scaled Value
Amp 1	a	a_1	a/a_1
Amp 3	b	b_1	b/b_1
Amp 5	c	c_1	c/c_1
Pot 9	1	—	a_1/c_1
Pot 10	1	—	b_1/c_1
Pot 1	$a(0)$	a_1	$a(0)/a_1$
Pot 2	k_2	—	$(b_1/a_1)k_2$
Pot 3	k_1	—	k_1
Pot 4	0	—	0
Pot 5	k_1	—	$(a_1/b_1)k_1$
Pot 6	k_4	—	$(c_1/b_1)k_4$
Pot 7	$k_2 + k_3$	—	$(k_2 + k_3)$
Pot 8	n	n	n/c_1

For a second order differential equation of the form $C_1(d^2y/d\Theta^2) + C_2(dy/d\Theta) + C_3 y = C_4 x$; the natural frequency of the equation is $\omega_n = (C_3/C_1)^{1/2}$. The natural frequency, for a third order differential equation of the form $C_1(d^3y/d\Theta^3) + C_2(d^2y/d\Theta^2) + C_3(dy/d\Theta) + C_4 y = C_5 x$; is $\omega_n = (C_4/C_2)^{1/2}$. There are no simple approximations for determining the natural frequency of differential equations higher than third order. However, if the coefficients of the low-order terms of an equation are quite different from the coefficients of the high-order terms, a change of time scale will probably be required.

Differential Equations. When it is found that a change in time scale is desirable for a differential equation, a substitution must be made. If t is the real time variable, and τ is the computer time variable, the time for solution of the equation may be changed by substituting τ/β for t. If the solution is to be slowed down, $\beta > 1$; and if the solution is to be speeded up, $\beta < 1$. As an example we will change the time scale of the following equation by the factor β.

$$C_1(d^2y/dt^2) + C_2(dy/dt) + C_3 y = C_4 \qquad (20)$$

We substitute τ/β for t.

$$C_1\,[d/d(\tau/\beta)]\;[dy/d(\tau/\beta)] + C_2\,[dy/d(\tau/\beta)] + C_3 y = C_4$$

$$C_1\beta^2\,(d^2y/d\tau^2) + C_2\beta\,(dy/d\tau) + C_3 y = C_4 \qquad (21)$$

The undamped natural frequency for the unscaled equation is $(C_3/C_1)^{1/2}$ and for the time scaled equation it is $(C_3/(C_1\beta^2))^{1/2}$ or $(1/\beta)(C_3/C_1)^{1/2}$. Thus, the rate at which the solution is obtained has been changed by the factor $1/\beta$. It should be noted that β appears only in terms containing time derivatives and in the forcing function if it is time dependent.

It is of interest here to see how time scaling of the last relation modifies the computer circuit. A circuit for the unscaled Equation (20) is shown in Fig. 9. The time-scaled Equation (21) is shown in Fig. 10. The circuit may then be rearranged to give Fig. 11.

The form of Fig. 11 is particularly significant. It should be noted that the circuit is identical to the unscaled circuit of Fig. 9 with the exception that the input to each integrator is scaled by the factor $1/\beta$, the time scaling factor. Thus, the process of time scaling is much simpler than magnitude scaling (See Part 2) and in general in-

TABLE 6—How Circuit Components Are Scaled

Physical Parameter	Numerical Value	Scaled Value
Amp 1	[0.01a]	[0.01a]
Amp 2	[0.01b]	[0.01b]
Amp 5	[0.01c]	[0.01c]
Pot 1	1.00	1.00
Pot 2	50	0.50
Pot 3	100	1.00
Pot 4	0	0
Pot 5	100	1.00
Pot 6	75	0.75
Pot 7	200	2.00
Pot 8	1.00	1.00

volves changing ...ator by the factor $1/\beta$.

Methods of Time Scaling. There are two general methods of time scaling a problem. One method involves the formal time scaling of the differential equations at the same time that the equations are magnitude scaled. The second method involves magnitude scaling the problem and subsequently time scaling the problem by changing each of the input pots to integrators by $1/\beta$ after the problem has been patched. The second method is usually recommended because it permits the magnitude and time scaling processes to be done separately and therefore is not as confusing as the first method.

If after magnitude scaling, it is found that pots to integrators have settings of less than 0.1 or greater than 30, time scaling will usually be necessary. In some cases after amplitude scaling a situation such as that shown in Fig. 12 arises, with the magnitude of other pots to integrators about 0.0001 and all other pots in the circuit between 0.1 and 30. A time scale factor of β about 0.0005 is required, for all the integrators except the integrator shown in the figure above. The pots which are inputs to the summer may be scaled by $1/\beta$ instead of the input pot to the integrator. The output from the integrator is then time scaled but the output of the summer contains a $1/\beta$ factor.

The steps in time scaling can be reduced in many cases to:

Step 1. Changing the input of each integrator by $1/\beta$. $\beta > 1$ slows the solution down, $\beta < 1$ speeds the problem up.

Step 2. Choose β such that pot settings are between 0.1 and 30. Settings close to 1 are the most desired.

Step 3. Change β by a factor of 0.5 or 2 and replot the solution. If the curves are identical the problem is properly time scaled.

Rate of Integration. It is of interest to see how integration is slowed down or speeded up by changing the magnitude of an input signal to an integrator. A simple integration circuit is given in Fig. 13.
The output voltage is

$$e_o = -(1/RC)\int_0^t e_i\,dt + E_o$$

where E_o is the value of e_o at $t = 0$. The group $1/RC$ has the units of reciprocal time and along with the voltage e_i controls the rate at which e_o changes. In many computers $R = 10^6$ ohms and $C = 10^{-6}$ farads so that RC normally equals 1 second. There is also usually a means for changing the capacitor C by a factor of 10. The resistance R can of course be varied by inserting a pot in the input of an integrator. If RC is one second then the rate at which the output voltage of the integrator changes is just e_i. Now if RC is greater than one second corresponding to $\beta > 1$ the rate of change of e_o will be decreased, and if RC is less than one second corresponding to $\beta < 1$ the rate of change of e_o will increase.

An Example Problem. To illustrate the rules for time scaling we consider a constant volume, isothermal, gaseous reaction represented by the following relation.

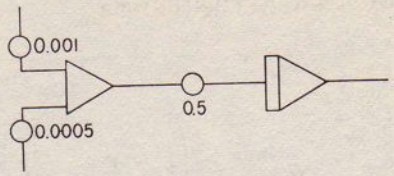


Fig. 12—Only one of these pots are within the proper range.

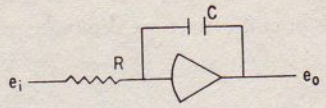


Fig. 13—A simple integration circuit.

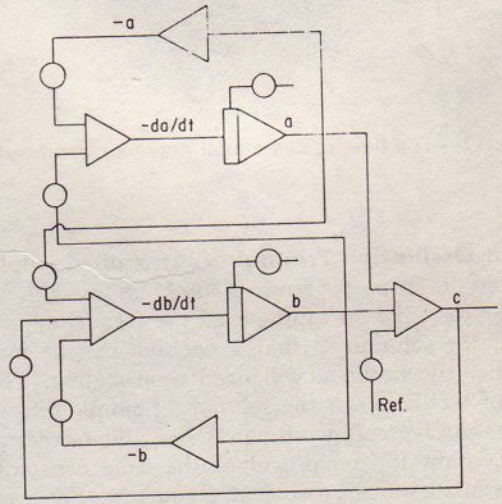


Fig. 14—A circuit to solve the simultaneous equations.

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B \underset{k_4}{\overset{k_3}{\rightleftarrows}} C \qquad (22)$$

We will let a, b and c be the moles of A, B and C respectively, at any instant and k_1, k_2, k_3 and k_4 will be the rate constants expressed in reciprocal seconds for the various reactions shown in Equation (22).

The rate equations for the change of A, B and C with time are:

$$da/dt = -k_1 a + k_2 b \qquad (23)$$

$$db/dt = k_1 a - k_2 b - k_3 b + k_4 c \qquad (24)$$

$$dc/dt = k_3 b - k_4 c \qquad (25)$$

Another relation expressing the fact that the total number of moles n remains constant may be written although the relation does not introduce any information not contained in Equations (23), (24) and (25).

$$n = a + b + c \qquad (26)$$

If it is desired to follow the concentration changes of a, b and c with time, Equations (23), (24) and (26)

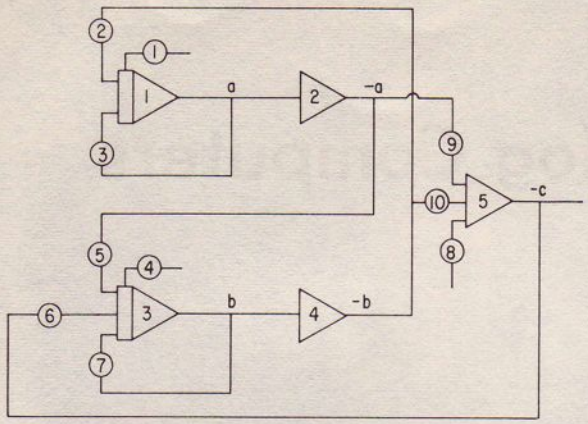


Fig. 15—Summation can be performed in the integrators.

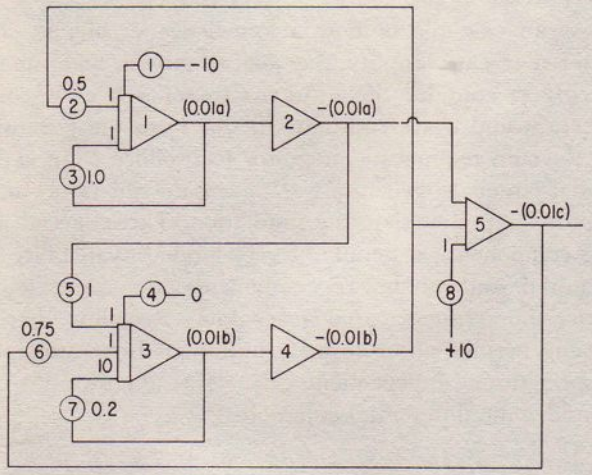


Fig. 16—After amplitude and time scaling is applied.

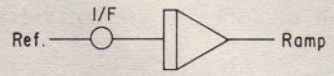


Fig. 17—The time signal for the plotter is also scaled.

must be programed on the computer. The physical parameters chosen for illustration are given below.

$$k_1 = 100 \text{ sec}^{-1}$$
$$k_2 = 50 \text{ sec}^{-1}$$
$$k_3 = 150 \text{ sec}^{-1}$$
$$k_4 = 75 \text{ sec}^{-1}$$
$$a(0) = 100$$
$$b(0) = 0$$
$$c(0) = 0$$

We may now draw a preliminary computer circuit to solve these simultaneous equations as shown in Fig. 14.

This circuit may be simplified if we are not interested in obtaining da/dt or db/dt by performing the summation in the integrator. The revised circuit is shown in Fig. 15.

We now must scale Equations (23), (24) and (26). We will first magnitude scale and then time scale if necessary. It should be noted that a, b and c each must be magnitude scaled. The reactions are constrained and the initial conditions are such that the concentrations of A, B or C at any time may not exceed 100, the initial concentration of A.

The numerical values of each of the physical parameters may now be determined, assuming $a_1 = b_1 = c_1 = 100$. These are shown in the second column of Table 6.

The large gains on the integrators indicate that the system is a naturally fast one and must be time-scaled to slow it down. Since it is desirable to have pot settings beween about 30 and 0.1 we choose the time scale factor β to be 100.

Only pots that are on inputs (but not initial condition pots) to integrators must be scaled. Pots 2, 3, 5, 6 and 7 are adjusted by dividing the numerical value found from magnitude scaling by $\beta = 100$. The magnitude and time scaled values are listed in the third column of Table 6. The final computer circuit (amplitude and time scaled) is given in Fig. 16.

If it is desirable to plot the concentration of A, B, or C as a function of time on an X-Y plotter, a time signal for the plotter may be supplied by the analog computer. It is important to note that the analog circuit for the time signal (a ramp increase in voltage) should be scaled just as the problem. Suppose the solution is to be recorded in F seconds of computer operating time. The scaled circuit for the ramp signal is shown in Fig. 17.

The ramp units are equal to τ/F, where τ is the computer operating time, and thus will reach a maximum value equal to that of the reference voltage after F seconds of operating time.

In order to obtain the relationship between actual problem time t and the length of computer chart travel, two additional factors must be known: the time scale factor, $\beta = \tau/t$; and the recorder chart setting, G, volts per inch. The relationship is developed in the following manner:

Ramp = (Ref. Volts) τ/F, volts

Since $\tau = \beta t$,

Volts Developed = (Ref. Volts) $\beta t/F$

Volts Developed per Unit Actual Problem Time = (Ref. Volts) β/F

Using a recorder chart setting of G volts per inch,

Inches of Chart Swept by Ramp per Unit Actual Problem Time = (Ref. Volts) $\beta/(FG)$

As an example, if the solution is to be recorded for 10 seconds of computer operating time using a 10-volt machine, a recorder set at 1 volt/inch, and $\beta = 10$, gives 10 inches of chart = 1 unit actual problem time.

In many problems it is desirable to check to see if the chosen time scale is such that the solution is recorded accurately. This may be done by plotting the solution for the chosen time scale and then replot the solution for a different value of β. If the two solutions do not overlap the chosen time scale is a poor one and some of the solution information is being lost. New time scales should be chosen until two different values of β give solutions which coincide.

Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Electricity-10, Engineering-4, Programing-10, Simulation-4.

Learn About Analog Computers

PART 4: PROCESS SIMULATION–There is a usual sequence of steps which are required to complete an analog simulation

Theodore G. Smith and **Theodore W. Cadman**
University of Maryland, College Park, Md.

NOW WE SHALL DISCUSS the steps before patching, standard modes of analog operation, suggestions to facilitate accurate patching, and the operation of the analog together with the interpretation of results. The aspects of analog simulation are considered first in general terms and then as they apply to the simulation of the vapor-phase dehydrogenation of benzene in a homogenous, isothermal, flow reactor.

Steps Before Patching. In order to adequately prepare a problem for analog simulation, four principal steps should be carried to as near completion as possible before patching is undertaken. These steps are:

1. The development of the mathematical model for the system to be simulated
2. The preparation of an analog diagram exclusive of scaling
3. Amplitude scaling of the analog circuit, and
4. Time scaling of the analog circuit.

Although the first step is an obvious one, it is perhaps the most crucial for all subsequent aspects of the simulation largely depend upon the results of this first step. Apart from the difficulties, familiar to all engineers, encountered in mathematically describing a physical system, several mathematically equivalent forms can frequently be obtained for a given system. Since the relative ease of incorporating the various forms as well as the accuracy of the analog simulation may differ, it is wise to capitalize on the advantages of the analog and to minimize potential analog trouble spots while developing the model. This is perhaps more readily done by considering Step 1 and Step 2 simultaneously even if the latter step is only partially completed. Further consideration will be given to analog trouble spots in the next article of this series.

As an example of how a knowledge of analog characteristics can simplify the analog circuit and inhance accuracy, consider the generation of $y = e^{-\alpha t} \cos \omega t$ where α and ω are constant. In this form the generation of y would require an integrator to produce t, an exponential circuit to generate $e^{-\alpha t}$, a cosine generator, and a multiplier to complete the simulation. Three special analog components, generally of very limited availability, are required and nonlinear components are connected in series thus reducing analog accuracy. Recalling that the analog permits accurate and continuous integration with respect to one independent variable at almost any speed, consider the differential equation

$$d^2y/dt^2 + 2\alpha\, dy/dt + \alpha^2 + \omega^2 = 0,$$

with initial conditions of 1 and $-\alpha$ for y *and* dy/dt respectively. Its solution $y = e^{-\alpha t} \cos \omega t$ is seen to result in a simpler and more accurate analog circuit. Two integrators and an inverter are the only major components required.

Frequently of equal or greater concern than ease and accuracy in simulation is flexibility in the analog circuit because the analog can be an excellent tool for rapidly examining the effect of changes in process parameters and characteristics. Flexibility arises from retaining a one-to-one correspondence between the physical variables and the analog variables. Thus although an electronic analog computer circuit is not an electrical analog of the physical system in the conventional sense (since all physical variables are represented by analog voltages), it should be considered as more than a group of components designed to perform specified mathematical operations. An analog circuit should represent flexible simulation of the physical system. Such a circuit, which is called an analog by many, is obtainable through the one-to-one correspondence of physical and computer variables. The degree of flexibility to be built in an analog circuit is, of course, dependent upon the modifications which may be made and this should be seriously considered during problem definition.

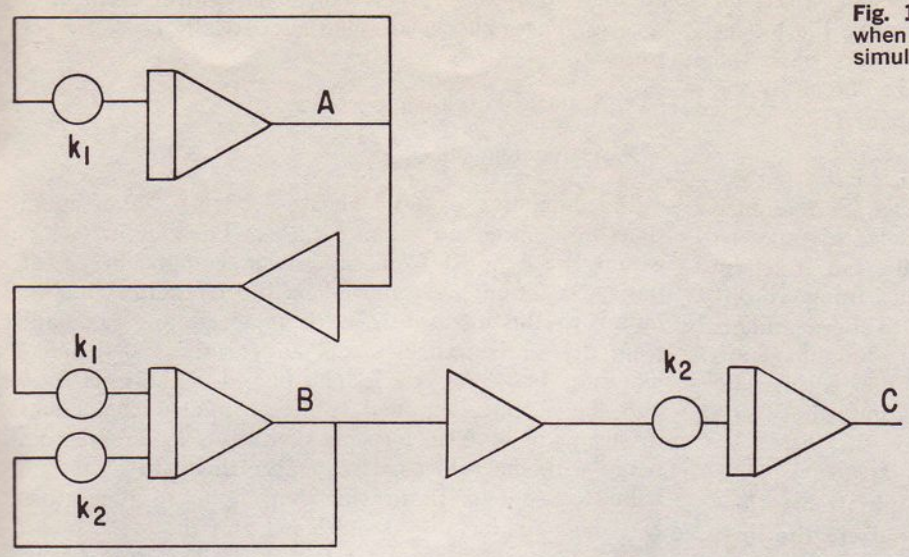


Fig. 18—Flexibility must be considered when setting up an analog computer simulation circuit.

Fig. 19—Although this circuit is simpler, it is not as flexible to changes.

As a simple example of flexibility, consider the consecutive reaction steps described by

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

and

$$dA/dt = -k_1 A \quad (27)$$

$$dB/dt = k_1 A - k_2 B \quad (28)$$

$$dC/dt = k_2 B \quad (29)$$

A preliminary analog circuit based on these equations is given in Fig. 18. An alternate, but equivalent, solution can be obtained by eliminating the dependent composition B to yield:

$$dA/dt = -k_1 A \quad (30)$$

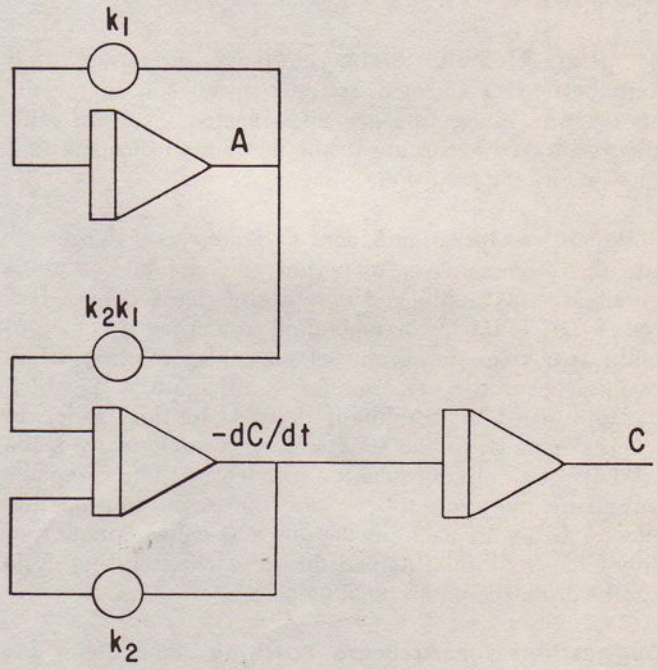
$$d^2C/dt^2 + k_2 (dC/dt) - k_2 k_1 A = 0 \quad (31)$$

The preliminary analog diagram for Equations 30 and 31 is shown in Fig. 19. Consider now the relative ease of changing $k_2 B$ to $k_2 B^2$ in Figs. 18 and 19. In the first case only a squaring card needs be added after the integrator for B. In the latter case, however, it is necessary to revert to the original equations and repeat the elimination of B. This yields

$$\frac{d^2C}{dt^2} + \frac{2k_2}{\sqrt{k_2}} \sqrt{\frac{dC}{dt}} \left(\frac{dC}{dt} - k_1 A \right) = 0 \quad (32)$$

the incorporation of which would require major modification of Fig. 19. Similar difficulties would be encountered for other model changes. Thus, although the circuits in both figures represent the same physical system, Fig. 18, in which the one-to-one correspondence is retained, is significantly more flexible.

Once the model has been completed, with due consideration to the simplicity, accuracy, and flexibility of the analog circuit, the details of the preliminary analog circuit can be completed and the scaling undertaken. In completing the scaled diagram, it is suggested that:



a. Each analog variable be labeled as to its physical meaning at each step. This will be of aid not only in the scaling process but in the remaining steps of a given simulation as well.

b. The process of unity scaling described in Part 2 of this series is recommended for completing amplitude scaling. If maximum magnitudes are unknown or may change from one run of the final simulation to another, amplitude scaling may be completed in a symbolic manner so that modifications may be readily made.

c. The process of time scaling as described in Part 3 of this series is a systematic way of completing this step. It is to be noted that time scaling does not affect amplitude scaling but that changes in amplitude scaling may affect the choice of an appropriate time scale factor. Thus time scaling should be completed after amplitude scaling.

Modes of Analog Operation. Before discussing the remainder of the steps generally involved in obtaining an analog simulation, it is convenient to describe the modes of analog operation. Most analog computers have the following modes of operation which can be chosen by the computer operator:

Pot Set Mode. When the computer is in the pot set mode, the values of the pots may be set. A reference voltage is applied to the input to the pot (this may be done automatically) and the value of the pot is set by monitoring the output voltage of the pot using a voltmeter or a digital voltmeter. The inputs to the amplifiers are disconnected and grounded and the amplifiers are effectively at zero gain. The analog computer is generally placed in the pot set mode when a simulation is not being carried out.

Reset Mode. In the reset mode, the initial conditions are imposed on the integrators. The inputs to the integrators are disconnected but the analog circuit is otherwise operable.

Operate Mode. In the operate mode, the inputs to all amplifiers are connected and the initial condition voltages to the integrators are disconnected. Problem solution is affected according to the mathematical operations specified by the analog circuit.

Repetitive Operation Mode. The purpose of the repetitive operation mode is to permit analog solutions to be obtained very rapidly. (β is typically changed by a factor of 0.02 to 0.002 corresponding to a speed up of 50 to 500.) It enables the display of an analog solution on an oscilliscope or the performance of calculations in which a rapid speed of solution is desired. In this mode, an internal change in the time scale is automatically made so that the simulation may be speeded up. The computer automatically cycles between the reset and operate modes, being in each mode for a specified amount of time. The solution obtained during each operating cycle can be displayed on an oscilliscope.

Suggestions for Accurate Patching. Patching is the term used to describe the process of connecting together the various analog components making up an analog circuit by means of external leads. Since the details vary from one type of analog to another and are adequately described by the manufacturer of each, they are not discussed here. The patching process is generally completed while the computer is in the pot set mode or while the removable patch panel is detached from the analog. Once the patching is complete and the patch panel in place on the computer, the pots may be set. Since the resistance of the pots will vary with the loading, it is important to set the pots after patching is complete and when the computer is in the pot set mode. (In this mode, the inputs to the amplifiers are grounded so that loading of the pots occurs.) Because of loading, the voltage output from the pot should be used for setting the value rather than the scale which may be indicated on the pot.

Although the analog circuit is now ready for use, the patching, the pot settings, and the operability of the components in use should be independently checked to eliminate solution errors which may arise from these sources. These checks are characteristically made by performing:

- A static check, and
- A dynamic check.

In completing a static check, arbitrary initial conditions are placed on all integrators. The outputs which would be obtained from all analog components if the initial conditions were placed on the integrators but the inputs to the integrators were removed are calculated from the mathematical model and/or the scaled analog diagram. The computer is then placed in the reset mode and the outputs obtained from the analog components by means of a voltmeter or a digital voltmeter are compared with the values calculated. In this manner the pot values (except for those which are inputs to integrators) and the patching may be checked and the static operability of the components established. The pots on the input lines to integrators can be checked separately.

The dynamic check corresponds to trial computer runs in which the dynamic operability of the analog components is established and the feasibility of the scale factors which have been assumed is checked. A computer run is carried out by first placing the computer in the reset mode to establish the initial conditions on the integrators and then in the operate mode, or simply placing the computer in repetitive operation mode. The computer is left in the operate mode for the desired time of the simulation.

Computer Operation. Once the static and dynamic checks have been made and errors corrected, computer runs can then be made for the purpose of recording the results. If only qualitative results are desired, they may be observed on an oscilliscope by placing the computer in repetitive operation mode. If a permanent record is desired, they may be obtained using an x-y recorder. Since the response time of a recorder is quite slow compared to that of an oscilliscope, the normal speed of computer operation must be used when recording. The computer is first placed in reset mode to establish initial conditions and then in the operate mode during which time the results are recorded.

The accuracy of a problem solution obtained on an analog computer is dependent upon several factors. Solution accuracy depends upon how faithfully the algebraic and differential equations represent the physical system, how accurately the physical constants are known, and upon how well the problem is programed so that each computer component is used in its most accurate range. Under the best of circumstances one might expect the computer solution to be accurate to at least three significant figures.

It should be noted that the solution or portions of the solution obtained on an analog computer may not be obtainable in a physical system. To illustrate: The differential equations describing liquid level in a tank as normally solved on an analog computer can yield negative heights. This of course is physically impossible. It is, therefore, important to have a physical feeling for the problem limitations when evaluating computer results.

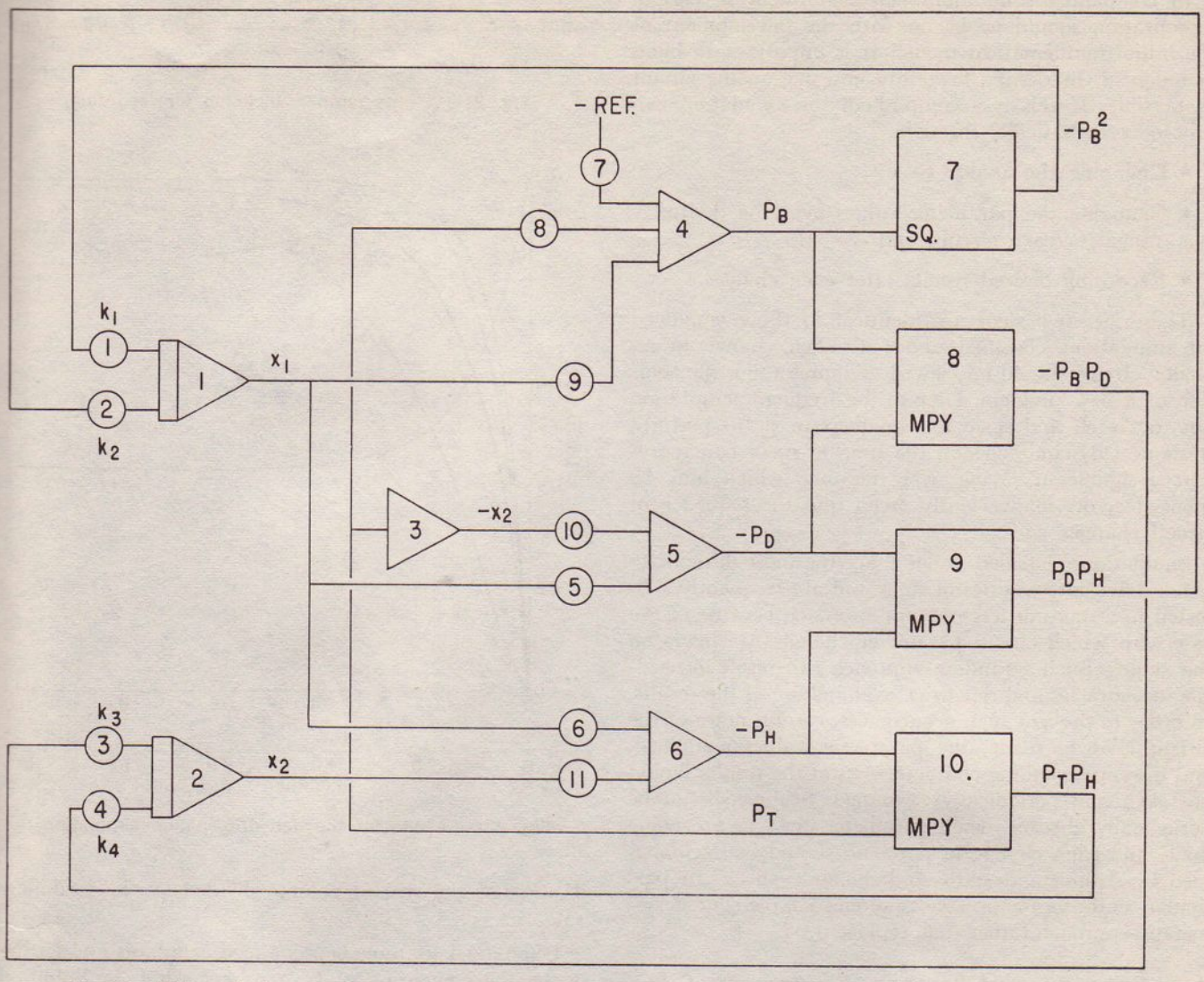


Fig. 20—This preliminary analog diagram retains one-to-one correspondence with the dehydrogenation problem.

Thus far in describing the steps of a simulation, attention has been directed toward the calculation of the values of known variables for a specified known system with specified known parameter values. This has permitted the sequential examination of

- The development of the mathematical model and the preliminary analog diagram
- The development of the scaled analog diagram
- The achievement of accurate patching, and finally
- Computer operation leading to the desired results.

As such, the presentation describes a rather narrow facet of analog simulation for frequently the simulation will be directed towards:

a. The calculation of the values of known variables for a specified, known system using numerous parameter values

b. The calculation of the values of known variables for numerous modifications of the simulated system using numerous parameter values

c. The choice modification of a simulated system and/or its parameters in order to obtain results possessing some characteristic, such as the determination of the optimum production rate for a chemical reactor system.

The simulations classified under **a** may be readily carried out after the circuit for the first set of parameters is prepared for operation by systematically:

- Setting new parameter values, and
- Recording the results for each set of parameter values.

If the parameter changes to be made are small, there is generally no need to rescale. However, if the changes are large, the assumed scaling factors should be periodically checked and the circuit rescaled if necessary. In the rescaling process, a clear concise circuit diagram together with tables of all analog variables and pot values, which presents the results of scaling obtained by symbolically retaining maximum values of all amplifier outputs, can be of great use. There is generally no need to perform additional static and dynamic checks.

In completing simulations classified under **b**, careful organization should be begun with the development of the initial mathematical model. It is important to build as much of the desired flexibility into one analog circuit as possible. If this is accomplished, the simulation can proceed systematically through

- Changing the analog circuit,
- Changing the parameter values over the desired range for each circuit, and
- Recording desired results after each change.

These last two steps are identical to those employed for simulations classified under **a**. Each change in an analog circuit should be viewed as representing the solution of a new problem. Despite the frequent temptation not to sketch and scale a new diagram or to perform static and dynamic checks, the time so spent can represent a significant saving over the time which may be spent if errors inadvertently creep into the sequence of circuit changes.

Simulations classified under **c** are the most difficult to break down into a series of steps and are frequently subjected to a more or less random approach because of the ease with which circuit parameter changes are made on the analog. Such a random approach can result in needless inaccuracies and repetitive examination of the results. In order to prevent such occurrences, careful notes of the circuit changes made, the parameter values examined, and the corresponding characteristics of the results should be taken and periodically examined. Scaling should be periodically checked when parameter changes are being made and each change in patching should be accompanied by scaling and static and dynamic check. In particular, enthusiasm for results should supplement a systematic approach rather than replace it.

Dehydrogenation of Benzene. For purposes of illustrating the steps of an analog simulation, the vapor-phase dehydrogenation of benzene in an isothermal, homogeneous, flow reactor has been chosen. The system as described in Smith[2] using the rate equations reported by Hougen and Watson[3] is used.

The vapor-phase dehydrogenation of benzene is assumed to proceed according to

$$2\ C_6H_6 = C_{12}H_{10} + H_2 \tag{33}$$

and

$$C_6H_6 + C_{12}H_{10} = C_{18}H_{14} + H_2 \tag{34}$$

At 1400°F the reaction of Equation 33 gives:

$$r_1 = \text{benzene reacted, lb. moles/(hr.) (cu. ft.)}$$

$$= 6.23\ [P_B^2 - (P_D P_H/0.312)] \tag{35}$$

and the reaction in Equation 34 gives:

$$r_2 = \text{triphenyl produced, lb. moles/(hr.) (cu. ft.)}$$
$$= 3.61\ [P_B P_D - (P_T P_H/0.480)] \tag{36}$$

In Equations 35 and 36, P denotes the partial pressure in atmospheres with subscripts B, D, H, and T representing benzene, diphenyl, hydrogen, and triphenyl, respectively. It is desired to calculate the conversion of an initially pure benzene feed at one atmosphere as a function of the

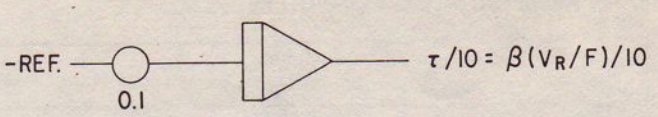


Fig. 21—A time ramp is included for recording.

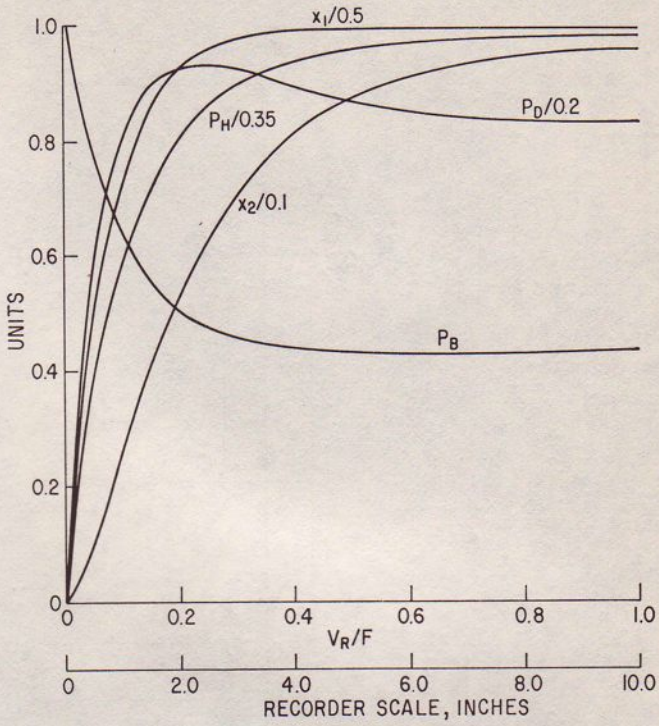


Fig. 22—Results for the dehydrogenation simulation.

V_R/F, i.e., the reactor volume divided by the feed flow rate.

Choosing 1 lb. mole benzene feed as a basis and letting x_1 be the conversion of benzene according to Equation 33 and x_2 be the conversion of benzene according to Equation 34, Smith[2] shows that

$$P_H = \text{moles of hydrogen} = (\tfrac{1}{2})\ x_1 + x_2 \tag{37}$$
$$P_D = \text{moles of diphenyl} = (\tfrac{1}{2})\ x_1 - x_2 \tag{38}$$
$$P_B = \text{moles of benzene} = 1 - x_1 - x_2 \tag{39}$$
$$P_T = \text{moles triphenyl} = x_2 \tag{40}$$

and that the design equations are

$$V_R/F = \int dx_1/r_1 \tag{41}$$

and

$$V_R/F = \int dx_2/r_2 \tag{42}$$

Smith then proceeds to solve Equations 41 and 42 numerically using the relationships given in Equations 35 to 40. The method employed is representative of the techniques which would be used to simulate such systems on a digital computer.

In order to obtain an analog solution, Equations 41 and 42 are first expressed in differential form and r_1 and r_2 are then replaced by the relationships given in Equations 35 to 42. This results in:

$$dx_1/d(V_R/F) = 6.23$$
$$[(1 - x_1 - x_2)^2 - (x_1/2 - x_2)\ (x_1/2 + x_2)/0.312] \tag{43}$$

TABLE 7—Unity Scaling, Time Scaling and Static Check

Amp	Physical Variable	Estimated Maximum
01	x_1	$x_1^* = 0.5$
02	x_2	$x_2^* = 0.1$
03	$-x_2$	$x_2^* = 0.1$
04	$P_B = 1 - x_1 - x_2$	$P_B^* = 1.0$
05	$-P_D = -x_1/2 - x_2$	$P_D^* = 0.2$
06	$-P_H = -x_1/2 - x_2$	$P_H^* = 0.35$
07	$-P_B^2 = (1 - x_1 - x_2)^2$	$(P_BP_B)^* = 1.0$
08	$-P_BP_D =$ $-(1 - x_1 - x_2)(x_1/2 - x_2)$	$(P_BP_D)^* = 0.2$
09	$P_DP_H =$ $(x_1/2 - x_2)(x_1/2 + x_2)$	$(P_DP_H)^* = .07$
10	$P_TP_H = x_2(x_1/2 + x_2)$	$(P_TP_H)^* = 0.035$

Pot	Before Scaling	After Amplitude Scaling
01	$k_1 = 6.23$	$(P_BP_B)^* k_1/x_1^* = 12.46$
02	$k_2 = 6.23/0.312$	$(P_DP_H)^* k_2/x_1^* = 2.795$
03	$k_3 = 3.61$	$(P_BP_D)^* k_3/x_2^* = 7.22$
04	$k_4 = 3.61/0.480$	$(P_TP_H)^* k_4/x_2^* = 2.632$
05	0.5	$0.5\ x_1^*/P_D^* = 1.25$
06	0.5	$0.5\ x_1^*/P_H^* = 0.714$
07	1.0	$1.0/P_B^* = 1.000$
08	1.0	$x_2^*/P_B^* = 0.100$
09	1.0	$x_1^*/P_B^* = 0.500$
10	1.0	$x_2^*/P_D^* = 0.500$
11	1.0	$x_2^*/P_H^* = 0.286$

Amp	Computer Variable	Static Check Initial Condition	Static Check Amplifier Output
01	$x_1/0.5$	0.500	0.500
02	$x_2/0.1$	0.800	0.800
03	$-x_2/0.1$	....	−0.800
04	P_B	....	0.670
05	$-P_D/0.2$	....	−0.225
06	$-P_H/0.35$	....	−0.585
07	$-P_B^2$	....	−0.449
08	$-P_BP_D/0.2$	....	−0.151
09	$P_DP_H/0.07$	....	0.132
10	$P_TP_H/0.035$	....	0.468

Pot	After Amplitude and Time Scaling ($\beta = 10$)
01	$(P_BP_B)^* k_1/(x_1^*\beta) = 1.246$
02	$(P_DP_H)^* k_2/(x_1^*\beta) = 0.2795$
03	$(P_BP_D)^* k_3/(x_2^*\beta) = 0.722$
04	$(P_TP_H)^* k_4/(x_2^*\beta) = 0.2632$
05	$0.5\ x_1^*/P_D^* = 1.25$
06	$0.5\ x_1^*/P_H^* = 0.714$
07	$1.0/P_B^* = 1.000$
08	$x_2^*/P_B^* = 0.100$
09	$x_1^*/P_B^* = 0.500$
10	$x_2^*/P_D^* = 0.500$
11	$x_2^*/P_H^* = 0.286$

$$dx_2/d\,(V_R/F) = 3.61$$
$$[(1 - x_1 - x_2)(x_1/2 - x_2) - (x_2)(x_1/2 + x_2)/0.480] \quad (44)$$

with $x_1 = 0$ and $x_2 = 0$ when $V_R/F = 0$.

Retaining a one-to-one correspondence between physical and analog variables, the preliminary analog diagram given in Fig. 20 is made. Pots 07 to 11 are included because they may be required after scaling although not required in the preliminary diagram. It is to be noted that the independent variable (V_R/F) is to be computer operating time. In Table 7, the physical significance of all amplifier outputs and all pot settings is summarized.

The processes of amplitude and time scaling are then sequentially completed as indicated in Table 7. In estimating the maximum magnitudes, the values of x_1 and x_2 corresponding to $V_R/F = \infty$ were rounded off to the nearest 0.1 on the high side (i.e., the equilibrium values were used); P_B^* was noted to be $= 1$; P_H^* and P_D^* were initially picked using $(1/2)\ x_1^* + x_2^*$ and $(1/2)\ x_1^* - x_2^*$ but P_D^* was changed to 0.2 when a dynamic check indicated it to be larger than 0.15; and the maximum magnitude for the products were chosen to be products of the maximum magnitudes for factors being multiplied.

To complete time scaling, the range of the pot values obtained after amplitude scaling were examined. Although all pot values between 0.1 and 30, the values of Pots 01 to 04, namely, those on inputs to integrators, were consistently greater than 1 (ranging 2.5 to 12.46) indicating that the simulation would be fast. Consequently $\beta = 10$ was chosen so that a slower simulation could be prepared for recording purposes.

The scaled analog diagram was then drawn. It is the same as Fig. 20 except that the amplifier outputs and pot values are changed to those quantities given in Table 7. Upon completion of the patching, a static check was performed as indicated in Table 7. A dynamic check was subsequently made to check the dynamic operability of the components used and the feasibility of the scale factors assumed. It was ascertained that the solution was completed in about 10 seconds. Following the setting of a time ramp for recording as shown in Fig. 21, the results using $\beta = 10$ and $\beta = 5$ were also recorded and compared.

The results shown in Fig. 22 were obtained using a scale factor on the recorder of one inch per volt and a 10-volt analog computer.

The next part of this series will discuss the generation of particular functions using common analog components. Consideration will be given to the operational aspects of the analog computer in order to assure stable, accurate simulation. Of particular concern will be methods for carrying out algebraic solutions using the analog computer.

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(Also see earlier parts.)

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Indexing Terms: Analogs-9, Aromatics-1, Benzene-1, Circuits-10, Compositions-6,7, Computations-4, Computers-9, Concentrations-6,7, Dehydrogenation-9, Descriptions-8, Diphenyl-2, Electricity-10, Engineering-4, Hydrocarbons-1,2, Hydrogen-2, Programing-10, Rates-7, Reactions-9, Simulation-4,10, Triphenyl-2.

Learn About Analog Computers

PART 5: CIRCUIT DESIGN–Stability, accuracy and flexibility must be considered before choosing from among several circuit designs

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

DURING THE COURSE of preparing a problem for analog solution, several mathematically equivalent methods may occur to the programer. At this point, he must make a judgment as to which will best suit his particular purposes. As indicated in the last article of this series, the amount of required analog equipment, the accuracy of required analog components, and the flexibility of the analog circuits can be significant factors in this choosing process. Attention can be given to such considerations, however, only after analog stability has been assured.

Below attention is drawn to those situations in which analog instability can arise. Particular emphasis is given to its occurrence during the solution of algebraic equations on the analog. Methods for insuring stability are discussed and are extended to indicate the applicability of the analog in optimization calculations. The article is concluded by considering the synthesis of transfer functions on the analog.

Feedback Stability. Although the analog computer permits the almost instantaneous solution of algebraic equations, precautions must be taken in the design of circuits to solve algebraic equations. As an example, consider the simple equation $y = a\,y + x, a > 0$, where it is desired to solve for y given x. An analog circuit is readily designed for the equation in the form given in Fig. 23.

The solution which might be expected is $y = x/(1 - a)$. In actuality, the circuit will become unstable if $a > 1$ and the amplifiers will readily saturate. This results from the phenomena known as positive feedback with excessive gain. To illustrate the reason for the instability, assume

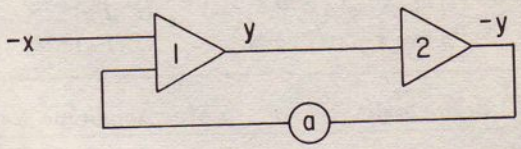

Fig. 23—An easy circuit to solve an algebraic equation although it may be unstable in operation.

that the output from amplifier 1 is momentarily in error by an amount ε. Following the progress of the error through the feedback loop in an approximate, sequential manner, the error ε is seen to result in an error of εa in the output from amplifier 1 after the first pass. Thus the initial error results in a subsequent error of the same sign, hence the term positive feedback. Now if $a < 1$, the error will soon die out. However, if $a > 1$ the error is propagated and the amplifiers soon overload. Thus if the gain of the feedback loop becomes excessive, $a > 1$, the circuit becomes unstable.

Positive feedback arises when an even number of amplifiers occur in a loop of an analog circuit. To insure stability in such cases, the total gain around the loop must be less than unity.

Negative feedback arises when an odd number of amplifiers occur in a loop of an analog circuit. As indicated by W. Brunner,[4] rather restrictive maximum permissible gains arise in this case also. These are less than 8, 2.9 and 2.1 for loops containing 3, 5 and 7 amplifiers respectively. The presence of integrators in the feedback loop, however, markedly enhances the stability, to the point where maximum permissible gains are higher than ever required.

To avoid feedback instability it is advisable to:

- Avoid, where possible, feedback loops which do not contain at least one integrator[5]
- Avoid summing-amplifier gains in excess of 30[5]
- Double check the occurrence of loops containing positive feedback (i.e. loops with an even number of amplifiers and integrators to insure that they are required by the physical system being examined).
- Adhere religiously to the maximum permissible feedback gains if loops with only amplifiers are used.

Such precautions are of particular significance in the design of analog circuits for solving algebraic equations.

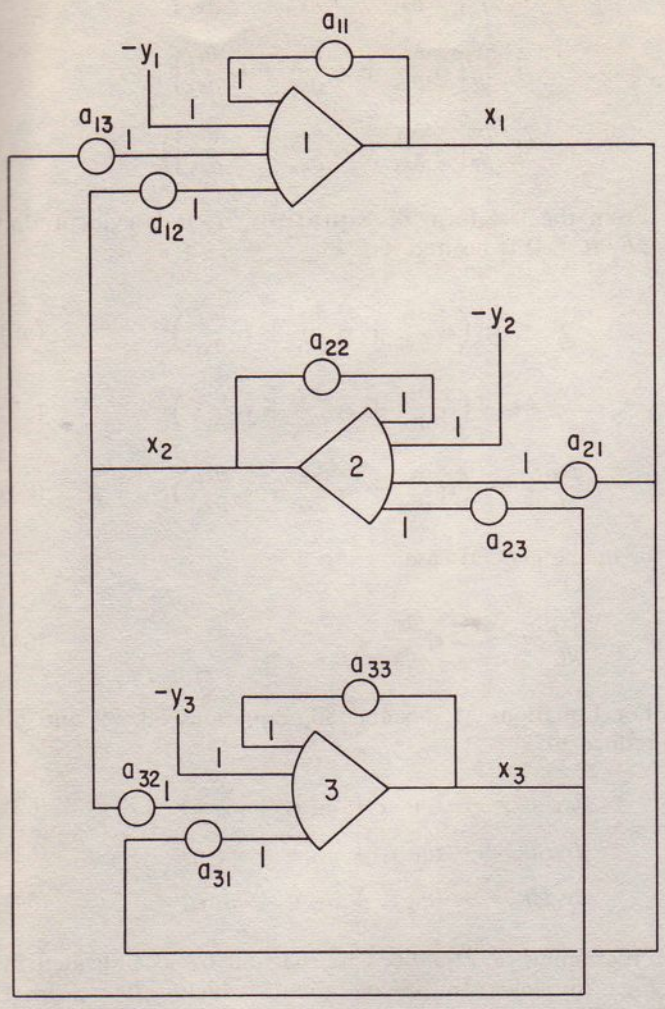

Fig. 24—Solving three equations simultaneously.

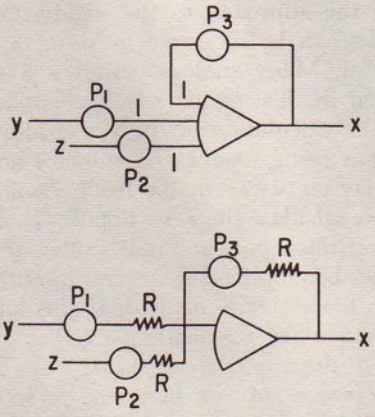

Fig. 25—The upper circuit is a shorthand symbol for the more complete circuit shown in the lower portion.

Algebraic Equations. Algebraic equations appear frequently in chemical and petroleum engineering as being representative of process performance, such as in steady-state mass and energy calculations, or as an integral part of a dynamic simulation. An example of the latter would arise during the simulation of the linear dynamics of multicomponent distillation on an analog. In this case, if Raoult's Law is assumed, it can be shown[6] that the linearized equilibrium relationship is

$$y_{j,i} = \bar{K}_{j,i}\, x_{j,i} + \frac{\bar{x}_{j,i}\,\bar{K'}_{j,i}}{\sum_{\beta=1}^{N} \bar{x}_{j,\beta}\,\bar{K'}_{j,\beta}} \sum_{\alpha=1}^{N} -\bar{K}_{j,\alpha}\, x_{j,\alpha}$$

where

$y_{j,i}$ = the deviation from its steady-state value of the mole fraction of component i in the vapor leaving tray j

$\bar{x}_{j,i}$ = the steady-state value of the mole fraction of component i in the liquid on tray j

$x_{j,i}$ = the deviation from its steady-state value of the mole fraction of component i in the liquid on tray j

$\bar{K}_{j,i}$ = ratio of the vapor pressure of component i evaluated at the temperature of tray j to the column pressure

$\bar{K'}_{j,i}$ = the derivative of $K_{j,i}$ evaluated at the temperature of tray j

N = number of components present.

To calculate the deviations $x_{j,i}$ given the deviations $y_{j,i}$, it is necessary to solve the coupled set of algebraic equations. Thus for a four-component system and a given tray, equations of the following form arise where the a_{ij}'s are constants

$$y_1 = a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 \quad (45)$$

$$y_2 = a_{21}\,x_1 + a_{22}\,x_2 + a_{23}\,x_3 \quad (46)$$

$$y_3 = a_{31}\,x_1 + a_{32}\,x_2 + a_{33}\,x_3 \quad (47)$$

where

$$y_4 = -y_1 - y_2 - y_3$$

$$x_4 = -x_1 - x_2 - x_3$$

One method of analog simulation would be to solve Equations 45, 46 and 47 simultaneously to yield

$$x_1 = b_{11}\,y_1 + b_{12}\,y_2 + b_{13}\,y_3 \quad (48)$$

$$x_2 = b_{21}\,y_1 + b_{22}\,y_2 + b_{23}\,y_3 \quad (49)$$

$$x_3 = b_{31}\,y_1 + b_{32}\,y_2 + b_{33}\,y_3 \quad (50)$$

and program Equations 48, 49 and 50 directly. Such an approach, however, requires considerable computation before the analog solution can be obtained and results in a relatively inflexible analog diagram since the known coefficients a_{ij}'s are not isolated on individual pots.

A much more direct approach is to use the analog to perform the calculation using the a_{ij}'s directly. This can be achieved by rearranging Equations 45, 46 and 47 to yield

$$x_1 = (y_1 - a_{12}\,x_2 - a_{13}\,x_3)/a_{11} \quad (51)$$

$$x_2 = (y_2 - a_{21}\,x_1 - a_{23}\,x_3)/a_{22} \quad (52)$$

$$x_3 = (y_3 - a_{31}\,x_1 - a_{32}\,x_2)/a_{33} \quad (53)$$

which can be programed in the manner shown in Fig. 24.

In Fig. 24, the symbol shown on the upper circuit of Fig. 25 is used to represent the same as the more complete components shown on the lower view of Fig. 25, where P_1, P_2, and P_3 are grounded pots. It is readily verified that $x = -y\,(P_1/P_3) - z\,(P_2/P_3)$. Thus a factor common to all inputs can be handled by the addition of the grounded pot P_3 in the feedback line.

Also note that Fig. 24 has not been scaled and that all

of the a_{ij}'s have been assumed to be positive. Negative a_{ij}'s are handled by the addition of inverters in the appropriate feedback lines.

An examination of Fig. 24 indicates that there are three positive feedback loops.

- The loop consisting of amplifiers 1 and 2 which has an over-all gain of $(a_{12}\,a_{21})/(a_{11}\,a_{22})$,
- The loop consisting of amplifiers 2 and 3 which has an over-all gain of $(a_{23}\,a_{32})/(a_{22}\,a_{33})$,
- The loop consisting of amplifiers 1 and 3 which has an over-all gain of $(a_{13}\,a_{31})/(a_{11}\,a_{33})$.

If a stable solution is to be obtained each of the three gains must be less than unity. For the particular case of multicomponent equilibrium, one would generally expect $a_{ii} > a_{ij};\ j \neq i$, in which case the stability criteria would be automatically satisfied. If, however Equations 45, 46 and 47 had been solved for x_2, x_3 and x_1 respectively, the resulting circuit would be unstable.

Although the direct method indicated above can frequently be used to great advantage, care must be taken to insure that maximum permissible feedback gains are not exceeded. Particularly troublesome are those cases in which the equations can not be rearranged to make $a_{ii} > a_{ij};\ j \neq i$, there is no unique relationship between the a_{ij}'s which can be used to the programer's advantage, or the a_{ij}'s are variable. In the latter case, the pots in Fig. 24 would be replaced by multipliers and the analysis of stability could become unduly complex. Under such circumstances the programer might be well advised to use a method of solution which eliminates the need for a stability analysis. The method of steepest descent is such an alternative.

The method of steepest descent results in the synthesis of a set of differential equations, the steady-state solution of which represents the solution of the algebraic equation(s). The method of synthesis is given below.

Choosing Equations 45, 46 and 47 for example, errors ε_1, ε_2 and ε_3 are defined in the following manner.

$$\varepsilon_1 = -y_1 + a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 \tag{54}$$

$$\varepsilon_2 = -y_2 + a_{21}\,x_1 + a_{22}\,x_2 + a_{23}\,x_3 \tag{55}$$

$$\varepsilon_3 = -y_3 + a_{31}\,x_1 + a_{32}\,x_2 + a_{33}\,x_3 \tag{56}$$

If the correct values of x_1, x_2 and x_3 are chosen, $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 0$. Choosing $E = \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2$, $E = 0$ is seen to result if and only if the correct solution is obtained.

Other forms for E may also be used. For example, $E = |\varepsilon_1| + |\varepsilon_2| + |\varepsilon_3|$ or $E = \varepsilon_1^4 + \varepsilon_2^4 + \varepsilon_3^4$, $E \geq 0$.

It is recognized that if an analog circuit is designed for which $dE/dt \leq 0$ for all t, the steady-state solution would result in $E = 0$ and thus solution. Letting x_1, x_2 and x_3 be functions of t, the following is obtained by the rules of differentiation

$$\frac{dE}{dt} = 2\left(\epsilon_1 \frac{d\epsilon_1}{dt} + \epsilon_2 \frac{d\epsilon_2}{dt} + \epsilon_3 \frac{d\epsilon_3}{dt}\right)$$

$$= 2\left(\epsilon_1\left[\frac{\partial\epsilon_1}{\partial x_1}\frac{dx_1}{dt} + \frac{\partial\epsilon_1}{\partial x_2}\frac{dx_2}{dt} + \frac{\partial\epsilon_1}{\partial x_3}\frac{ax_3}{dt}\right]\right.$$

$$+ \epsilon_2\left[\frac{\partial\epsilon_2}{\partial x_1}\frac{dx_1}{dt} + \frac{\partial\epsilon_2}{\partial x_2}\frac{dx_2}{dt} + \frac{\partial\epsilon_2}{\partial x_3}\frac{ax_3}{dt}\right]$$

$$\left. + \epsilon_3\left[\frac{\partial\epsilon_3}{\partial x_1}\frac{dx_1}{dt} + \frac{\partial\epsilon_3}{\partial x_2}\frac{dx_2}{dt} + \frac{\partial\epsilon_3}{\partial x_3}\frac{dx_3}{dt}\right]\right)$$

$$= 2\left(\frac{ax_1}{dt}\left[\epsilon_1\frac{\partial\epsilon_1}{\partial x_1} + \epsilon_2\frac{\partial\epsilon_2}{\partial x_1} + \epsilon_3\frac{\partial\epsilon_3}{\partial x_1}\right]\right.$$

$$+ \frac{ax_2}{dt}\left[\epsilon_1\frac{\partial\epsilon_1}{\partial x_2} + \epsilon_2\frac{\partial\epsilon_2}{\partial x_2} + \epsilon_3\frac{\partial\epsilon_3}{\partial x_2}\right]$$

$$\left. + \frac{dx_3}{dt}\left[\epsilon_1\frac{\partial\epsilon_1}{\partial x_3} + \epsilon_2\frac{\partial\epsilon_2}{\partial x_3} + \epsilon_3\frac{\partial\epsilon_3}{\partial x_3}\right]\right) \tag{57}$$

From the last form of Equation 57, it is evident that $dE/dt \leq 0$ is insured if

$$\frac{ax_1}{dt} = -\left(\epsilon_1\frac{\partial\epsilon_1}{\partial x_1} + \epsilon_2\frac{\partial\epsilon_2}{\partial x_1} + \epsilon_3\frac{\partial\epsilon_3}{\partial x_1}\right) \tag{58}$$

$$\frac{dx_2}{dt} = -\left(\epsilon_1\frac{\partial\epsilon_1}{\partial x_2} + \epsilon_2\frac{\partial\epsilon_2}{\partial x_2} + \epsilon_3\frac{\partial\epsilon_3}{\partial x_2}\right) \tag{59}$$

$$\frac{dx_3}{dt} = -\left(\epsilon_1\frac{\partial\epsilon_1}{\partial x_3} + \epsilon_2\frac{\partial\epsilon_2}{\partial x_3} + \epsilon_3\frac{\partial\epsilon_3}{\partial x_3}\right) \tag{60}$$

or in the general case

$$\frac{dx_j}{dt} = -\sum_i \epsilon_i \frac{\partial\epsilon_i}{\partial x_j} \tag{61}$$

For Equations 54, 55 and 56, Equations 58, 59 and 60 reduce to

$$ax_1/dt = -(a_{11}\,\epsilon_1 + a_{21}\,\epsilon_2 + a_{31}\,\epsilon_3) \tag{62}$$

$$dx_2/dt = -(a_{12}\,\epsilon_1 + a_{22}\,\epsilon_2 + a_{32}\,\epsilon_3) \tag{63}$$

$$dx_3/dt = -(a_{13}\,\epsilon_1 + a_{23}\,\epsilon_2 + a_{33}\,\epsilon_3) \tag{64}$$

Programing of Equations 62, 63 and 64 as indicated in Fig. 26 yields an analog circuit which, after a brief period of operation, will produce the desired values of x_1, x_2 and x_3 without the necessity of performing a stability analysis.

To speed the approach to the steady-state, the speed of integration can be increased by using a smaller feedback capacitor. Many analogs permit a $\beta = 0.1$ or less to be selected in this manner. In the application of this technique, the calculation of the ε_i's is also crucial since a null point is being sought. To enhance accuracy, feedback pots may be placed in the feedback line of the amplifiers which calculate the ε_i's—Pots P_1, P_2 and P_3 in Fig. 26. By setting these pots at small values, the errors, ε_i's, generated can be amplified by several hundred so that the null point is more clearly defined. If this latter approach is taken, momentary overloading of the amplifiers may occur prior to the approach to steady-state. It is common to limit the values of ε_i's between $\pm$ reference, using techniques which are to be described in the next article, in order to prevent such overloading. After the analog circuit has attained a steady-state for a set of fixed y_1, y_2 and y_3, variable values of y_1, y_2 and y_3 can be handled. The values of x_1, x_2 and x_3 obtained from the circuit will essentially be the instantaneous solution of the algebraic set for the variable y_i's.

The method of steepest descent as described above for linear algebraic equations has several other applications and extensions which can be of considerable use to the practicing engineer:

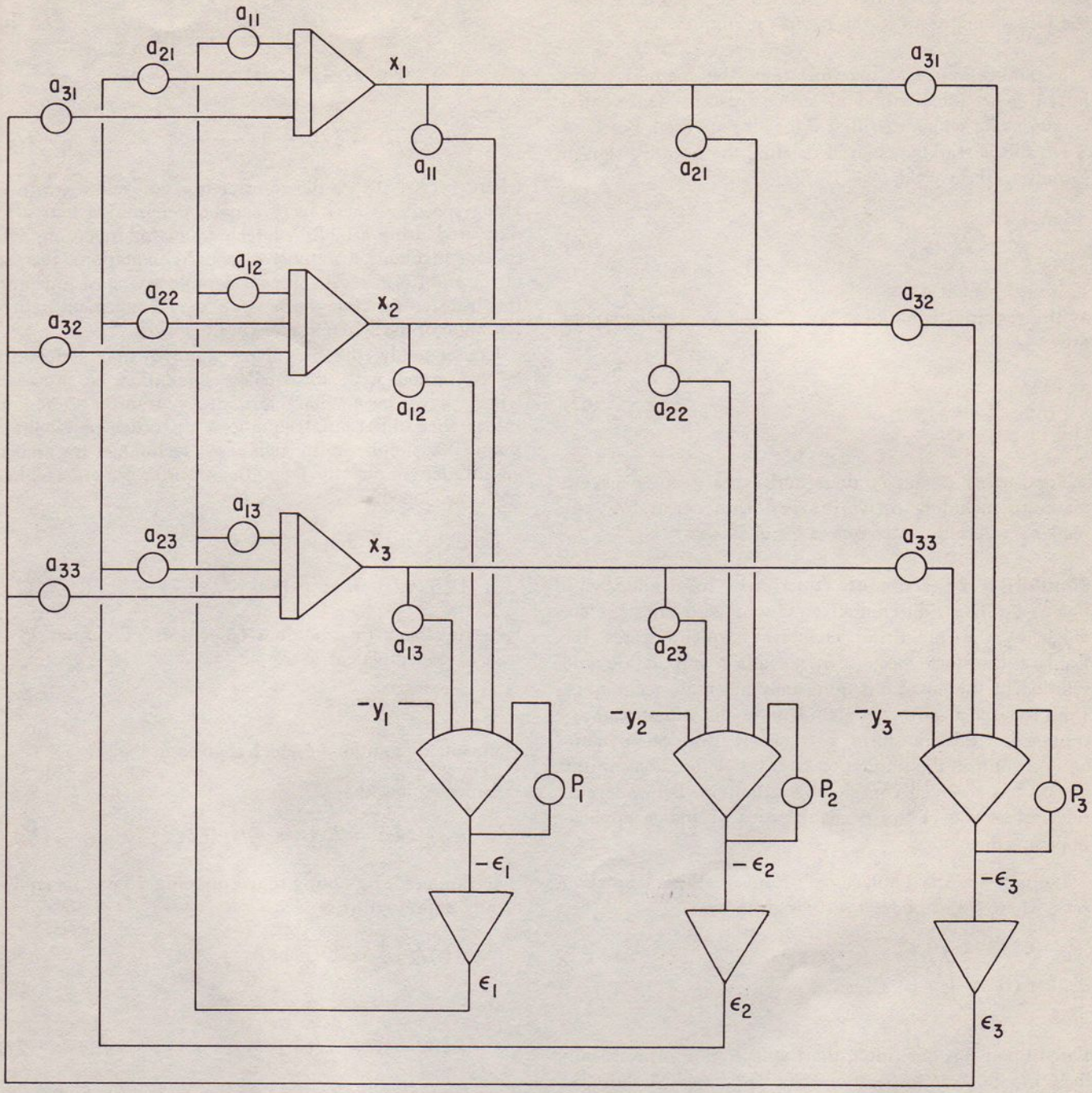

Fig. 26—The method of steepest descent as a circuit.

Nonlinear Algebraic and Transcendental Equations. Appropriate ε_i's are defined so that ε_i's $= 0$ corresponds to solution. Equation 61 then forms the basis for the synthesis of differential equations whose steady-state response is the solution. If multiple solutions exist, the analog solution will proceed in the direction in which $dE/dt \leq 0$ for all t from the initial conditions to the nearest solution.

When Number of Equations Exceed the Number of Unknowns. For these cases, no change needs to be made in the approach. The individual ε_i's will, however, reach non-zero values at steady-state corresponding to a minimization of E. Thus the "best" solution can be obtained according to the relationship chosen between E and the ε_i's. The squared error form, $E = \Sigma\ \varepsilon_i^2$, is probably the most frequently used.

Minimization. In light of the application given in the preceding method, the extension to the general use of minimization becomes a natural one. The approach remains the same. If $E = \Sigma\ \varepsilon_i^2$ is to be minimized, Equation 61 details the differential equations to be used. If $E = \Sigma\ \varepsilon_i$ is to be minimized, it may be verified that the equations to be used are:

$$\frac{ax_j}{dt} = -\sum \frac{\partial \epsilon_i}{\partial x} \qquad (65)$$

If multiple minimums exists, the analog solution will proceed in the direction in which $dE/dt \leq 0$ for all t from the initial conditions to the nearest minimum.

Maximization. For maximization, the method is referred to as the method of steepest ascent. Differential equations for which $dE/dt \geq 0$ for all t are used. For $E = \Sigma\, \varepsilon_i^2$, this is readily achieved deleting the negative sign in Equation 61 to yield

$$\frac{dx_j}{dt} = \sum_i \epsilon_i \frac{\partial \epsilon_i}{\partial x_j} \tag{66}$$

as the required equations. For $E = \Sigma\, \varepsilon_i$, the equations are

$$\frac{dx_j}{dt} = \sum_i \frac{\partial \epsilon_i}{\partial x_j} \tag{67}$$

For further details of these and other steepest descent methods, including optimization with constraints, the reader is referred to References 4 and 5.

Simulation of Transfer Functions. In dealing with linear, ordinary, differential equations with constant coefficients, the practicing engineer frequently uses the Laplace transform because it permits manipulation and solution of the equations using only algebraic techniques. (See Reference 7 for details.) Due to the widespread acceptance of this transform, particularly in process dynamics and control, the simulation of transfer functions on the analog has received considerable attention. Below several relevant aspects of this particular area of analog applications are developed.

Letting s be the Laplace transform, $f(s)$, of a function $f(t)$, where $f(t) \equiv 0$ for $t < 0$, is given by

$$f(s) = \int_o^\infty f(t)\, e^{-st}\, at.$$

Based upon this definition, the Laplace transform of standard functions and operations can be derived. A short list is given in Table 8.

The usefulness of the transform is indicated by considering the set of differential equations

$$ay/at + y = x, y(0) = 0 \tag{68}$$

$$dx/dt + x = z, x(0) = 0 \tag{69}$$

Upon transforming Equations 68 and 69 they become

$$sy(s) + y(s) = x(s) \tag{70}$$

$$sx(s) + x(s) = z(s) \tag{71}$$

which can be algebraically manipulated to yield

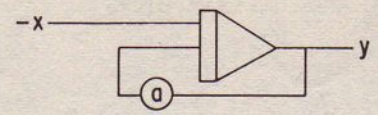

Fig. 27—y(s)/x(s) = 1/(s + a).

$$y(s)/z(s) = 1/(s+1)^2 \tag{72}$$

where $1/(s+1)^2$ is the transfer function relating z to y. Upon specifying $z(s)$, $y(s)$ can be determined and $y(t)$ recovered using established techniques for inversion. For systems involving a number of coupled equations, the use of the transform results in considerable saving of time and the transfer function becomes a very convenient representation of the system under consideration.

Consequently, the practicing engineer may frequently be concerned with the analog simulation of processes which have been characterized by transfer functions rather than differential equations. In order to facilitate the analog simulation in such cases, techniques for analog circuit design directly from the transfer functions have been developed.

Consider for example

$$v(s)/x(s) = 1/(s+a) \tag{73}$$

Referring back to Equations 68 and 70, Equation 73 is seen to be equivalent to

$$av/at + av = x \tag{74}$$

the analog solution of which is given in Fig. 27.

Suppose now that

$$y(s)/x(s) = K/(s+a)(s+b) \tag{75}$$

is encountered. By noting that Equations 75 can be equivalently expressed as

$$v(s)/z(s) = 1/(s+a) \tag{76}$$

and

$$z(s)/x(s) = K/(s+b) \tag{77}$$

the analog circuit is readily designed as given in Fig. 28.

Adding the acceptable circuit given in Fig 29 for

TABLE 8—Laplace Transforms

$f(t)$	$f(s)$
A	A/s
t	$1/s^2$
e^{-at}	$1/(s+a)$
$f'(t), f(0) = 0$	$sf(s)$
$\int_o^t f(t)\, at$	$\frac{f(s)}{s}$
$f(t-T)$, T constant	$e^{-sT} f(s)$

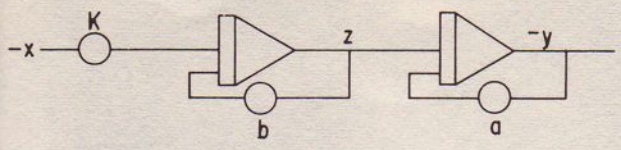

Fig. 28—y(s)/x(s) = K/(s + a) (s + b).

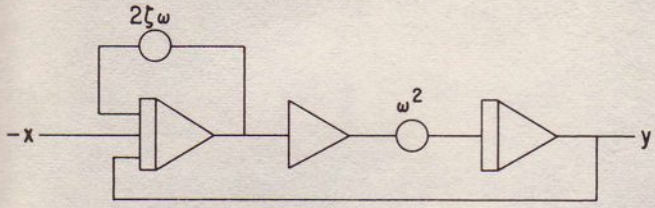

Fig. 29—An acceptable circuit for a transfer function.

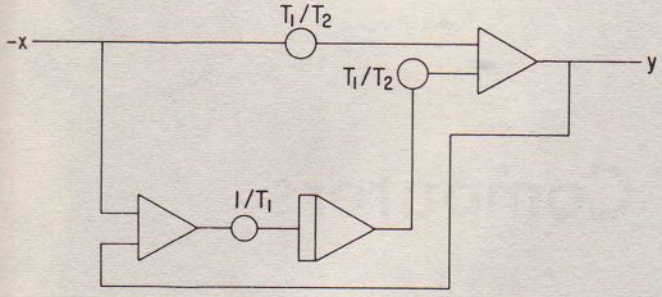

Fig. 30—y(s)/x(s) = (T₁s + 1)/(T₂s + 1).

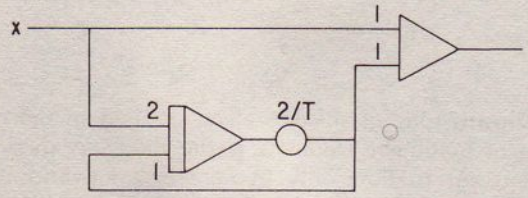

Fig. 31—y(s)/x(s) = [1 — (Ts/2)]/[1 + (Ts/2)].

$$\frac{y\,(s)}{x\,(s)} = 1\Big/\left(\frac{s^2}{w^2} + \frac{2\zeta s}{w} + 1\right), \tag{78}$$

all transfer functions of the form

$$\frac{y\,(s)}{x\,(s)} = \frac{K}{s^n(s^m + a_1 s^{m-1} + \cdots + a_m)} \tag{79}$$

can be handled when it is noted from Table 8 that multiplication by $1/s$ is equivalent to another integration. Thus with knowledge of the analog circuits for the basic transfer functions, the programer can design directly an analog program for more complicated transfer functions.

The basic transfer function

$$\frac{y\,(s)}{x\,(s)} = \frac{T_1 s + 1}{T_2 s + 1} \tag{80}$$

appears to be more difficult to simulate because the differential equation from which this result is

$$T_2\,(dy/dt) + y = T_1\,(dx/dt) + x \tag{81}$$

which implies the need for differentiating the input signal x, an operation which is generally unsatisfactory due to analog noise. This problem is alleviated by noting that Equation 81 is equivalent to

$$dz/dt = (x/T_1) - (y/T_1) \tag{82}$$

$$y = (T_1/T_2)\,x + (T_1/T_2)\,z \tag{83}$$

Equations 82 and 83 permit the simulation of Equation 80 without differentiation as is shown in Fig. 30.

An approximation to $y(s)/x(s) = T_1 s + 1$ is obtained by making the value of T_1/T_2 very large.

For a more complete listing of analog circuits for standard transfer functions than can be given here, the reader is referred to References 4 and 8. Note that neither the circuits presented here nor in the references are scaled and that numerous acceptable circuits may exist for a given transfer function.

The material presented above briefly describes the synthesis of transfer functions consisting of ratios of polynomials in s. One of the most important transfer functions in chemical and petroleum engineering, however, is

$$y\,(s)/x\,(s) = e^{-Ts} \tag{84}$$

the time delay, which is equivalent to the physical situation in which $y(t) = x(t - T)$. This transfer function can not be simulated exactly on the analog using only standard analog components. In order to approximate the time delay, numerous circuits based on expansions of e^{-Ts} have been developed.[4, 7, 8] The most frequently used is the first-order Padé approximation

$$\frac{y\,(s)}{x\,(s)} = \frac{1 - Ts/2}{1 + Ts/2} \tag{85}$$

the circuit for which is given in Fig. 31.

Other approximations used for greater accuracy are the second and fourth Padé approximations and the Stubbs-Single approximation. In Reference 8, typical responses to step and sinusoidal inputs are given for the various approximations. As indicated there, the time delay of a step is particularly difficult to approximate. Analog simulations using these approximations do, however, represent marked improvements over simulations completed by neglecting the presence of time delays.

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Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Electricity-10, Engineering-4, Programing-10, Simulation-4.

Learn About Analog Computers

PART 6: DIODE SWITCHING—A key element in the design of circuits for non-linear problems, the diode acts as a switch in an operation analogous to a check valve

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

PROBLEMS WHICH ARE DISCONTINUOUS in nature are often solved on analog computers. Problems with discontinuities can arise in several ways: from a discontinuous physical system or from the piecewise linear approximation of a nonlinear differential equation with a set of linear differential equations, each of which is applicable over a fixed interval. In the hydrocarbon processing industry it is not unusual to find systems which have time delays, hysteresis or backlash, coulomb friction, limitations on physical quantities, or are forced with discontinuous forcing functions. Each of these nonlinearities as well as others may be simulated on the analog computer.

The Diode. One of the key elements used in the circuit design of nonlinear elements is the diode. A diode permits current to flow only in one direction and its operation is analogous to the operation of a check valve. There are in general three types of diodes used in analog computers. These are the vacuum tube diode, usually called a "hot diode," and two "cold diode" solid state devices, the germanium diode and the silicon-junction diode often called a Zener diode. The symbols for the "hot" and "cold" types are shown in Fig. 32.

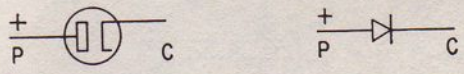


Fig. 32—Vacuum tubes (left symbol) and solid state devices can be used as switching diodes.

The latest solid state analog computers use only "cold type" diodes which have forward resistances on the order of one hundred ohms. If the anode or plate *P* is positive with respect to the cathode *C*, electrons will flow from the cathode to the plate and the direction of current flow will be from the plate to the cathode. If the plate is made negative with respect to the cathode, electrons are repelled, and, as a consequence, no current flows. When a diode is conducting, its resistance is a nonlinear function of voltage and current.

Some complex non-linear circuits are possible by combining several simpler circuits

Diodes in Switching. Diodes are used extensively as switching devices in digital computers, but are rarely used strictly as switches in analog computers. They are often used with operational amplifiers and relays to form switching circuits. Diodes switch currents rather than voltages and the state of the switch and the magnitude of the current is dependent upon the voltage drop across the diode.

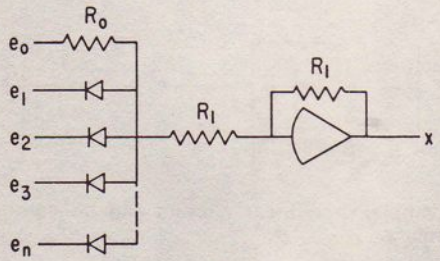


Fig. 33—Minimum selection where $x = -\min (e_1, e_2, e_3 \ldots e_n, e_y)$.

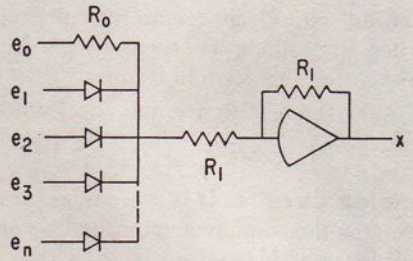


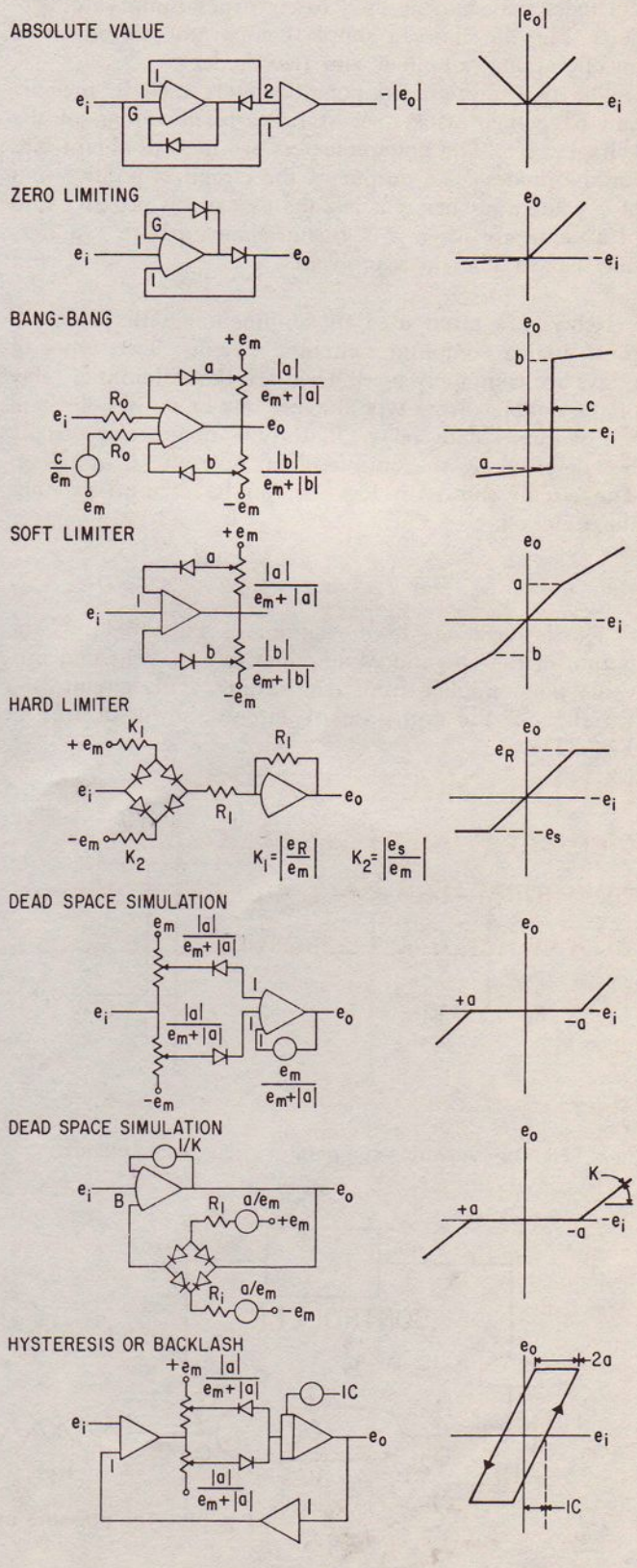
Fig. 34—Maximum selection where $x = -\max (e_1, e_2, e_3 \ldots e_n, e_y)$.

Diodes are often used in the design of selection and comparator circuits. Fig. 33 shows a circuit that may be used to obtain the minimum of a set of input voltages, while Fig. 34 shows a circuit that may be used to obtain the maximum of a set of input voltages. In either case,

$$e_y = \left[\frac{R_1}{R_o + R_1}\right] e_o$$

These circuits require that the source and diode forward resistance be negligibly small compared with resistances R_o and R_1. The voltage e_o may be either positive or negative. If R_o is equal to R_1 and e_o is twice the positive reference voltage, then e_y will be the positive reference voltage, and the circuit in Fig. 33 will find the minimum of the set of input voltages. When e_o is positive in the circuit in Fig. 33 the circuit is equivalent to the **AND** circuit used in digital computers. If e_o is negative in the

TABLE 9—Non-linear Analog Computer Diode Circuits



circuit in Fig. 34, the circuit is equivalent to the **OR** circuit used in digital computers.

Diodes may also be used to construct comparator circuits. Fig. 35 shows a simple comparator circuit using an operational amplifier and two diodes.

The two ungrounded potentiometers used in the circuit have their wipers set at ratios of a_1 and a_2 of the voltages $\pm e$. The potentiometers are used to obtain bias for the diodes. The output of the circuit is positive and of a value $a_2 e$ when x is less than e_2 and is negative and of a value $a_1 e$ when x is greater than e_2. Both x and e_2 may be variables in a problem.

Relays are often used in conjunction with diodes to form analog computer switching circuits. Two types of relays are commonly used. They are the differential relay of the double throw type, having one or more poles and the sensitive-plate relay. Plate-type relays can usually be energized by the output of an operational amplifier. The circuit shown in Fig. 36 can be used to produce the function:

$$z = \begin{cases} a & \text{if } x - y \leq o \\ x & \text{if } x - y > o \end{cases}$$

The lower diode in the circuit of Fig. 36 limits the output of the operational amplifier to $-e_o$ volts and prevents the amplifier from overloading. This circuit is a variation of the comparison circuit shown earlier in Fig. 35.

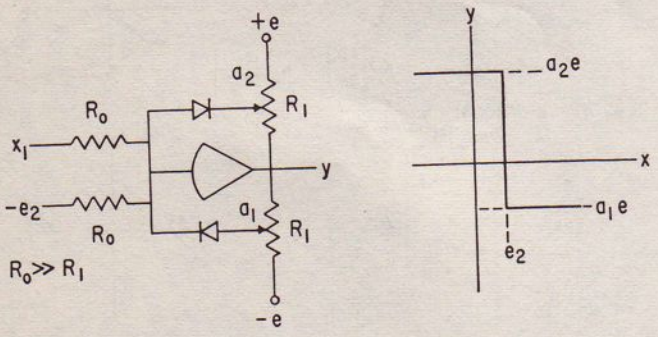


Fig. 35—A simple comparator circuit using diodes.

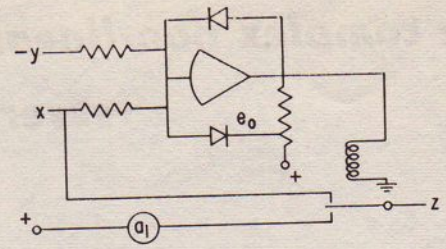


Fig. 36—A relay circuit for switching.

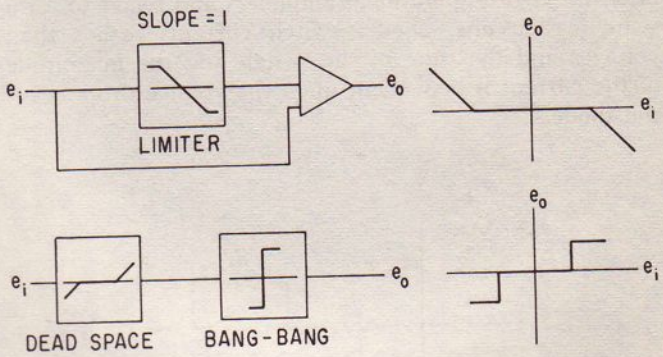


Fig. 37—Complex non-linear circuits can be combined from simpler circuits.

A number of simple circuits have been developed to simulate the discontinuous phenomena that arises in many physical problems. Table 9 contains some of the most often used diode circuits. Each of these circuits usually has an equivalent relay circuit replacing the diodes. When the diode conducts the relay switch is closed. Otherwise, the switch is open.

Several other diode circuits may be found in the literature.[1, 4, 8-10]

More Complex Circuits. It is sometimes possible to construct more complex nonlinear circuits by combining relatively simple nonlinear circuits in series or parallel. Two examples of such circuits are shown in Fig. 37.

Scaling Nonlinear Circuits. The scaling of nonlinear components is accomplished in the same manner as linear components. They are scaled by changing the gain of integrator inputs. Nonlinear components are affected by amplitude scaling of their inputs and it is not unusual to have to scale both the input and output. Scaling can sometimes be done simply by patching the nonlinear ele-

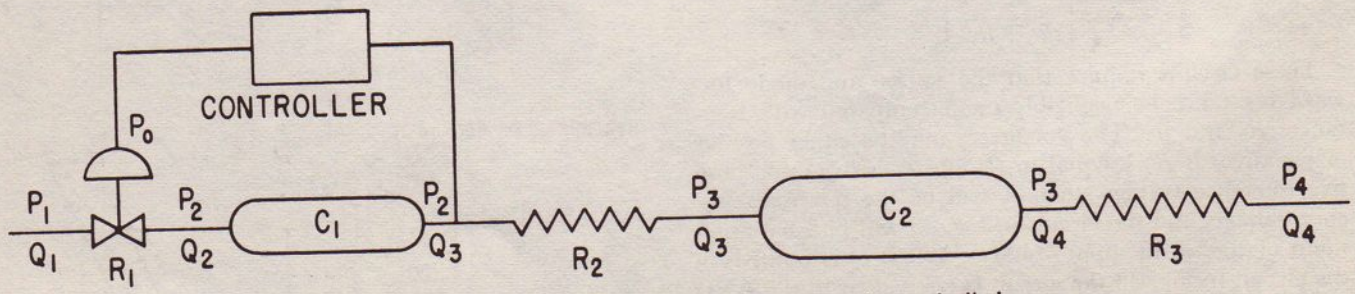


Fig. 38—The pressure in the first tank is to be controlled.

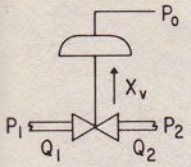


Fig. 39—Pneumatic control valve parameters.

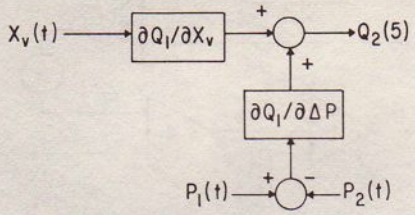


Fig. 40—Block diagram of the control valve.

ment on the computer and then scale it while forcing the element with a variable input such as a ramp function.

A Process Control Example. As an example of the use of a diode circuit in an analog computer problem we consider the system of Fig. 38 in which it is desired to control the pressure in a tank by employing a pneumatic control valve to throttle the flow. For this example the pressure P_2 in the first tank is to be controlled. The symbols are defined as follows:

C = Capacitance, cf./psi
R = Resistance, psi/cfm
P = Pressure, psi
Q = Flow rate, cfm

In this system there are several nonlinear elements. Each resistance must usually be considered to be nonlinear and the pneumatic control valve is nonlinear. For this example we will linearize each resistance for small departures from the steady state and will consider only the control valve as nonlinear.

A pneumatic valve is usually designed so that it operates over a pressure range from 3 to 15 psi. If the valve is normally closed, it will begin to open when the signal from the controller is 3 psi and will be fully open when the signal reaches 15 psi. A normally open valve operates in the reverse fashion. The simulation of the control valve requires the use of a nonlinear element (a limiter) because the controller output signal range is normally 0 to 20 psi while valve movement is restricted to the 3 to 15 psi range.

The outflow Q_2 from the control valve is a function of the upstream pressure P_1, the downstream pressure P_2, and the valve stem position X_v (or the degree to which the valve is open). For this problem we assume that the valve is very fast so that valve stem position is linearly related (no dynamic element) to the pressure P_o supplied to the valve bonnet. The relationship between the valve elements is shown in Fig. 39.

The relationship between outflow, pressure drop and valve stem position is given in the following linearized equation:

$$Q_2(t) = \frac{\partial Q_1}{\partial X_v} X_v(t) + \frac{\partial Q_1}{\partial P_2} P_2(t) + \frac{\partial Q_1}{\partial P_1} P_1(t) \quad (86)$$

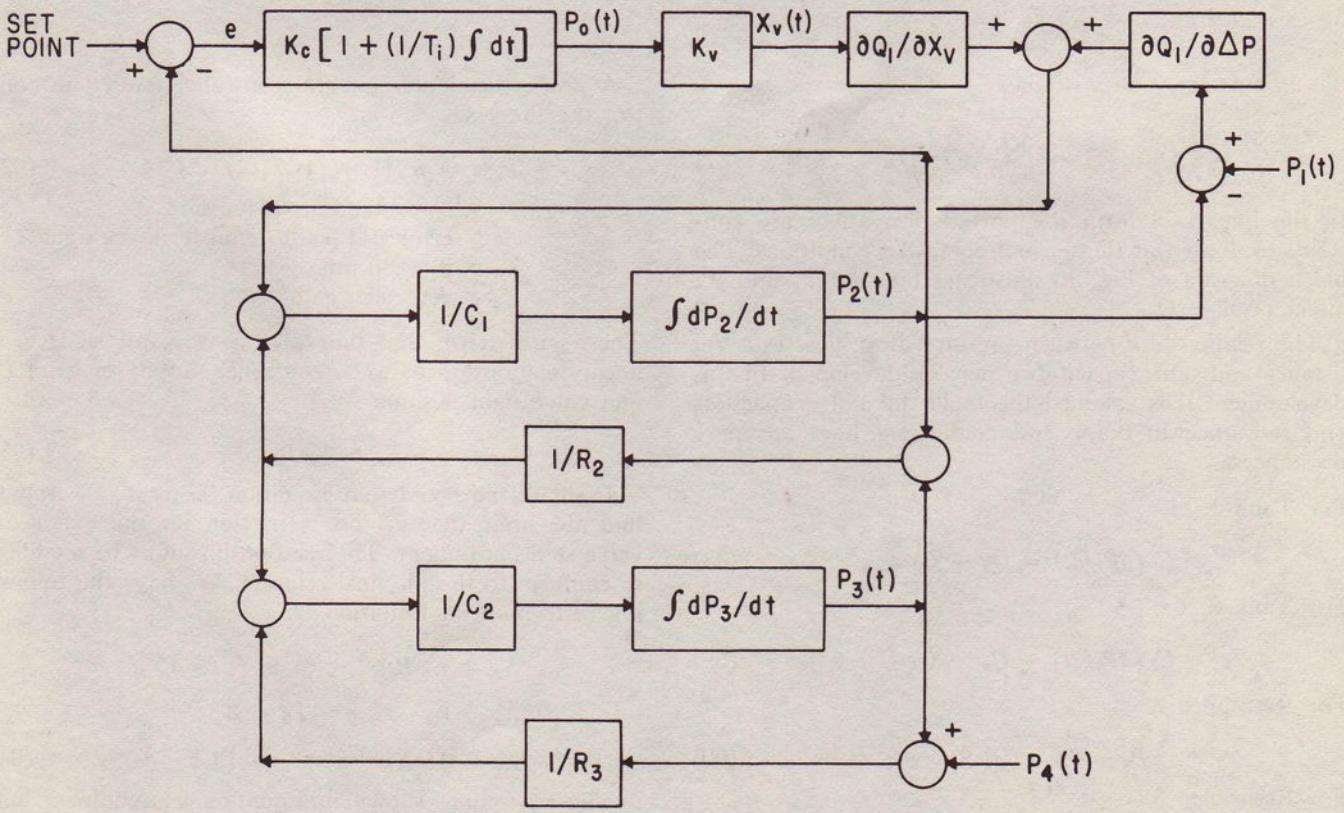


Fig. 41—Block diagram of the pressure control system.

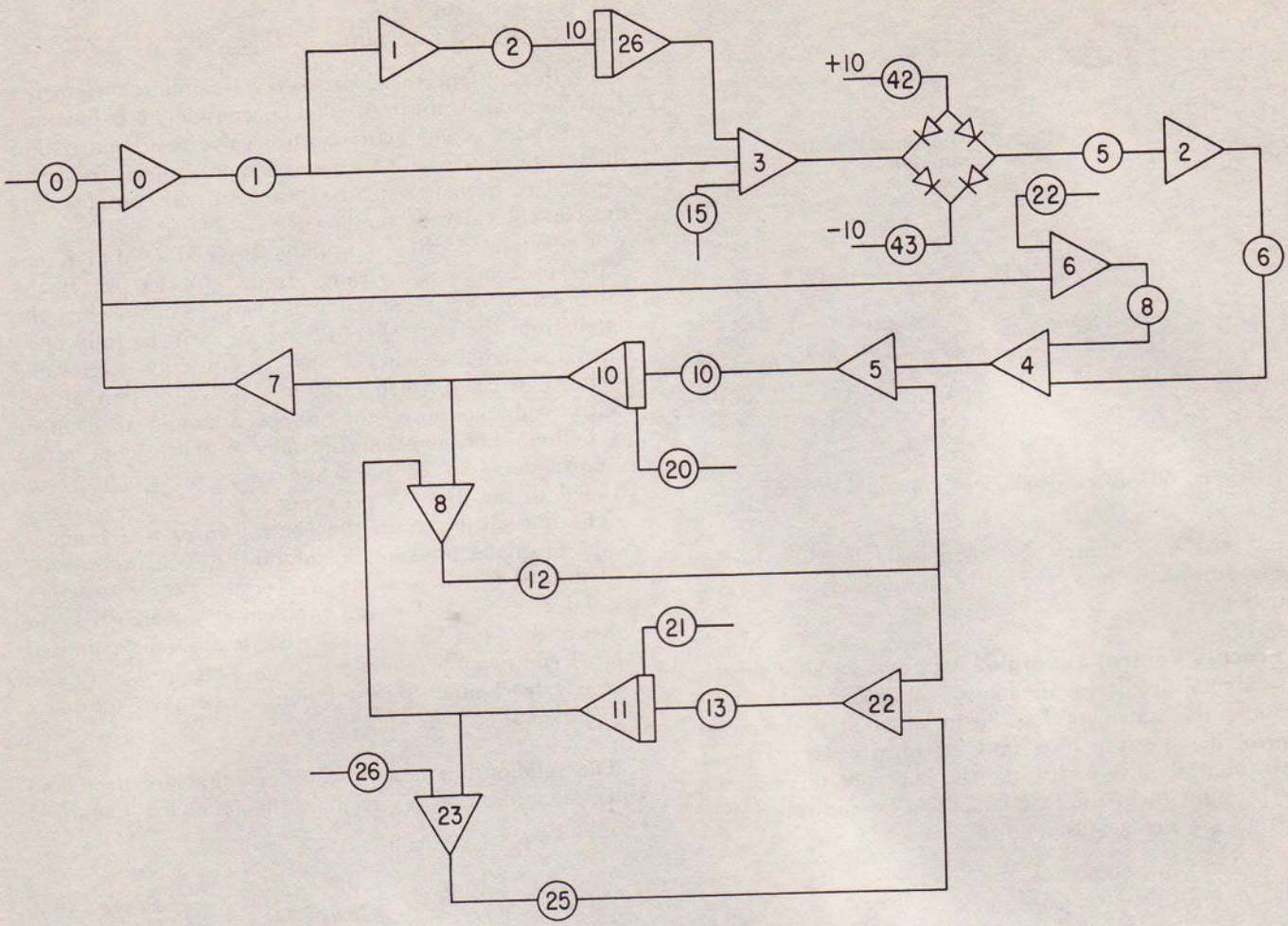


Fig. 42—An analog diagram for the example problem.

this in turn may be written as

$$Q_2(t) = \frac{\partial Q_1}{\partial X_v} X_v(t) + \frac{\partial Q_1}{\partial \Delta P} \Delta P(t) \tag{87}$$

In the linearized form the partial derivatives are constants evaluated at the normal operating conditions. The block diagram of Fig. 40 illustrates how P_1, P_2 and X_v affect outflow Q_2.

The relationships between pressure drop, flow rate, resistance and tank capacitance may be developed. In this development it is assumed the tanks are pure capacitors (no resistance to flow) and connecting lines are pure resistances.

For Tank 1

$$C_1 (dP_2/dt) = Q_2 - Q_3 \tag{88}$$

For Tank 2

$$C_2 (dP_3/dt) = Q_3 - Q_4 \tag{89}$$

For Resistance 2

$$P_2 - P_3 = Q_3 R_2 \tag{90}$$

For Resistance 3

$$P_3 - P_4 = Q_4 R_3 \tag{91}$$

A proportional plus integral controller is used to control the process

$$P_o/e = K_c [1 + (1/T_i) \int dt] \tag{92}$$

where P_o = controller output pressure
e = error (set point minus feedback signal)
T_i = integral time
K_c = controller gain

The assumption that the valve is very fast leads to a linear relationship between controller output pressure P_o and valve stem position X_v.

$$X_v = K_v P_o \tag{93}$$

It should be noted that Equation 93 as it now stands indicates that there is no restriction on the extent of valve stem movement. The relationship must be modified to conform to the physical relation. We have the following restriction on Equation 93.

$$\begin{aligned} X_v &= K_v P_o \qquad && 3 \leqslant P_o \leqslant 15 \\ X_v &= 0 && P_0 < 3 \\ X_v &= 15\, K_v && P_o > 15 \end{aligned} \tag{94}$$

The restrictions shown in Equation 94 require a limiter circuit to be placed in the pressure line before the valve bonnet.

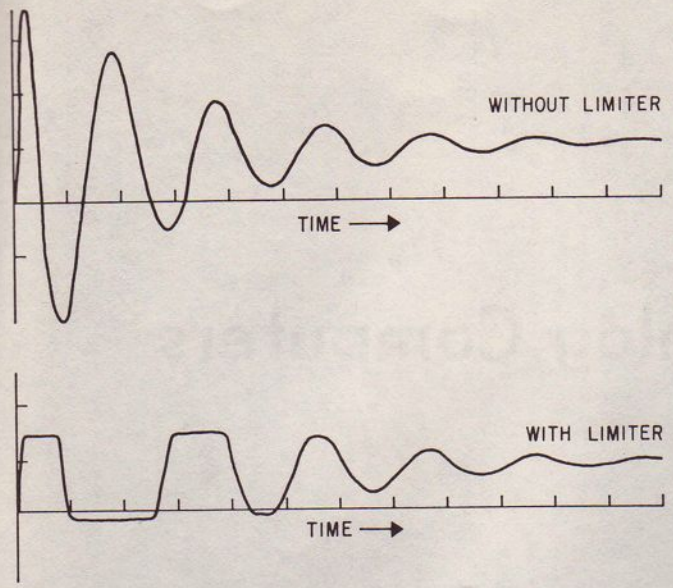


Fig. 43—Valve stem position, $-X_v$.

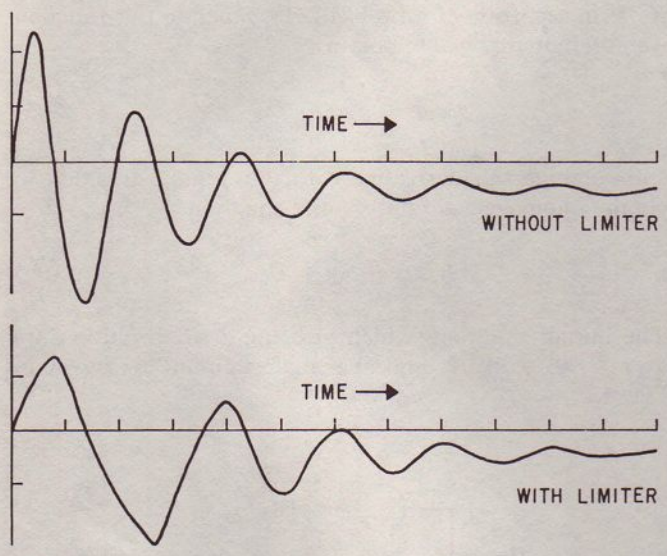


Fig. 44—Tank pressure, P_2.

In process control problems it is often helpful to draw a block diagram of the system. This type of diagram shows how signals flow through the system and how the various elements are affected by the signals. Fig. 41 is a block diagram for the system under discussion.

An analog circuit may be constructed using the block diagram and the limitations on valve stem movement. The circuit is given in Fig. 42.

The normal value of each of the constants in the problem is given in Table 10.

Typical pot settings, determined after magnitude and time scaling, are given in Table 11.

It is now of interest to determine the effect of the limiter upon the valve displacement and upon the pressure P_2 in the first tank. The disturbance is a step change

TABLE 10—Normal Values of Constants

Function	Value
Sp/10	2.56 psi
K_c	0.7 psi/in.
T_i	36 min.
P_o	0.036 psi
K_v	0.044 in./psi
$\partial Q/\partial X_v$	10 cfm/in.
$\partial Q/\partial \Delta P$	0.083 cfm/psi
R_2	45 psi/cfm
R_3	590 psi/cfm
$P_{4/10}$	3 psi
C_1	0.007 cf/psi
C_2	0.0001 cf/psi

TABLE 11—Typical Pot Settings

Pot	Function	Value
0	Sp/10	0.023
1	K_c	0.683
2	$1/T_i$	3.82
5	K_v	0.44
6	$\partial Q/\partial X_v$	1.00
8	$\partial Q/\partial \Delta P$	0.083
10	$1/C_1$	0.146
12	$1/R_2$	2.22
13	$1/C_2$	0.927
15	P_o (0)	0.038
20	P_2 (0)	0.305
21	P_3 (0)	0.305
22	$P_1/10$	0.848
25	$1/R_3$	0.170
26	$P_4/10$	0.305
42	Limiter	0.072
43	Limiter	0.326

in pressure caused by a setpoint change. Fig. 43 shows how the output from amplifier 2 (in this case $-X_v$) changes as a function of time with the limiter circuit and without the limiter circuit. Fig. 44 shows how the output of amplifier 10 (in this case P_2) changes with time with the limiter circuit and without the limiter circuit. Because of the nature of the control system (closed loop feedback control), the effect of the limiter shown in Fig. 43 is not just to truncate the unlimited sinusoidal decay curve of X_v. The curve in which the limiter is used has been significantly changed in both amplitude and frequency and this in turn has changed the pressure curve shown in Fig. 44. For this particular case the limiter has helped to reduce the wild pressure fluctuations in the first tank due to a set point change.

This example has illustrated the importance of designing the analog circuit to incorporate physical limitations of the system. The example was simplified to illustrate just the effect of the limiter. A more realistic system might take into account nonlinearities in resistances, valve dynamics and hysterisis in valve motion. Each of these may readily be incorporated in an analog simulation.

LITERATURE CITED

[1-8] In earlier parts.
[9] Levine, *Methods for Solving Engineering Problems Using Analog Computers*, McGraw-Hill, 1964.
[10] Ashey, *Introduction to Analog Computation*, Wiley, 1963.

Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Diodes-10, Electricity-10, Engineering-4, Programing-10, Simulation-4.

Learn About Analog Computers

PART 7: FUNCTION GENERATION—Usually the best way to generate mathematical functions in an analog computer is to simulate differential equations.

Theodore G. Smith and **Theodore W. Cadman**
University of Maryland, College Park, Md.

IT IS POSSIBLE to generate a function either as the solution of a differential equation or by employing a memory device which stores the functional relationships. The solution of differential equations is the strong point of analog computers, while storage is one of their weakest attributes. Whenever possible one should try to use the differential equation method of function generation.

Differential Equations. We have referred to differential equation function generation in a previous article in this series. If we have a function of the form $y = f(x)$, we may generate the function as a solution of a n^{th} order homogeneous differential equation if the function and each of its first n derivatives are continuous and if each of the derivatives can be calculated. The procedure to follow in forming a function by this method is to differentiate the function a number of times until a homogeneous equation may be formed. The solution of the homogeneous equation with the proper boundary conditions will be the desired function.

As an example, suppose we required the function $y = Ke^{-at}$ in a portion of a problem. To generate this function we differentiate once to obtain

$$dy/dt = -aKe^{-at} \tag{95}$$

and combine this derivative with the original function to obtain a homogeneous differential equation

$$(dy/dt) + ay = 0 \tag{96}$$

The initial conditions which give the desired solution are at $t = 0$, $y = K$, and the analog circuit is shown in Fig. 45.

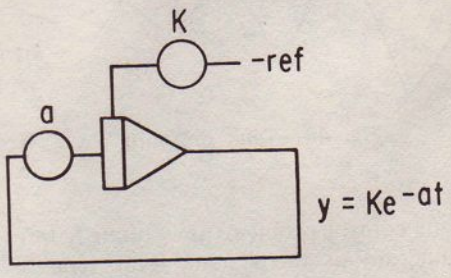


Fig. 45—A homogenous differential equation is obtained by combining an equation with its derivative.

If we wish to generate the previous function in a variable other than machine time we employ a similar method. For example, consider the generation of the exponential

$$y = Ke^{-ax} \tag{97}$$

whose first derivative is

$$dy/dt = -Kae^{-ax}\,(dx/dt) \tag{98}$$

or using symbols gives

$$\dot{y} = -ay\dot{x} \tag{99}$$

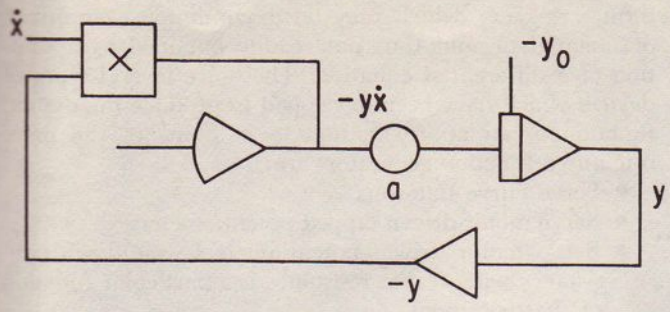


Fig. 46—This differential equation generator requires a derivative input.

The solution of this equation may be obtained from the circuit shown in Fig. 46, where $y_o = Ke^{-ax}{}_o$. The generation of this function requires the derivative input $\dot{x}$.

Sine and cosine functions of dependent variables are used quite frequently and may be generated as solutions of differential equations or by a special device called a resolver. If we wish to generate functions of the form

$$y = \sin h(t) \tag{100}$$

We construct a differential equation as follows

$$\dot{y} = \dot{h} \cos h(t) \tag{101}$$

$$\ddot{y} = \ddot{h} \cos h(t) - (\dot{h})^2 \sin h(t) \tag{102}$$

combining equations we obtain

$$\ddot{y} - (\ddot{h}/\dot{h})\dot{y} + (\dot{h})^2 y = 0 \tag{103}$$

For the special case $y = \sin wt$ we obtain $\ddot{y} + w^2 y = 0$ and the analog circuit is shown in Fig. 47.

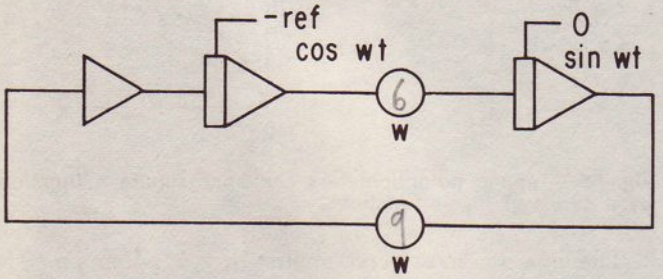


Fig. 47—Sine and cosine functions can be generated from the solution of a differential equation.

If $h(t)$ is a function of a variable other then time the circuit is somewhat more complex. For example if $h(t) = x$, then we must generate $y = \sin x$, where x and its derivatives with respect to time are available. We must solve the equation

$$\frac{d^2y}{dx^2} + y = 0 \tag{104}$$

A computer circuit for this function contains multipliers in place of potentiometers as shown in Fig. 48.

When generating integer powers of t, multipliers may be used. However, a very convenient method involves integrators in cascade with the initial condition on each integrator set at zero. These are shown in Fig. 49.

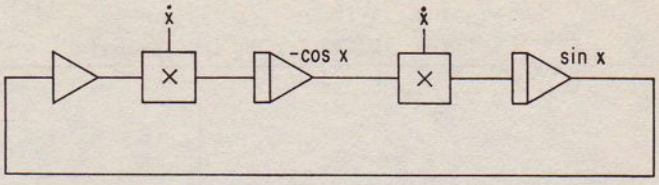


Fig. 48—Multipliers are used instead of potentiometers if the sine and cosine are to have variable frequency.

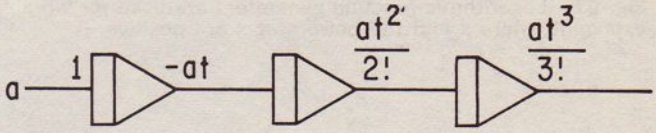


Fig. 49—Integrators in cascade can be used to generate power functions of time.

Fractional powers of functions can readily be generated if the function is not complex or imaginary and if multipliers and logarithmic elements are available. For example the square root, cube root and 2/3 power of x may be generated by the circuits shown in Figs. 50, 51 and 52.

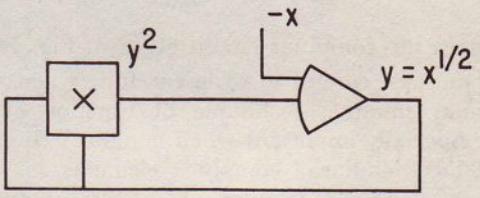


Fig. 50—This circuit generates square roots if the value of x are positive.

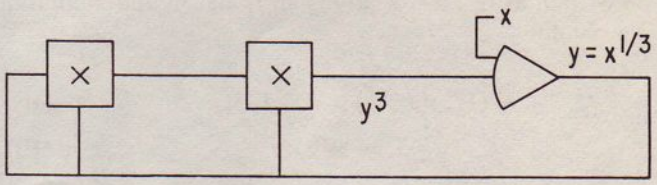


Fig. 51—This circuit generates the cube root.

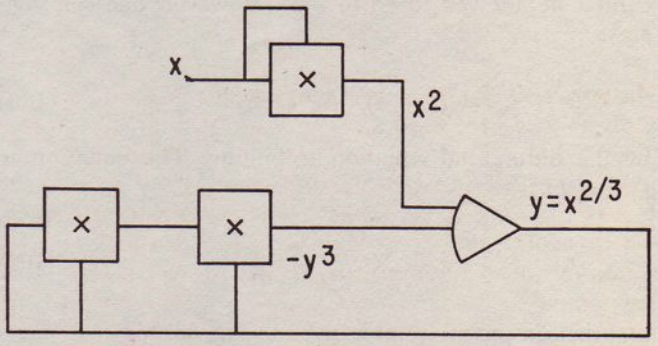


Fig. 52—Fractional exponents also can be generated.

Variable powers may also readily be generated. The solution of $y = x^z$ where both x and z are variables can be obtained by using logarithmic function generators. The function may be generated using the circuit in Fig. 53.

The logarithm of a function may be generated by the use of function generators as well as by the solution of differential equation. For example to obtain $z = \ln x$ we take the time derivative of both sides,

$$dz/dt = (1/x)dx/dt$$

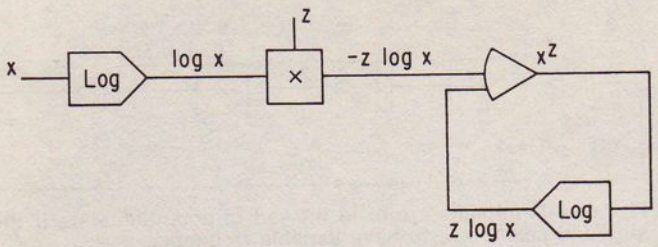


Fig. 53—Logarithmic function generators are used for variable exponent where x and the powers of x are positive.

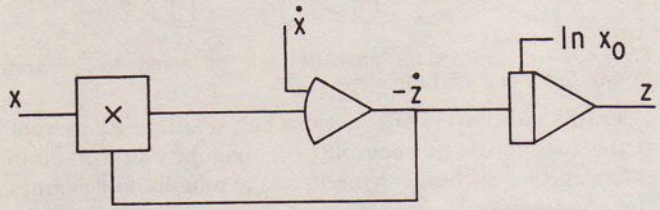


Fig. 54—A time derivative can generate a logarithm.

and obtain the computer circuit given in Fig. 54.

One must be careful to scale carefully when using the differential equation technique of function generation. This is especially important when nonlinear equations are solved since nonlinear computer elements may become overloaded within the range of interest of one of the variables. For example, suppose we wished to generate $z = t^{1/3}$ by the differential equation technique. This may be written as $\ln z = \times (1/3) \ln t$, and by differentiating we obtain

$$(1/z)(dz/dt) = \times 1/3t \tag{106}$$

or

$$\dot{z} = \times z/3t \tag{107}$$

This cannot be instrumented directly on the computer since at the start of the problem t is zero and a divisor cannot be allowed to go to zero. However, one can generate

$$z = (t + a)^{1/3} \text{ for } a > o \tag{108}$$

by the differential equation technique. The equation to be solved is

$$\dot{z} = \times \frac{z}{3(t + a)} \tag{109}$$

and the computer circuit is given in Fig. 55.

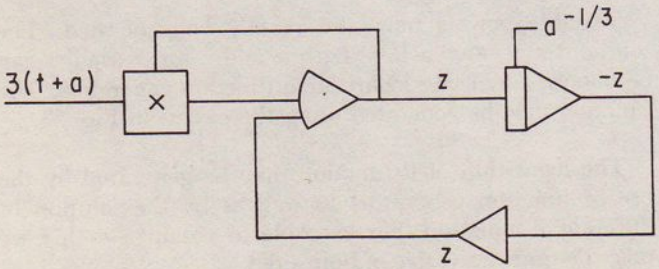


Fig. 55—Proper scaling must be used when generating a function with the differential equation technique.

Function Generation Devices. In some types of problems the engineer may have to generate functions of the form $y = f(x)$ which may be discontinuous, empirical, or nonanalytic and thus not readily obtained as a solution of a differential equation. There are several types of devices which have been developed to produce the desired function or an approximation to it. Some of the more often used function generators are:

- Servo curve followers
- Servo motor driven tapped potentiometers
- Servo motor driven potentiometers wound with resistance wire so that resistance is a particular function of shaft position
- Diode function generators which approximate functions with straight line segments.

The tapped servo motor driven potentiometer and the diode function generator are the most commonly used function generators. Both of these types of function generators approximate the function of interest by a series of straight line approximations.

A tapped potentiometer which may be used to approximate a function $f(x)$ by straight line segments is shown in Fig. 56. Voltages are impressed at the taps and when the slides are in some position x between two taps the voltage $f(x)$ is a linear interpolation of the voltages between the two taps. Servo motor driven tapped potentiometers are usually provided with from 10 to 20 taps so that a function may be approximated with from 10 to 20 straight lines. Fig. 56 shows how the function represented by the solid curve may be approximated by the dotted straight lines.

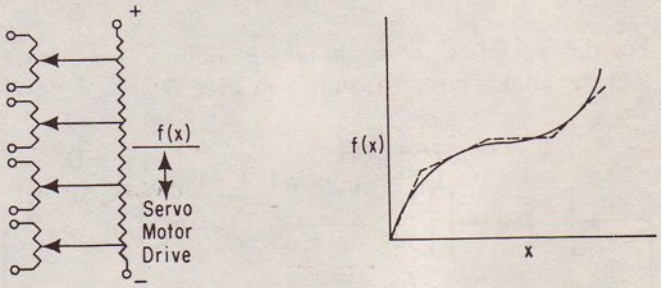


Fig. 56—Tapped potentiometers can approximate a function by a series of linear functions.

The taps on most servo motor driven potentiometers are usually located a fixed distance apart. This feature may limit the usefulness of this device for a complex function which has several points of inflection which are close together.

Servo motor driven potentiometers wound with resistance wire so that resistance is a function of the potentiometer shaft position are usually found only in analog systems that require repeated use of a particular complex function. This type of device can not be varied and must be carefully chosen and scaled for the particular application.

Modified X-Y recorders are often used as a curve follower type of function generator. The function of interest is plotted using conducting ink and by using a special signal pickup on the X-Y recorder the functional relation may be retraced and the resulting signal used in the analog computation.

The use of function generating devices employing servo motors requires careful time scaling of the analog

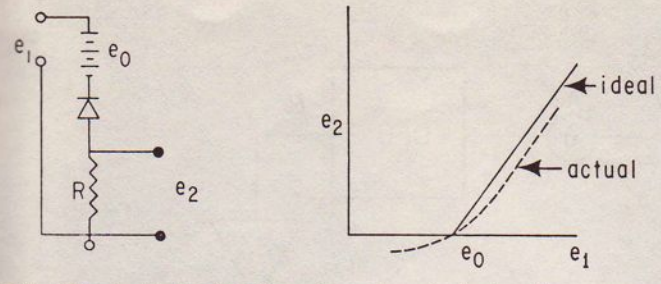


Fig. 57—A diode function generator is faster than servo-motor-driven potentiometers.

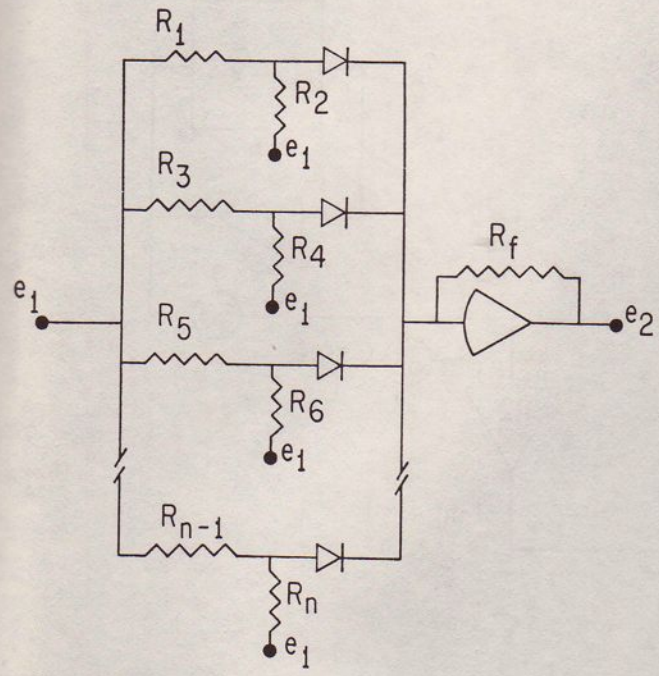


Fig. 58—The simplest diode function generators do not have a means of varying the breakpoints.

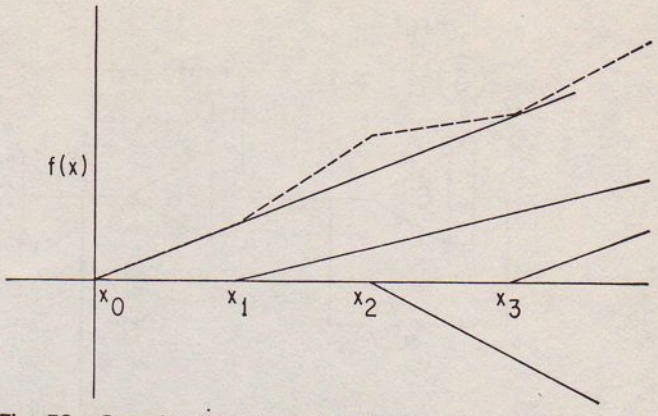


Fig. 59—Complex lines can be simulated by adding the output from several diode function generators.

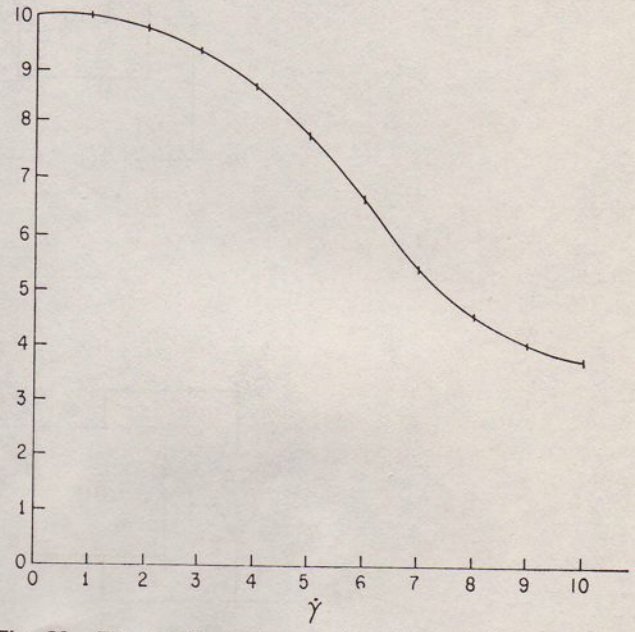


Fig. 60—The relation between viscosity and shear rate is divided into segments.

circuit so that the problem is scaled within the frequency limitations of the servo motors. This means that fast repetitive operation employing oscilloscope display can not be used, and the solution must usually be recorded with a servo recorder.

Diode Function Generation. Much of the servo motor driven function generation equipment has been replaced by diode function generators in modern analog computers. Although diode function generators represent functions by straight line segments just as servo motor driven potentiometer function generators, the diode function generator is an all electronic system and is therefore much faster than servo motor driven systems.

These are two general types of diode function generators: fixed and variable breakpoint generators. The voltage at which two line segment approximations intersect (a breakpoint) is fixed by the computer manufacturer in a fixed breakpoint function generator, while the engineer solving the problem may decide, within certain limitations, the location of breakpoints for a variable breakpoint function generator. The diode has such an important function in diode function generation, that it is essential its operation be understood. In a previous article in this series it was shown that if the plate voltage of a diode is larger than the cathode voltage the diode permits a current to pass through it. If the reverse is true, the diode acts as an infinite resistance and no current can pass through it. Fig. 57 illustrates the properties of a diode.

In the circuit of Fig. 57 the diode acts as a switch. When the applied voltage e_1 is less than the bias voltage e_o, the diode acts as an infinite resistance. At values of applied voltage equal to or greater than the bias voltage the diode acts as if it has zero resistance and current may flow. The entire voltage drop e_2 due to the flow of current though the diode appears across the resistance R as

$$e_2 = (e_1 - e_0)/R \qquad (110)$$

The solid curve in Fig. 57 illustrates how e_2 would vary with an increase in e_1 if the bias voltage were set at e_o for an ideal diode. Actual diodes have characteristics more closely represented by the dashed curve. The value of e_o of bias voltage in Fig. 57 is called a breakpoint. The gradual rather than sharp change of slope at the breakpoint of the diode characteristic curve permits a more accurate representation of many functions which do not have sharp changes in slope.

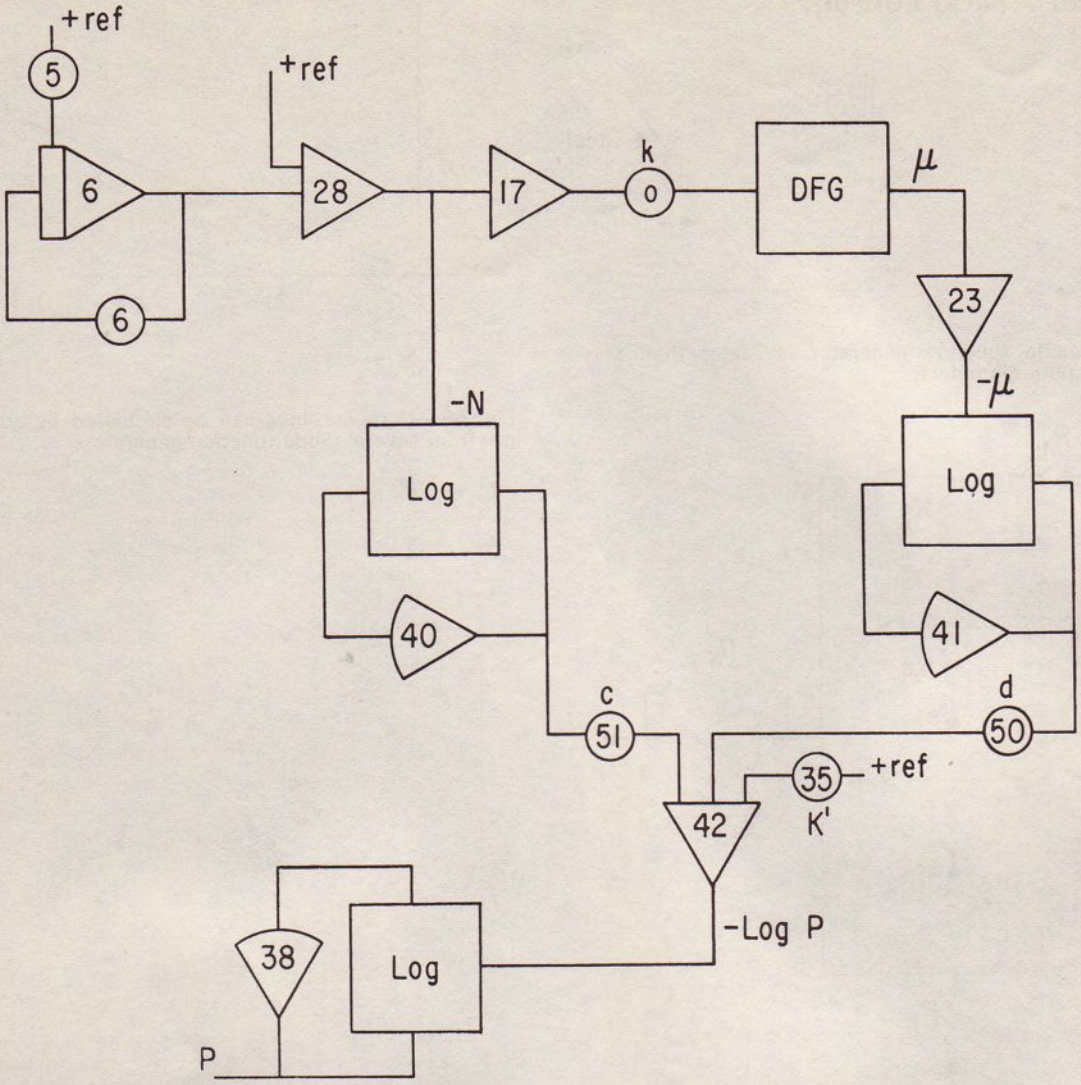


Fig. 61—This circuit solves the example problem.

Function Simulation. The process of simulating a function with diode function generators is one which involves setting the slopes and breakpoints of the various line segments which make up the approximation. It is clear that by setting e_o in Equation 110 a breakpoint may be fixed, and by setting R a slope may be fixed. The simplest diode function generators do not have a means of varying the location of breakpoints. Fig. 58 shows a simplified fixed breakpoint diode function generator.

A 10-volt computer with a 10-diode fixed breakpoint function generator would normally have breakpoints at 1-volt intervals. The slopes of each of the line segments are set by adjusting the values of resistors in the circuits shown in Fig. 58. Fig. 59 shows how the slopes of the first four line segments might be set to obtain the composite function shown as a dashed line.

It should be noted that as the independent variable x increases from x_o the dependent variable $f(x)$ follows the curve starting at x_o until x reaches the value x_1. At this point the next diode circuit conducts and the value of $f(x)$ is the sum of the curve starting at x_o and the curve at x_1. As x continues to increase each line segment adds in as the value of the breakpoint voltage corresponding to the function is reached. Most diode function generators contain an adjustment which permits the operator to translate the entire function $f(x)$ between the two extremes of machine voltage.

A fixed breakpoint diode function generator should only be used for functions that do not have sharp or closely spaced changes in slope. The variable breakpoint diode function generator has greater utility than the fixed breakpoint type because of the ease with which breakpoints may be adjusted to conform to the variations of the function. The procedure for the adjustment of breakpoints and slopes may vary depending upon the construction of the computer. Before attempting to generate a function by this technique the computer manual should be consulted for procedural details.

A simple method of setting up and checking a function is to follow these steps:

Step 1. Plot the desired function on a sheet of graph paper to a large scale.

Step 2. Locate breakpoints. If a fixed breakpoint function generator is used, the breakpoints are usually located at even voltages. If a variable breakpoint function generator is used, convenient points to locate breakpoints are at points of inflection. A great deal of judgment is needed

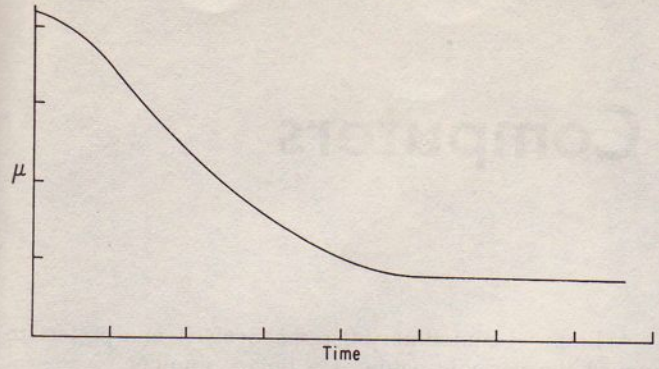


Fig. 62—How viscosity changes with startup time.

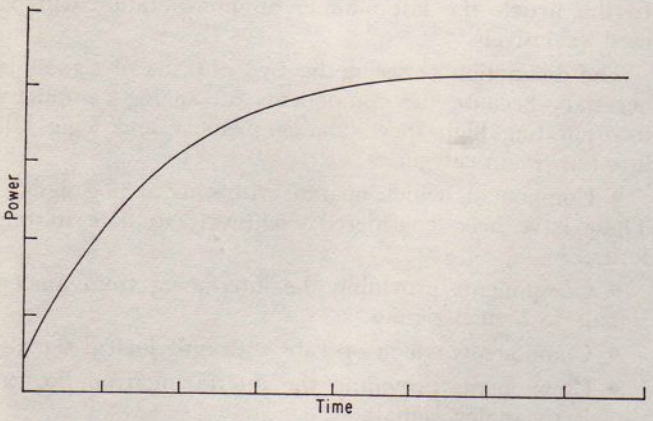


Fig. 63—Power requirements increase during startup.

TABLE 12—Diode Function Generator Settings

$\dot{\gamma}$	μ
0	1.000
1	0.998
2	0.977
3	0.932
4	0.865
5	0.780
6	0.667
7	0.537
8	0.462
9	0.412
10	0.378

TABLE 13—Pot Settings

Pot	Setting
0	0.788
5	0.884
6	0.176
35	0.011
50	0.021
51	0.834

to determine the best location of breakpoints. It should be noted that breakpoints must be separated by a specified voltage depending upon machine construction. Otherwise the diodes will interact.

Step 3. A table should be prepared listing breakpoint voltage and the value of the function at each breakpoint. It is some times helpful to approximate the function on the graph with straight lines between the breakpoints to obtain an idea of the shape of the function to be generated.

Step 4. Potentiometers may now be adjusted to obtain the proper value of $f(x)$ corresponding to each breakpoint voltage x. This may be conveniently done in the operate mode.

Step 5. A time ramp may now be applied as the independent variable and the generated function plotted with an x-y plotter. The plotted curve may be compared with the desired function and potentiometers adjusted until the two curves conform as well as possible.

An Example. Now consider the use of a diode function generator in a computer for a problem in which a non-Newtonian fluid is to be mixed. We are interested in the power required to mix this fluid and in particular the power required as the mixer starts and accelerates to its final speed. We assume that the mixer speed characteristics can be approximated by an exponential. The relationship between viscosity μ and shear rate $\dot{\gamma}$ for the non-Newtonian fluid is shown in Fig. 60. This relationship will be approximated with a 10-segment fixed breakpoint diode function generator. We will assume that there is a linear relationship between mixer speed N and shear rate γ of the form $N = k\dot{\gamma}$. We assume that the relationship

$$\frac{Pg_c}{\rho N^3 D^5} = K\left(\frac{\rho ND^2}{\mu}\right)^a \left(\frac{N^2 D}{g_c}\right)^b \qquad (111)$$

describes the mixing process, where:

P = power
N = speed
D = impeller diameter
ρ = fluid density
μ = viscosity
a,b = negative constants
K = constant

This relation may be reduced to

$$P = K' N^c \mu^d \qquad (112)$$

where
$$K' = K \rho^{1+a} D^{2a+b+5}/g_c^2 \qquad (113)$$
$$c = a+2b+3$$
$$a = -c$$

We may solve this equation with the computer circuit shown in Fig. 61.

By using Fig. 60 we may determine the functional values at each breakpoint. The function generator used in solving this example problem is of the fixed breakpoint type with breakpoints at 10 equally spaced intervals. The values of the function at each breakpoint are contained in Table 12. The pot settings used in this simulation are given in Table 13. The results of the simulation shown in Figs. 62 and 63 show that the viscosity decreases rapidly to a steady value and the power required increases almost exponentially.

Indexing Terms: Analogs-9, Calculus-6, Circuits-10, Computations-4, Computers-9, Descriptions-8, Diodes-10, Electricity-10, Engineering-4, Functions-6, Programing-7,10, Simulation-4.

Learn About Analog Computers

PART 8: MEMORY AND LOGIC–Only modest increases in these will give an analog computer a marked increase in problem-solving capabilities

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

The memory and logic aspects of analog computer implementation are of particular significance to the practicing engineer because of the marked increase in problem-solving capacity which results with even a modest increase in memory and logic capability. Trial and error procedures may be automated, the quantitative effect of parameter changes may be automatically determined, and operating conditions may be changed automatically during a simulation according to criteria specified by the programmer. With such options, among others, capable of being exercised during normal or repetitive analog operation, the analog computer becomes a very rapid and powerful tool for the solution of many problems of particular significance to chemical and petroleum engineers.

This particular area of analog computation is quite extensive and, with increasing sophistication, merges into the large field of techniques better described by the word hybrid. However, the material which will be presented here shall be restricted to the discussion and illustration of the use of analog memory and logic capabilities which are now commercially available on moderate size analog facilities.

The Distinction Between Analog Signal and Logical Signal. Before discussing the individual components used to achieve high speed analog memory and logic, it is convenient to first make the distinction between an analog signal and a logical signal. Thus far in this series, discussions have revolved around analog signals. These are the outputs from common analog components such as the summer, integrator, multiplier, etc. and have values which may range from plus reference to minus reference. Logical signals, on the other hand, have only two possible voltage values. For example, either 0 or 5 volts. These two possible values may be referred to in several equivalent manners as follows:

- HIGH and LOW respectively if one prefers to refer to the relative voltage levels.
- Binary 1 and Binary 0 respectively if one prefers to regard the variable value as a binary number.
- TRUE and FALSE respectively, thereby, retaining perhaps more closely the concept of a logical signal.

In this article the last manner of interpretation will be used exclusively.

The distinction between the two classes of signals is necessary because the components on analog computers incorporating high speed analog memory and logic fall into four main categories:

- Components which operate with only analog signals. These have been considered exclusively to date in this series.
- Components providing the interfacing from analog signals to logical signals.
- Components which operate with only logical signals.
- Components providing the interfacing from logical signals to analog signals.

An example perhaps best illustrates the types of components which falls into each of these four categories.

An Example. Consider the physical system indicated schematically in Fig. 64 in which the overflow from Tank 1 forms the input stream into Tank 2.

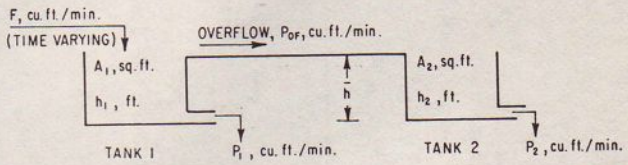


Fig. 64—The overflow from Tank 1 is the input stream into Tank 2.

Balances around Tank 1 and Tank 2 yield

$$A_1 (dh_1/dt) = F - P_1 - P_{OF} \tag{114}$$

and

$$A_2 (dh_2/dt) = P_{OF} - P_2 \tag{115}$$

Assuming $P_1 = f_1(h_1)$ and $P_2 = f_2(h_2)$ such that the mathematical model will not predict negative values of h_1 or h_2 nor permit the overflowing of Tank 2, the model is complete once the proper conditions are placed on $P_{OF} \equiv$ Overflow. These conditions are

$$P_{OF} = F - P_1 \text{ if } h_1 > \bar{h} \text{ and if } F > P_1 \tag{116}$$

otherwise

$$P_{OF} = 0 \tag{117}$$

The simulation of this system using components from each of the four component categories resolves into the following:

- Designing an analog circuit assuming the proper value of P_{OF} is available.
- Obtaining a logical signal (L_1) which is TRUE if $h_1 > \bar{h}$ and FALSE otherwise, and a logical signal ($\bar{L}_2$) which is TRUE if $F > P_1$ and FALSE otherwise.
- Obtaining a logical signal (L_3) which is TRUE if L_1 = TRUE and $\bar{L}_2$ = TRUE but FALSE otherwise.
- Choosing between $F - P_1$ and 0 for the value of P_{OF} depending on the value of L_3.

A preliminary circuit for the first step, assuming F is available, is completed as shown in Fig. 65.

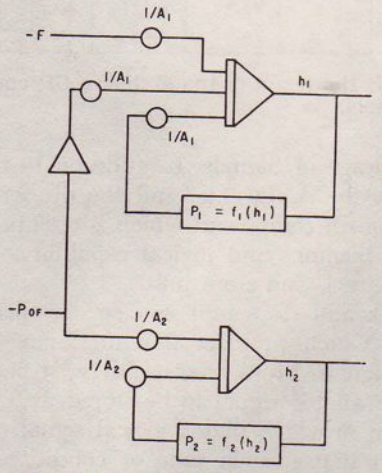
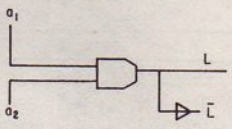


Fig. 65—This preliminary circuit determines the relation between feed rate and the heights in the two tanks.

The logical signals L_1 and $\bar{L}_2$ may be obtained using a component, known as the electronic comparator, having the symbol and characteristics given in Fig. 66. The indicated characteristics for this and other components presented may vary from machine to machine. It is suggested that compatability be established before using the circuits presented. The signals a_1 and a_2 are input analog signals, and L and $\bar{L}$ are output logical variables.



IF	THEN	
	L	L̄
$a_1 + a_2 > \epsilon$	TRUE	FALSE
$a_1 + a_2 < \epsilon$	FALSE	TRUE

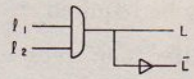
Fig. 66—The logic signal comes from an electronic comparator.

In Fig. 66, ε is the small voltage difference required for activation. It is of the order of a millivolt. The symbol $\bar{L}$ is called the logical complement of L and is obtained from an "Inversion" of a logical signal.

It is worth noting that the bang-bang circuit given in Part 6 of this series can be used as a comparator by making the proper choice for the lower and upper voltage levels.

Using an electronic comparator, the desired signal L_1 can be obtained by letting $a_1 = h_1$, $a_2 = -\bar{h}$, and $L = L_1$. Similarly $\bar{L}_2$ can be obtained by letting $a_1 = -F$, $a_2 = P_1$, and $\bar{L} = \bar{L}_2$.

The logical signal L_3 is obtained by operation on L_1 and $\bar{L}_2$ using a component known as the AND gate. The symbol and characteristics are given in Fig. 67 and l_1 and l_2 are input logical signals and L and $\bar{L}$ are output logical signals. L is referred to as the AND signal and $\bar{L}$ as the NAND (not AND) signal.

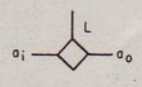


IF		THEN	
l_1	l_2	L	L̄
TRUE	TRUE	TRUE	FALSE
TRUE	FALSE	FALSE	TRUE
FALSE	TRUE	FALSE	TRUE
FALSE	FALSE	FALSE	TRUE

Fig. 67—The AND gate gives the logic signal L_3.

Letting $l_1 = L_1$, $l_2 = \bar{L}_2$, and $L = L_3$, the third step of the example is completed.

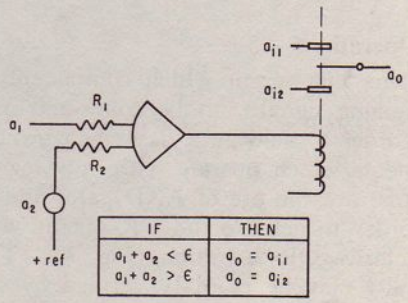
The final step incorporates the use of a component known as the electronic switch. Its characteristics and symbol are given in Fig. 68 where L is an input logical signal, a_i is an input analog signal, and a_o is an output analog signal.



IF L IS	THEN
TRUE	$a_o = a_i$
FALSE	OUTPUT IS GROUNDED

Fig. 68—An electronic switch is used to let the input logical signal control the analog output signal.

As noted in Part 6 of this series, relay switches operating with only analog signals are available. A schematic diagram, together with operational characteristics, of one such switch is given in Fig. 69.



IF	THEN
$a_1 + a_2 < \epsilon$	$a_o = a_{i1}$
$a_1 + a_2 > \epsilon$	$a_o = a_{i2}$

Fig. 69—Analog signal switching can also be accomplished with a relay circuit.

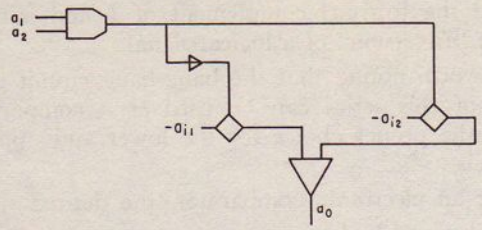


Fig. 70—This electronic circuit is equivalent to the relay signal switching shown in Fig. 69.

The electronic equipment required to achieve the equivalent is given in Fig. 70.

For normal speed of analog operation the relay switch is usually quite satisfactory. For repetitive, high speed operation, however, the wear and required switching time can be excessive. The electronic switch has no such limitations and its use is highly recommended over the use of the relay switch for those cases in which a rapid switching rate may be required.

The results of the four steps may now be combined in order to obtain a circuit for the example problem. The circuit, exclusive of scaling, is given in Fig. 71.

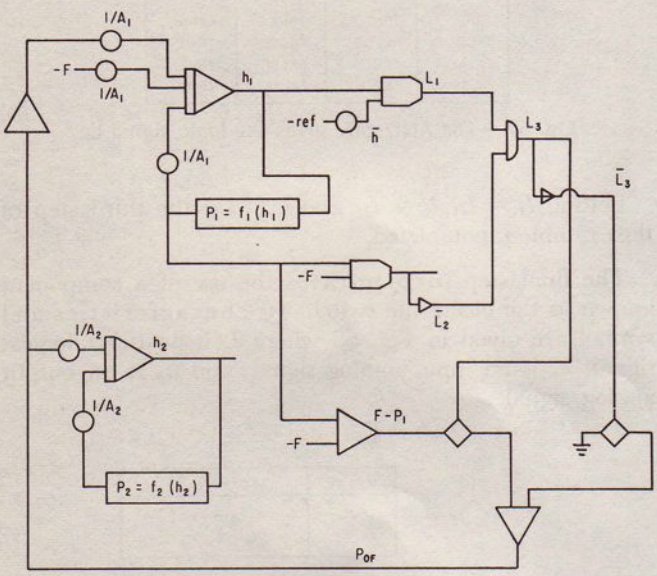
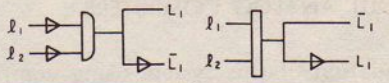


Fig. 71—This combined circuit for the overflow program does not include scaling.

The reader may verify that the example could also be solved using a relay switch and a limiter in order to impose the conditions on P_{OF}. Speed limitations and diode rounding would, however, restrict accuracy of solution, particularly for high speed, repetitive operation.

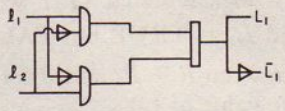
The OR Operations

In the same manner in which components operating with only analog signals can be connected in a variety of ways in order to achieve a desired operation, so may the components which operate with only logical signals. Two examples are the use of AND gates and logical inverters in order to achieve the OR operation (Fig. 72) and the exclusive OR operation (Fig. 73). The validity of the circuits may be readily verified by sequentially following the possible sets of input values through the circuit.



IF		THEN	
l_1	l_2	L_1	$\bar{L}_1$
TRUE	TRUE	FALSE	TRUE
TRUE	FALSE	FALSE	TRUE
FALSE	TRUE	FALSE	TRUE
FALSE	FALSE	TRUE	FALSE

Fig. 72—The symbol on the right is a simplified schematic of the one on the left. This is an OR operation.

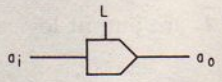


IF		THEN	
l_1	l_2	$\bar{L}_1$	L_1
TRUE	TRUE	TRUE	FALSE
FALSE	TRUE	FALSE	TRUE
TRUE	FALSE	FALSE	TRUE
FALSE	FALSE	TRUE	FALSE

Fig. 73—L_1 is the result of the exclusive OR operation on the l_1 and l_2 signals.

Point Storage of Signals. In addition to the electronic comparator, the AND gate, and the electronic switch, there is a fourth component which is essential for a basic, high speed memory and logical capability. This component is the track and store unit.

The track and store unit can be classified as being a component which provides the interfacing from logical to analog signals. More specifically, it permits a point value of an analog signal to be stored at a specific time or condition provided that a logical signal change corresponding to that specific time or condition can be synthesized. The symbol and characteristics are detailed in Fig. 74 where a_i is the input analog signal, a_o is the output analog signal, and L is the input logical signal. During the condition referred to as track, an internal capacitor is charged by the input analog signal. During the condition referred to as store, the input analog signal is not connected to the capacitor and the charge which existed on the capacitor the last time the input was connected provides the output analog signal.



IF	THEN	
L	CONDITION	
TRUE	TRACK	$a_o = -a_i$
FALSE	STORE	$a_o = -a_i$ LAST TIME L WAS TRUE

Fig. 74—This is a track and store unit.

Track and Store Units. There are numerous ways in which the track and store units can be used to great advantage during the solution of engineering problems on the analog. Several of these are outlined below.

Use of a Single Track and Store Unit. It is frequently the case during the completion of process designs that a particular value of a particular analog variable is of primary concern. This may be the maximum value of the

temperature in a reactor, the length of a reactor required to achieve a desired conversion, the percent recovery obtained with a given gas absorber, etc. The process of finding this particular value can be automated using a single track and store unit provided the proper logical signal can be synthesized. The restriction is that the logical signal must change only at the desired condition.

Suppose, for example, that it is desired to determine the maximum temperature in a flow reactor. First an analog circuit is designed for calculating T versus reactor bed length, x. If preliminary calculations have shown that the temperature increases with length to the maximum and then continuously decreases, the maximum temperature may be automatically determined as shown in Fig. 75.

During a single computer run, A will be equal to T until $dT/dx = 0$ and thereafter A will remain constant at T_{max}.

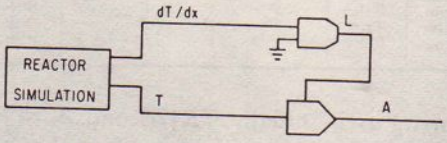


Fig. 75—A circuit to determine the maximum temperature of a flow reactor bed.

Transfer of a Point Value from One Analog Circuit to Another. The output of the track and store unit can be used for further analog calculation in the same manner that the output from a summer, integrator, etc. may. Consider, for example, the case in which a reactor-absorber system such as shown in Fig. 76 is to be simulated.

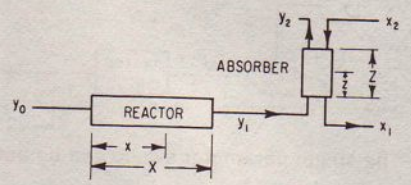


Fig. 76—The output composition y_2 depends upon all of the other compositions and dimensions shown here.

Given an analog circuit for finding y vs. x, by integrating dy/dx, for the reactor and another for finding y vs. z, by integrating dy/dz, within the absorber, assume that it is desired to determine the absorber height required to reduce y_2 to $f(y_1)$, $0 < f < 1$, when y_o and X are known. The process of first solving the reactor and then the absorber is to be automated by making one run to determine $y|_{x=X}$ from the reactor (during which time the absorber results are ignored) and then a second run in which the absorber equations are to be solved for Z. Determining $y|_{x=X}$ is indicated in Fig. 77. However, upon placing the computer in reset mode so that the absorber circuit may be initialized before solving, x drops to zero and the track and store unit begins to track $y = y_o$. As a consequence, $y|_{x=X}$ is lost. In order to achieve the transfer, two track and store units must be used in series as shown in Fig. 78. This arrangement is commonly referred to as the "bucket bridgade."

The sequence of events which occur for the example

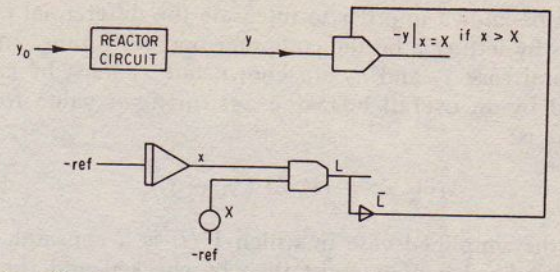


Fig. 77—The reactor-absorber in Fig. 76 is simulated.

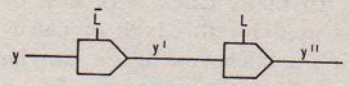


Fig. 78—A bucket brigade circuit.

problem during the process of making two runs are as follows:

- During the first run, y' is initially equal to $-y$ since $\bar{L}$ is TRUE. y'' is equal to the value of $-y'$ the last time L was TRUE since L is now FALSE (This value is zero in this case if the computer was placed in the pot set, the reset, and then the operate mode when the run was started).
- When $x > X$ occurs, $\bar{L}$ becomes FALSE and $y' = -y|_{x=X}$. However, L becomes TRUE and y'' represents the tracking of $-y'$. Consequently, $y'' = y|_{x=X}$.
- Upon placing the computer in the reset mode in order to begin the second run, $\bar{L}$ becomes TRUE and $y' = -y_o$. L is now, however, FALSE and thus y'' is equal to the value of y' the last time L was TRUE. ($y'' = y|_{x=X}$ obtained during the first run.)
- When the computer is placed in the operate mode for the second run, y'' will remain $= (y|_{x=X}$ obtained during the first run) until $x > X$, at which time $y'' = (y|_{x=X}$ obtained during the second run).

Using the bucket bridgade to insure the proper transfer of $y|_{x=X}$, the reactor-absorber system may be solved automatically in two runs by incorporating the circuit indicated in Fig. 79. The signal A will be equal to the desired value of Z during the latter portion of the second run.

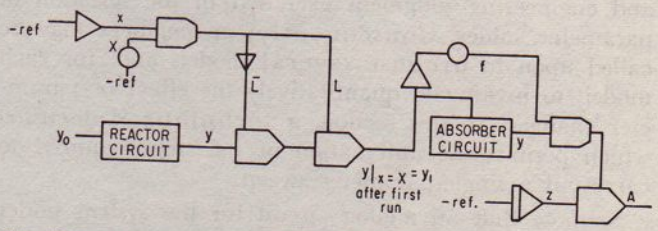


Fig. 79—A complete simulation of the reactor-absorber shown in Fig. 76.

Iterative Solutions Using Point Analog Values. In the above example, the bucket bridgade was used to transfer a point analog value from one analog circuit to another during the reset period between runs. A closely analogous situation arises in those cases in which point analog values are used in iterative solutions.

Consider as an example the calculation of the percent recovery in a gas absorber of known height. (Refer to Fig. 76 for a schematic of an absorber). Assuming that a differential equation of the form $dy/dz = f(x,y)$ is available for the absorber, the value of y_1 and x_1 must

both be known in order to integrate the differential equations by letting z be the computer operating time. In the general case y_1 and x_2 are known but x_1 must be calculated by an overall balance assuming a value for y_2. That is:

$$x_1 = x_2 + (V/L)\,(y_1 - y_2) \qquad (118)$$

for the simplified case in which V/L is a constant. The assumed value of y_2 must then be checked and the calculation repeated using another assumed value if a significant error is observed. In many cases, a process of iterative substitution can be used for this type of calculation. The manner in which a bucket bridgade can be used for the iterative solution of the recovery in an absorber is indicated in Fig. 80.

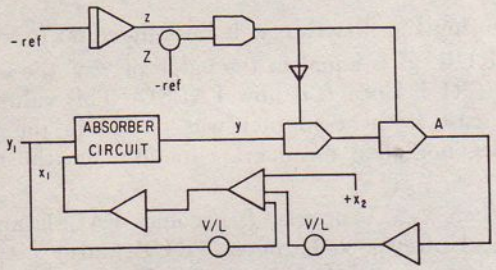


Fig. 80—A iterative solution can be employed.

The signal A, during the period of calculation in which $z < Z$, will be equal to the value of y_2 which was calculated during the last run. When $z > Z$, y_2 is updated. By then placing the computer in reset, a new run may be begun using the updated value of y_2. Such an iterative calculation can be completed automatically by placing the computer in repetitive operation mode during which time the computer is automatically cycled between the reset and the operate modes.

Single Parameter Sweep. Very seldom is the practicing engineer's primary concern the solution of a neatly defined mathematical model. In the general case, assumptions of dubious physical validity must be investigated and engineering judgment exercised in the selection of parameter values. Consequently, an engineer may be called upon to propose several models and, for each model, to investigate quantitatively the effect of parameter changes. In this section, a technique is discussed which permits the automation of the steps required to carry out a single-parameter sweep.

Suppose that an analog circuit for the system under consideration is available and that a bucket bridgade has been designed so that a desired point value of an important analog signal can be retained for plotting versus the parameter P. (See Fig. 81)

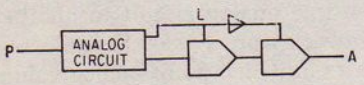


Fig. 81—A bucket brigade for a single parameter.

Assuming that the analog circuit is in the repetitive operation mode with an operate period of at least Z, which is in turn greater than the time required for L to change to FALSE, it is desired to automate the following procedure:

- Maintain P at a fixed value during the operating period for Z time units.
- When the computer resets, increment (or decrement) the fixed value of P by an amount ΔP. The value of A will then be plotted versus P while the computer is in repetitive operation.

The solution utilizes a configuration of track and store units called the accumulator which is given in Fig. 82.

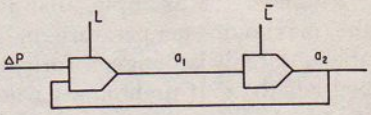


Fig. 82—The accumulator circuit.

TABLE 14—The Sequence of Events in an Accumulator

Event	L	$\bar{L}$	a_1	a_2
1	True	False	$-P-\Delta P$	P
2	False	True	$-P-\Delta P$	$P+\Delta P$
3	True	False	$-P-\Delta P-\Delta P$	$P+\Delta P$
4	False	True	$-P-\Delta P-\Delta P$	$P+\Delta P+\Delta P$
5	True	False	$-P-\Delta P-\Delta P-\Delta P$	$P+\Delta P+\Delta P$

Assuming L is initially TRUE and $a_2 = P_1$, the sequence of events occurs as L changes as shown in Table 14. Thus from the time at which $\bar{L}$ becomes FALSE to the time it becomes FALSE again, a_2 remains constant, but a_2 is incremented by ΔP each time $\bar{L}$ becomes FALSE.

In order to automate the steps for the parameter sweep, one needs only use the output of the accumulator for the parameter value and use the operating time z to synthesize the logical signal L. The completed circuit is given in Fig. 83.

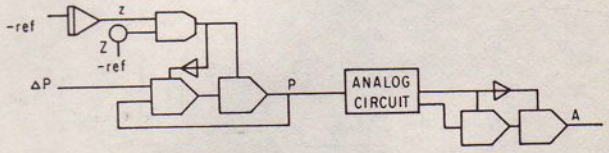


Fig. 83—The single parameter sweep can be automated.

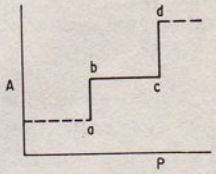


Fig. 84—The results from the circuit of Fig. 83.

A plot of A versus P would have the characteristics given in Fig. 84. The desired point values of the analog variable as a function of P are given by the points b, d, etc. If P is sufficiently small, the plot will appear to be continuous.

Two Parameter Sweep. Consider next the case indicated schematically in Fig. 85 for which it is desired to automatically determine A as a function of P_1, in increments of ΔP_1, and P_2, in increments ΔP_2, by operating the

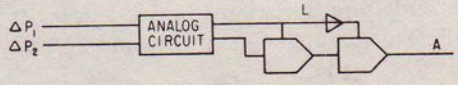


Fig. 85—A two parameter sweep circuit.

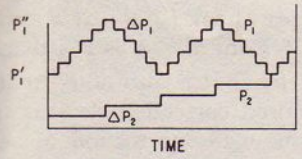


Fig. 86—The results from the circuit of Fig. 85.

circuit in the repetitive operation mode. It is desired to design a circuit which will change P_1 and P_2 in the manner shown in Fig. 86.

With ΔP_1 sufficiently small and ΔP_2 rather large, a plot of A versus P_1 will appear continuous with P_2 being a parameter on the plot.

The circuit in Fig. 87 permits the desired changes to be made in P_1.

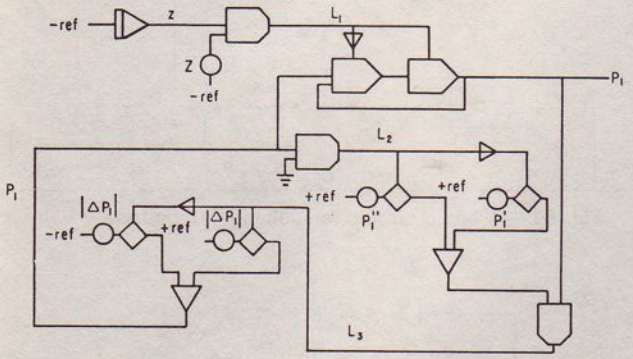


Fig. 87—A circuit to determine the change in P_1.

The logical signal L_1 determines the rate at which P_1 is incremented. The logical signal L_2 establishes whether ΔP_1 is positive or negative. If ΔP_1 is positive, P_1 is compared with P_1''; otherwise with P_1'. The logical signal L_3 permits the sign of ΔP_1 to be changed. If ΔP_1 is initially positive and $P_1 - P_1'' < \varepsilon$, a positive ΔP_1 is retained. However, when $P_1 - P_2'' > \varepsilon$ occurs, a negative ΔP_1 is specified. The negative ΔP_1 causes P_1 to be compared with P_1'. The sign of ΔP_1 becomes positive again when $P_1 - P_1' < \varepsilon$ first occurs and P_1 is again compared with P_1''. In this manner, the cycling of P_1 is insured.

In order to increment P_2 in the desired manner, the circuit given in Fig. 88 has been used. The signals P_1 and L_3 are obtained from the circuit in Fig. 87.

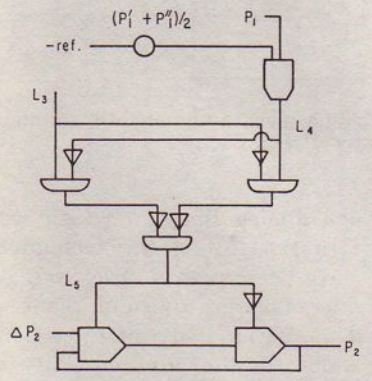


Fig. 88—A circuit to determine the change in P_2.

It is to be noted L_5 is the result of an exclusive OR operation on L_3 and L_4. Thus L_5 is TRUE if only L_3 is TRUE or if only L_4 is TRUE and L_5 is FALSE otherwise. The sequence of events given in Table 15 occurs as P_1 undergoes cycling. Assume ΔP_1 is initially positive and P_1 is at the minimum.

TABLE 15—The Sequence of Events as P_1 and P_2 Undergoe Cycling

Event	ΔP_1	L_3	L_4	L_5	P_2
	+	False	False	False	P_2
P_1 surpasses $(P_1'' + P_1')/2$	+	False	True	True	P_2
P_1 surpasses P_1''	+	True	True	False	$P_2 + \Delta P_2$
ΔP_1 changes sign	−	True	True	False	$P_2 + \Delta P_2$
P_1 becomes less than $(P_1'' + P_1')/2$	−	True	False	True	$P_2 + \Delta P_2$
P_1 becomes less than P_1'	−	False	False	False	$P_2 + \Delta P_2 + \Delta P_2$
ΔP_1 changes sign	+	False	False	False	$P_2 + \Delta P_2 + \Delta P_2$

The next event will again be the first entry into Table 15 and thus the desired changes in both P_1 and P_2 have been logically achieved.

The final circuit for a two-parameter sweep is obtained by combining the circuits shown in Figs. 85, 87 and 88.

Solution of Boundary Value Problems. Boundary value problems can be regarded as the generalization of the class of problems mentioned earlier in the section, "Iterative Solutions Using Point Analog Values." There an unknown input to the analog circuit was identical to a desired analog output. In the general case, it is known that an unknown input is a function of a desired output but the functionality is not available. The manner in which the required trial and error calculations may be automatically completed is discussed in this section by

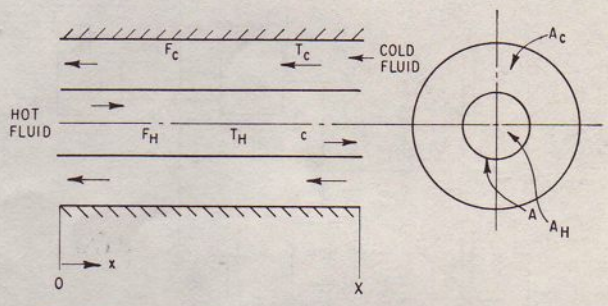


Fig. 89—A double-pipe reactor with heat exchange.

TABLE 16—Nomenclature for the Boundary Value Problem

Variable	Definition	Units
A	surface area per unit length	sq. ft./ft.
A_H	crosssectional area available for flow of hot fluid	sq. ft.
A_c	crosssectional area available for flow of cold fluid	sq. ft.
c	mass fraction of reactive species	lb_c /lb
c_p	heat capacity	BTU/(lb) (°R)
D	diameter of inner pipe	ft
E	activation energy divided by the gas constant	°R
F_H	mass flow rate of hot fluid	lb/sec
F_c	mass flow rate of cold fluid	lb/sec
ΔH	heat of reaction	BTU/lb_c
k	reaction rate constant	(cu ft, sec)$^{-1}$
X	length of exchanger	ft.
T_H	temperature of hot fluid	°R
T_c	temperature of cold fluid	°R
v_H	velocity of hot fluid	ft/sec
v_c	velocity of cold fluid	ft/sec
U	overall heat transfer coefficient	BTU/(sec) (sq. ft.) (°R)
x	length along exchanger	ft
y	reaction rate	(cu. ft., sec)$^{-1}$
ρ	fluid density	lb/cu. ft.

Special Symbols Used With Variables

* superscript to indicate expected maximum value of a variable.
– overscore to indicate an initial or a desired value.
· dot over variable to indicate the first derivative with respect to exchanger length.

TABLE 17—System's Equations

Cold Fluid:

$\dot{T}_c = U\,A\,(T_c - T_H)/(F_c\,C_p)$

where U, A, F_c, C_p, and T_c at $x = X$ are assumed to be known.

Reaction Rate:

$y = k\,e^{-E/T_H}$

or

$\dot{y} = E\,\dot{T}_H\,y/(T_H^2)$

where E and k are assumed to be known.

Reactive Species:

$\dot{c} = c\,y/v_H$

where v_H and c at $x = 0$ are assumed to be known.

Hot Fluid:

$\dot{T}_H = U\,A\,(T_c - T_H)\,(F_H\,C_p) + \Delta H\,y\,c/(v_H\,C_p)$

where F_H, ΔH, and T_H at $x = 0$ are assumed to be known.

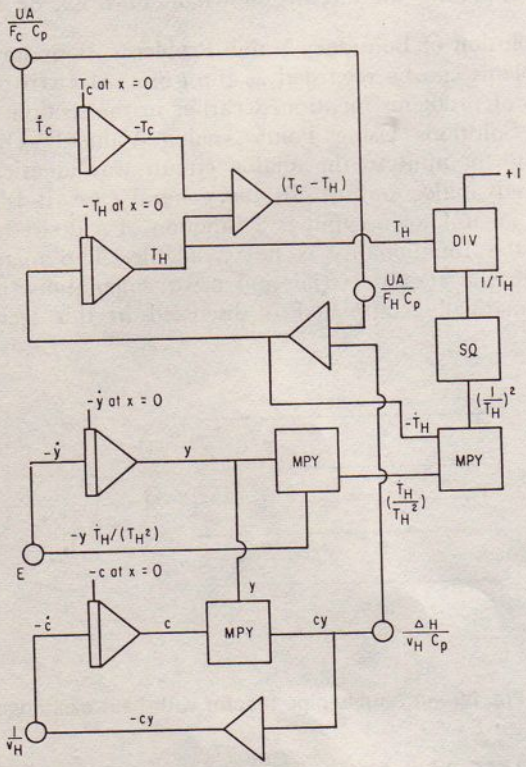


Fig. 90—The preliminary circuit for the reactor of Fig. 89.

considering the simulation of an exothermic reaction in a double-pipe heat exchanger. A schematic of the chosen system is given in Fig. 89. Table 16 summarizes the notation used.

If it is assumed that component c undergoes an exothermic, irreversible, first-order, temperature dependent reaction as it flows through the reactor, the differential equations presented in Table 17 may be derived in order to describe the system. The preliminary analog diagram given in Fig. 90 may be designed.

Since the value of T_H and c at $x = 0$ are assumed known, $\overline{T}_H = T_H$ at $x = 0$, $\bar{c}$, and $\bar{y}$ are known. However, the value of T_c is known at $x = X$. In order to solve the problem it is necessary to assume a value of T_c at $x = 0$, check to see if $T_c = \overline{T}_c$ at $x = X$, and to repeat the calculation using a new value if an appreciable error exists. The relationship between T_c at $x = 0$ and at $x = X$ is not explicitly known, but from physical considerations it is noted that if T_c at $x = 0$ increases, T_c at $x = X$ will also.

Thus if T_c at $x = X$ is larger than $\overline{T}_c$, T_c at $x = 0$ should be decreased. Similarly if T_c at $x = X$ is less than $\overline{T}_c$, T_c at $x = 0$ should be increased. It is also noted that as the error decreases, the required correction decreases. As a first approximation assume the correction to be made is proportional to the error. With this assumption, letting K be the proportionality constant, it may be verified that the addition of an accumulator to the preliminary circuit will permit the proper corrections to be made as the analog circuit is cycled between the reset and operate modes. The resulting unscaled circuit is given in Fig. 91.

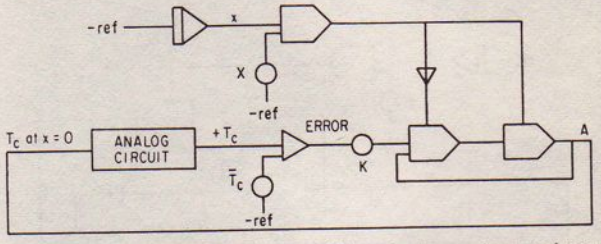


Fig. 91—A basic circuit for solving for boundary values.

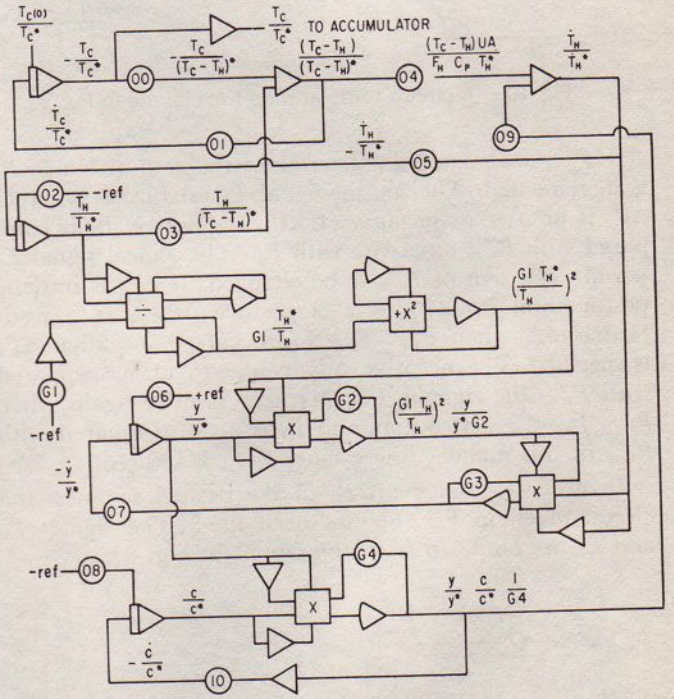


Fig. 92—A scaled analog circuit gives a numerical illustration of the solution of the reactor of Fig. 89.

Fig. 92 presents a scaled analog diagram which was prepared for numerical illustration of this technique. Pots G_1, G_2, G_3, and G_4 have been used in order to scale the outputs from the divider, squarer, and multipliers so that errors are minimized in the serial use of these nonlinear components. The values of the required pots are summarized in Table 18.

Using the numerical values given in Table 19, the plot given in Fig. 93 was obtained by guessing T_c at $x = 0$ to be zero initially, and then cycling the computer between

reset and operate. From the plot it is seen that $\bar{T}_c - T_c$ at $x = X$ was reduced to an insignificant amount after only 6 trials. In Fig. 94, the profiles obtained for T_H, T_c, c, and y after convergence was achieved are summarized.

The illustrated technique finds general applicability in the solution of boundary value problems. It is necessary to know only the following:

TABLE 18—Pot Settings for Fig. 92

Pot	Value
00	$T_e^*/(T_e - T_H)^*$
01	$U\,A\,(T_e - T_H)^*/(F_c\,c_p\,T_e^*\,B)$
02	$\bar{T}_H/T_H^*$
03	$T_H^*/(T_e - T_H)^*$
04	$U\,A\,(T_e - T_H)^*/(F_H\,c_p\,T_H^*)$
05	$\dot{T}_H^*/(T_H^*\,B)$
06	$\bar{y}/y^*$
G1	Such that $(G1\,T_H^*/T_H)_{max} \simeq$ **REF**
G2	Such that $[(G1\,T_H^*/T_H)^2\,(y/y^*)\,(1/G2)]_{max} \cong$ **REF**
G3	Such that $[(G1\,T_H^*/T_H)^2\,(y/y^*)\,(1/G2)\,(\dot{T}_H/\dot{T}_H^*)\,(1/G3)]_{max} \cong$ **REF**
07	$E\,G2\,G3\,\dot{T}_H^*/(G1^2\,T_H^{*2}\,B)$
08	$\bar{c}/c^*$
G4	Such that $[y\,c/(y^*\,c^*\,G4)]_{max} \cong$ **REF**
09	$[\Delta H]\,y^*\,c^*\,G4/(v_H\,c_p\,\dot{T}_H^*)$
10	$y^*\,G4/(v_H\,B)$

TABLE 19—Numerical Values of Parameters

$\bar{T}_H$ = 500° R	k = −1750 (sec)$^{-1}$	$(T_e - T_H)^*$ = 800° R
$\bar{T}_e$ = 500° R	E = 3000 °R	$\dot{T}_H^*$ = 2000° R/ft
$\bar{c}$ = 1 lb_c/lb	ΔH = −330 BTU/lb_c	y^* = −100 (sec)$^{-1}$
X = 10 ft	ρ = 60 lb/ft^3	B = 1 sec/ft
U = 0.1 BTU/(sq. ft.) (sec) (°R)	v_e = 4 ft/sec	G1 = 0.5
	F_c = F_H	G2 = 0.235
D = 1/12 ft	T_H^* = 1000° R	G3 = 1.0
v_H = 4 ft/sec	T_e^* = 800° R	G4 = 0.240
c_p = 1 BTU/(lb) (°R)	c^* = 1 lb_c/lb	

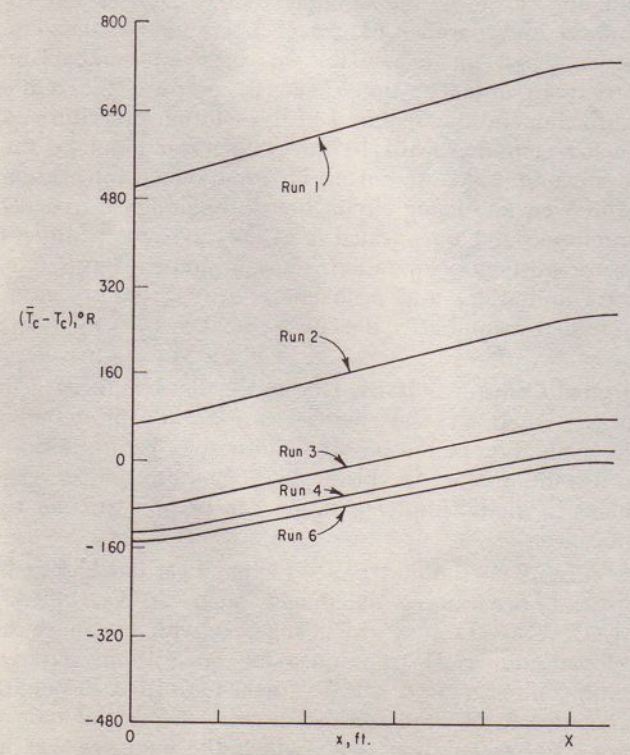


Fig. 93—The computer was cycled between reset and operate.

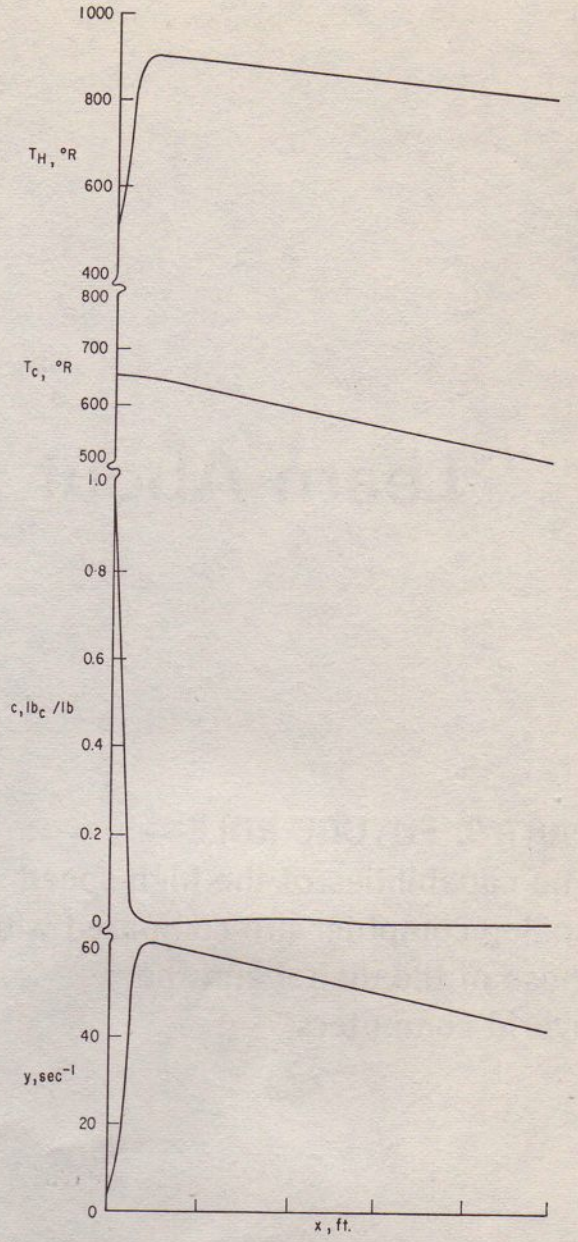


Fig. 94—Other numerical values from the computer program.

- Direction in which a correction must be made when an error exists.
- Approximate magnitude of the required correction. The latter is generally determined by trial and error on the value of K.

By placing the computer in the repetitive operation mode, the required trial and error is generally completed so rapidly that the time for a solution is not noticed. Due to the high speed, parameter changes may be made and, for all practical purposes, the instantaneous solution is continuously shown on the output oscilloscope.

In the next article of this series, more sophisticated applications and capabilities will be qualitatively discussed and a summary will be given of this series in retrospect to the developments in the field of digital simulation.

Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Electricity-10, Engineering-4, Logic-9, Memories-9, Programing-10, Simulation-4.

Learn About Analog Computers

PART 9: FUTURE ROLE— The capabilities of the high-speed analog computer are compared with those of the digital and the hybrid computers

Theodore W. Cadman and **Theodore G. Smith**
University of Maryland, College Park, Md.

THROUGHOUT THIS SERIES, attention was drawn repeatedly to the use of the analog computer for solving sets of ordinary—linear or nonlinear—differential equations such as those frequently used to describe the dynamic or steady-state characteristics of processing systems. The applicability of the analog was noted to result from the availability of the hardware integrator which permits integration over a wide range of time scales, the continuous and parallel nature of analog operation, and the availability of analog components which perform other required mathematical operations on the voltages used to represent the independent variables. These characteristics, coupled with provisions for oscilliscope and x-y plotter displays made the analog computer an excellent tool for the rapid solution and convenient examination of the solutions of differential equations.

The achievement of the full potentials of the analog did not, however, immediately follow. Due to the continuous and parallel nature of operation, analog components had to be available in sufficient numbers and variety in order to simultaneously perform the mathematical operations required in the solution procedure. An analog computer with 10 integrators could not be used to solve a problem requiring 11 simultaneous integrations. Moreover, an analog circuit had to be designed, patched, amplitude and time scaled, and checked out in order to insure satisfactory operation. Thus, in simplest terms, hardware limitations and problem preparation procedures were detrimental attributes of the analog.

Digital Computer Uses. Due to the disadvantages of the analog computer, the engineer is naturally interested in the evaluation of the possible alternatives before deciding to use the analog. In this evaluation, the recent developments in digital implementation can be of particular significance.

Since about the mid 1950s, the engineer has had at his disposal programing languages such as FORTRAN, MAD, ALGOL, etc., which, together with previously developed numerical techniques for integration, differentiation, interpolation, and so forth, permitted the digital computer to be used for the discrete, sequential type of numerical calculations with which the engineer was already familiar. Such languages permit digital programing

An engineer should evaluate alternatives when deciding to use the analog computer

to be achieved fairly easily and allow the programer to make full use of the flexibility of the digital computer.

Programing the digital computer is, however, quite detailed and care must be taken to insure the proper logical sequence of operations required for solution. Moreover, a program, once developed, tends to be specific in nature and not readily subject to extensive modification. If one neglects the comparison of the time required for solution and chooses a problem which is amenable to both analog and digital solution, the balance between the time spent on analog setup and the time devoted to the development of a digital program using a procedure oriented language heavily depends on the past experience of the potential user.

The state of affairs with regard to ease of digital programing has, however, been markedly changing during the past few years. First, there has been a proliferation of user-oriented languages aimed at reducing to a minimum the complexity of programing certain specific classes of problems. Particularly to be noted in conjunction with this series are a group of languages (MIDAS, MIMIC, DSL/90, just to name three of several dozen) referred to as digital simulation languages. Some of their important characteristics are:

- They are specifically oriented towards the numerical solution of ordinary differential equations and are principally aimed at simulating analog operation on the digital exclusive of the scaling and storage restrictions of the analog.
- Very little previous exposure is required for their comprehensive use.
- The burden of prescribing solution procedure as well as the error check of numerical procedures such as integration are removed from the user.
- Their use permits a very significant reduction in the time spent in problem preparation over that required for a comparable solution on the analog or with a procedure-oriented digital language.[11]

Digital simulation languages are becoming ever increasingly more popular. Developments will undoubtedly continue and potentially can very markedly reduce the time required for programing a digital to provide numerical solutions to partial as well as ordinary differential equations, boundary value problems, and classes of iterative calculations. The use of one of these languages requires a large computer because of the storage needed for the program.

The second marked change in digital inplementation which can be observed is the continual increasing in the degree of user-machine communication. Remote teletype terminals are now commonly used at installations equipped with a time sharing digital facility. These systems are very convenient for digital "debugging" of procedure-oriented based programs and on-the-spot solution of small to moderate sized problems. The future may very well witness the extensive development of user-oriented languages for use with teletype terminals, thereby significantly enhancing even more user-machine communication.

Other possibilities for the future revolve around active work being done to communicate with the digital computer by means of the written word. Here the objective is to develop means by which the user can write his problem on specially prepared paper and have the digital computer formulate his problem in detailed terms, construct a program, run the program, and finally deliver the results to the user. Communication by means of voice is also being seriously considered.

Of particular interest to design engineers is work currently being carried out with the objective of communicating with the digital by means of large oscilliscopes. Technology has probably advanced to the point where today it would be possible to develop a system which would require the following sequence of steps for an engineer to calculate the dynamic response of a plant complex:

- Specify the equipment and interconnections in the plant complex, using a light pen, on an oscilliscope.
- Specify, either on the scope or by means of cards and/or tapes, the parameters required, the conditions to be imposed, and the results desired.
- Press a button and have the digital solve the problem and display the desired dynamic response(s) on the scope.

Although such a facility would be inherently complex in its makeup, the user could be completely unaware of the complexity and be directly concerned only with drawing lines using a light pen, specifying operating conditions, and interpreting results.

Potential of Analog Computers. With the digital simulation languages now available and with the possibility of reducing communication with the digital computer to typewritten material, oscilliscope displays, the hand written word, or even voice, is the use of the analog in engineering to become passé in the forseeable future? The answer is an emphatic NO!

In contrast to an analog computer, a digital computer is slow. The digital operates on discrete values in a sequential manner in order to obtain a solution. For a given problem and procedure the number of discrete values

which must be used in order to obtain a satisfactory approximation has a fixed lower value. Consequently for a given machine, the time required for a satisfactory solution also has a fixed lower value since the values must be operated on sequentially according to the procedure being used. For the simulation of inherently continuous systems, this required time may be excessive. The presence of nonlinearities and higher frequency fluctuation of problem values tend to markedly increase the required time. The size of the problem to be solved has a direct bearing on the required time.

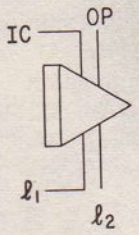
Analog operation is, however, continuous and parallel in nature. Its speed of operation can be chosen by the user. A solution may be obtained over a period of several minutes or in a few thousandths of a second for a great variety of problems. The time required is virtually independent of nonlinearities and frequency fluctuations can cover a very wide range. Solution time does not depend on the number of equations being simultaneously solved. As a consequence of these analog characteristics, the time required for a comparable solution on the digital can be several orders of magnitude larger than the time required for an analog solution. Thus the long term potential of the analog lies in its ability to simulate continuous systems in a very rapid fashion. This speed potential coupled with already developed mechanisms for a high degree of user-machine interaction establishes the analog as a very powerful engineering tool for the foreseeable future despite the present and projected advances in digital software for programing ease and user-machine communication.

The more recent developments in the field of analog computation have been directed towards the more efficient utilization of the inherent power of the modern electronic analog. In Part 8 of this series, four high-speed components which permitted automation in several aspects of analog implementation were presented. Particularly noted was the role of directly or indirectly synthesized logical signals in their use. The electronic comparator provided means for generating logical signals by comparing analog signals; the AND gate permitted comparison of logical signals; the electronic switch permitted an appropriate analog signal to be logically chosen, and the track and store unit permitted logical storage of the point value of an analog signal. Used collectively they were shown to provide means for automating trial and error calculations, the imposition of conditions during a computer run, and the process of obtaining parameter sweeps. These applications, together with the numerous others possible, relieve the user of the necessity of making many tedious changes in the analog parameters or circuit during or between analog runs and permit the effective utilization of analog solutions which may be obtained at a rate of up to about 1,000 per second.

Even the impressive applications which have been discussed are, however, overshadowed by the capabilities of the larger modern analog computers commercially available. It is our objective here to indicate briefly some of these more sophisticated capabilities.

Automatic Control of Integrator Operation. Essential to the more effective utilization of the speed potential of the analog is the ability to automatically control its operation. We have already seen the additional degree of control which the electronic switch permits and the usefulness of the track and store unit for controlled memory of point values of analog variables. The basic control of an analog circuit lies, however, in the integrators.

On smaller analogs the operation of the integrators may be specified manually to be reset, hold, or operate or the integrators may be operated in repetitive mode, cycling between reset and operate for specified periods of time. On the modern larger analogs, integrators may be logically controlled in a manner such as that indicated in Fig. 95.



If		Then
IC	OP	State of Integrator
True	True or False	Reset
False	True	Operate
False	False	Hold

If		Then
l_1	l_2	Time Constant = 1/RC
False	False	1 second
False	True	0.1 second
True	False	0.001 second
True	True	0.0001 second

Fig. 95—Logical control for an integrator.

With the logical signals *IC* and *OP*, the user has the ability to automatically control the state of the integrator. The logical signals l_1 and l_2 permit the speed of integration to be varied from a time constant of 1 second, corresponding to normal speed of operation, to 10,000 times faster than normal.

One can use the resulting capabilities in completing a parameter sweep, for example. The parameter to be varied could be the output from an integrator which remains in operate with a time constant of 1 second while the system being simulated is run in repetitive mode with a considerably smaller time constant.

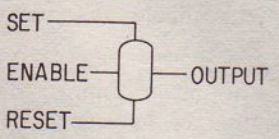
During one analog run simulating the system, the change in the parameter will be negligibly small. During several thousand runs (which may take only a few seconds), the parameter is swept, however, and a parameter sweep is completed with less equipment requirements than those noted in Part 8 of this series.

Reversing the method of operating the system and the parameter generation permits complex parameter generation, such as representing an equilibrium state in the system by the steady-state solution of a set of differential

equations, to be achieved automatically and continuously. The user might also automatically change the time constant so as to operate very rapidly during a trial and error solution and then slow down the solution rate after convergence so that a permanent record may be made on the logically controlled x-y recorders available. The possibility of multispeed calculations and automatic selection of the mode of individual integrator's operation thus open a whole new realm of analog applications which can be used to great advantage in engineering.

Patchable Digital Logic. A necessary prerequisite for the automatic control of integrators, electronic switches, and track and store units is the synthesis of the appropriate logical signals. The electronic comparator provides one means for generating logical signals but is dependent on an instantaneous comparison of analog signals. The AND gate provides means for continuously comparing logical signals. These, together with others to be briefly discussed later, constitute what is referred to as the patchable digital logic capability of the modern analog and provide the user with the capability of logical signal synthesis.

The flip-flop is an essential element in patchable digital logic. In order to insure proper logical operations for circuits using flip-flops, their operation on many analog computers is governed by carefully timed pulses (10^6 per second, 10^5 per second, etc.). Essentially each pulse can be thought of as a spike. During the rising part of the spike the flip-flop "decides" what it is to do. During the falling part of spike, the action is completed. The schematic and characteristics of operation of a flip-flop are given in Fig. 96.



If During Rising Part of Spike			Then Following Falling Part of Spike
Enable	Set	Reset	Output
False	....	....	No change
True	True	False	True
True	False	True	False
True	False	False	No change
True	True	True	Changes state

Fig. 96—The flip-flop is an essential element.

As one example of the flip-flop's applicability suppose that an electronic switch is to be thrown the first time that an analog variable exceeds a certain value and is to remain thrown throughout the remainder of an analog run. (Such an application would arise if there were a change in the method of operating a physical system once a certain condition was reached.) In this case, the enable input on the flip-flop could be made TRUE. Then during the *IC* period of the integrators, the set input would be made FALSE and the reset input made TRUE so that the output would be initialized to FALSE. During the operate period, the reset input would be made FALSE and the set input would be the output from an electronic comparator governed by the desired analog comparison. The first time the output from the comparator becomes TRUE, the flip-flop will set on the falling part of the next spike and the output will remain TRUE for the remainder of the run regardless of the subsequent result of the analog comparison.

Further insight into the operation of a flip-flop can be obtained by examining a schematic representation of a component known as the differentiator such as is given in Fig. 97. In this case, assume the enable input to the flip-flop remains TRUE.

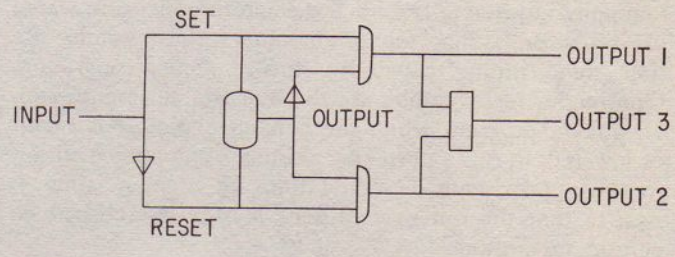


Fig. 97—Schematic representation of a differentiator.

To understand how the differentiator works, assume that input and output are initially FALSE. The sequence of events which occurs when the input becomes TRUE for a length of time and then becomes FALSE again is shown in Table 20.

TABLE 20—Sequence for a Differentiator

Timing	Input	Set	Reset	Output	Output 1	Output 2	Output 3
Rising spike.....	False	False	True	False	False	False	False
Falling spike.....	True	True	False	False	True	False	True
Between pulses....	True	True	False	False	True	False	True
Rising spike.....	True	True	False	False	True	False	True
Falling spike.....	True	True	False	True	False	False	False
While Input remains TRUE...	True	True	False	True	False	False	False
Falling spike.....	False	False	True	True	False	True	True
Between pulses....	False	False	True	True	False	True	True
Rising spike.....	False	Flase	True	True	False	True	True
Falling spike.....	False	False	True	False	False	False	False
While Input remains FALSE..	False	False	True	False	False	False	False

Examination of the sequence of events shows that Output 1 becomes TRUE for only one pulse after the input becomes TRUE. Output 1 is termed the leading edge differentiation of the input. Output 2 becomes TRUE for only one pulse after the input becomes FALSE and is termed the trailing edge differentiation of the input. Output 3 is the result of the OR operation on Output 1 and Output 2 and thus is TRUE for only one pulse after the input changes from TRUE to FALSE or from FALSE to TRUE.

The differentiator's outputs are used when it is desired to note the change of logical signals by a TRUE signal

only one pulse long. They are frequently used in conjunction with a component known as the monostable timer. The monostable timer is given the symbol shown in Fig. 98.

Fig. 98—The symbol for a monostable timer.

If the input to the monostable timer becomes TRUE, even for one pulse, the output from the monostable timer will remain TRUE for a period of time specified by $\triangle T$ and then become FALSE. The period $\triangle T$ is generally manually adjustable from a few microseconds to upwards of 100 seconds. The monostable timer thus permits the user some timing capability during analog operation. One might, for example, use the monostable time to stop an analog program while the pen on a plotter is raised or lowered, to run a particular portion of an analog circuit for an approximate period of time, or to allow time to pass so that the initial conditions may be established on certain integrators.

For more precise timing operations than are possible with the monostable timer, analogs incorporating a patchable digital logic capability are equipped with counters and registers. Counters permit, for example, the generation of a TRUE signal only after a logical signal has been TRUE for a specified number of pulses. Registers permit a sequence of events to be carried out according to a rigidly determined time table.

One of the documented applications of the use of patchable digital logic which has particular applications in control studies involves the completion of a double parameter sweep with the automatic plotting of the values of the parameters for which the system is stable.[12] In this particular application, the system is tested for stability using many thousand possible parameter values in the matter of a few minutes. Such an application of modern analog techniques can but impress on the engineer the power of the modern analog and the very significant time savings which are possible with the analog in the simulation of continuous systems requiring numerous iterative and complex calculations.

Other groups of problems for which patchable digital logic is particularly useful are those requiring dynamic optimizations, the fitting of multiple boundary values, complex sequencing of analog simulations, and in short, those problems in which the full potential of the analog can not be achieved because of the insufficiency of ordinary methods for controlling analog operation. These classes of problems are among the most complex in engineering and are more often than not, those for which possible alternative methods of solution are very time consuming.

The Hybrid Computer. An analog computer equipped with patchable digital logic capabilities is frequently called a hybrid computer. In this series, however, the term hybrid computer has been reserved to describe the even more powerful computational facility which results when an analog computer and a digital computer *per se* are operated as one system, being coupled by a linkage subsystem which permits the transfer of operating and control information to and from the one computer system to the other.

The need and usefulness of the hybrid are many. From the digital standpoint, the inclusion of the analog permits very significant reductions to be made in the time which would be required to simulate continuous systems and systems described by differential equations in particular. From the analog standpoint, the digital provides the severely needed storage capacity which the analog lacks and provides a means for completing arithmetic operations which may require an excessive amount of analog capacity or a degree of accuracy for which the analog is insufficient. Examining the hybrid system as a whole, it is observed that the combined use of the analog and digital, with appropriate interfacing, permits a system to be obtained which retains the advantages of each computer subsystem while minimizing the deterimental effect of their individual disadvantages.

The achievement of the full advantage of each computer subsystem places a great deal of importance on the ability to transfer, to receive, and to use received information. The linkage is understandably very important and its design has been proven to be more complex than may be first realized.[13,14] Essential in the analog subsystem are means for effective control. Here the capabilities provided by patchable digital logic are particularly convenient. In addition, the availability of servo-set potentiometers on the analog are required in order to permit the full utilization of information available from the digital.

Particularly important to effective digital utilization is the availability of a full complement of software specifically designed for use in the hybrid system. These desirable characteristics, as well as others, too numerous to mention, are now available on commercially produced hybrids.[15]

A few examples are now examined to show the applicability and application of hybrid computers in chemical and petroleum engineering:

One of the important general uses of the digital in a hybrid system is to facilitate problem setup and checking out of the analog computer before operation. Satisfactory digital software can be used during this initial period to complete the calculation of scaled pot settings, set the pots by means of servo-set pots on the analog, automatically complete a static check and inform the user of the most likely trouble spots should one of the provided checks fail. Such a capability can reduce programing and setup time on the analog by two-thirds.[15]

During the actual solution period the digital may be used to control the analog, to readjust pot settings after an analog run, and to solve a portion of the problem itself. Such a capability permits the simulation of complex pieces of processing equipment. Fixed bed catalytic reactors[14] and tubular reactors[16] (which may require simulation by several hundred continuous stirred tank reactors), multicomponent separation,[14] and a reacting distillation column[17] have been simulated by using the digital for intermediate calculations and control of analog

"subroutines." The digital's operation sequentially chooses a continuous stirred tank reactor or distillation tray for analog simulation, scales the analog circuit, specifies the initial conditions and period of analog simulation, permits the analog run to be completed, stores the required information from the analog simulation, performs the required intermediate calculation, and proceeds on to the next reactor stage or tray. Problems of this type require a prohibitive amount of time if only the digital is used and are too large for simulation if only the analog is used.

Other hybrid applications have been primarily oriented towards the solution of mathematical relationships and application of mathematical techniques commonly encountered in engineering. Solution of boundary value problems,[18] application of the state variable concept[19] and Monte Carlo method,[20, 21] statistical studies and correlation, [22, 23] and implementation of optimization schemes[15, 24, 25] are examples of the wide range of application and applicability of the hybrid in engineering. In all cases the use of the hybrid is highly recommended over either analog or digital computation alone.

Of particular interest to the chemical and petroleum engineer is the use of the hybrid in solving partial differential equations. Certain of these equations can be reduced to ordinary differential equations by an appropriate change of variable such as the familiar Blausius equation describing the laminar boundary layer on a flat plate[26] and numerous physical systems involving diffusion.[26, 27] Frequently a boundary value problem which is amenable to analog solution is obtained. In other cases the separation of variables technique which has direct analog utility may be used.[4]

The solutions of other partial differential equations on the analog require finite differencing of all but one independent variable[4] since only one independent variable can be continuous simulated on the analog. The use of this technique with only the analog can require an excessive amount of equipment although two independent variables can be simulated[8]. The alternative of digital simulation can lead to excessive computer time due to the large number of discrete values which must be handled in solving these equations.

The hybrid affords the opportunity of time sharing the solution of partial differential equations resulting in a significant savings in analog equipment and time. The simulation of reactors previously noted[14, 16] represents one such use. The time required to simulate a two dimensional equation on a hybrid is substantially reduced over the time required for digital simulation since finite differencing need be used for only one independent variable. For third order equations, one independent variable can be represented by analog operating time, a second by finite difference approximations on the analog such as is done when solving second order equations on the analog,[8] and the third by finite difference calculations on the digital.

The hybrid possesses the power which permits the solution of very large systems. Of importance to chemical and petroleum engineering are applications such as model building for large systems,[28] the simulation of the wet end of a paper manufacturing machine,[29] and the simulation of a chemical plant in order to train operators and optimize design.[30, 31, 32]

The modern electronic analog computer is an inherently powerful and rapid computational tool. The addition of analog memory and patchable digital logic capabilities establishes the analog as an important tool in engineering for the forseeable future. Despite the advances in digital software, the marked speed advantage of the analog permits very large and complex engineering problems to be simulated in a reasonable amount of time.

The combination of the analog and the digital, with appropriate interfacing, yields the most powerful and flexible computational tool available today, the hybrid computer.

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Indexing Terms: Analogs-9, Circuits-10, Computations-4, Computers-9, Descriptions-8, Digital-9, Electricity-10, Engineering-4, Simulation-4.

How to Simulate Recirculation Reactor With Analog Computer

Assuming recycle-fresh feed concentration for analog simulation proved reactor design was limited by turbulence level

P. G. Cooper, Gulf Research & Development Co., Pittsburgh, Pa., and
E. F. Schagrin, International Minerals & Chemical Corp., San Jose, Calif.

FOR MANY HIGHLY exothermic reactions, it is necessary to dilute the feed to a commercial reactor with a recycle stream for temperature control. Often, means for determining the initial composition to the reactor are not available; thus, an initial condition problem is encountered in the mathematical description of the process. In other words, the composition of the fresh feed is known, but the unknown composition of the recycle-fresh feed mixture is needed for the solution of the simulation equations. The schematic diagram in Fig. 1 illustrates this type of reactor.

After the startup of a Gulf processing unit incorporating a recirculation reactor, it was found that an unusually low conversion was being obtained. It was suggested that the reactor design was unsound since the feed was quickly circulated to the exit point and could "short-circuit" through the reactor. However, low reaction rate due to poor agitation could also give low conversion. It was decided to check the soundness of the reactor design by simulating it, assuming that the agitation was good. If the computer results indicated high conversion, then the reactor design was sound and poor agitation was causing the trouble.

The feed to the reactor is a two-phase liquid-liquid mixture and the heavy phase catalyzes the reactions in the light phase. Experimental measurements in a laboratory continuous flow stirred tank reactor had shown that the rate constants k_1, k_2, and k_3 are a function of the turbulence level. The rate constants increased with increasing stirrer speed up to a certain level.

From the chemistry of the system, a simplified kinetics model can be determined. There are primarily three reactions that occur. AB_2 is the desired product.

$$A + B \xrightarrow{k_1} AB \qquad (1)$$

$$AB + B \xrightarrow{k_2} AB_2 \qquad (2)$$

$$A \xrightarrow{k_3} C \qquad (3)$$

The rate of heat transfer is sufficiently high so that the reactor is essentially isothermal and the reaction rate is

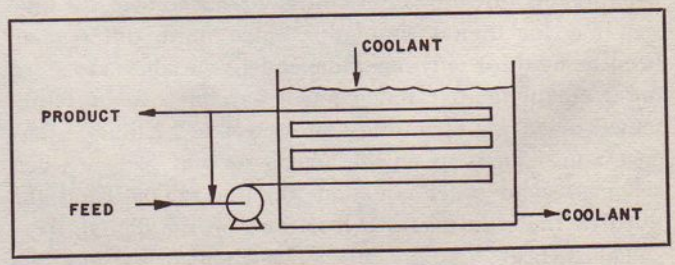

Fig. 1—Shows schematic diagram of jacketed recirculation reactor.

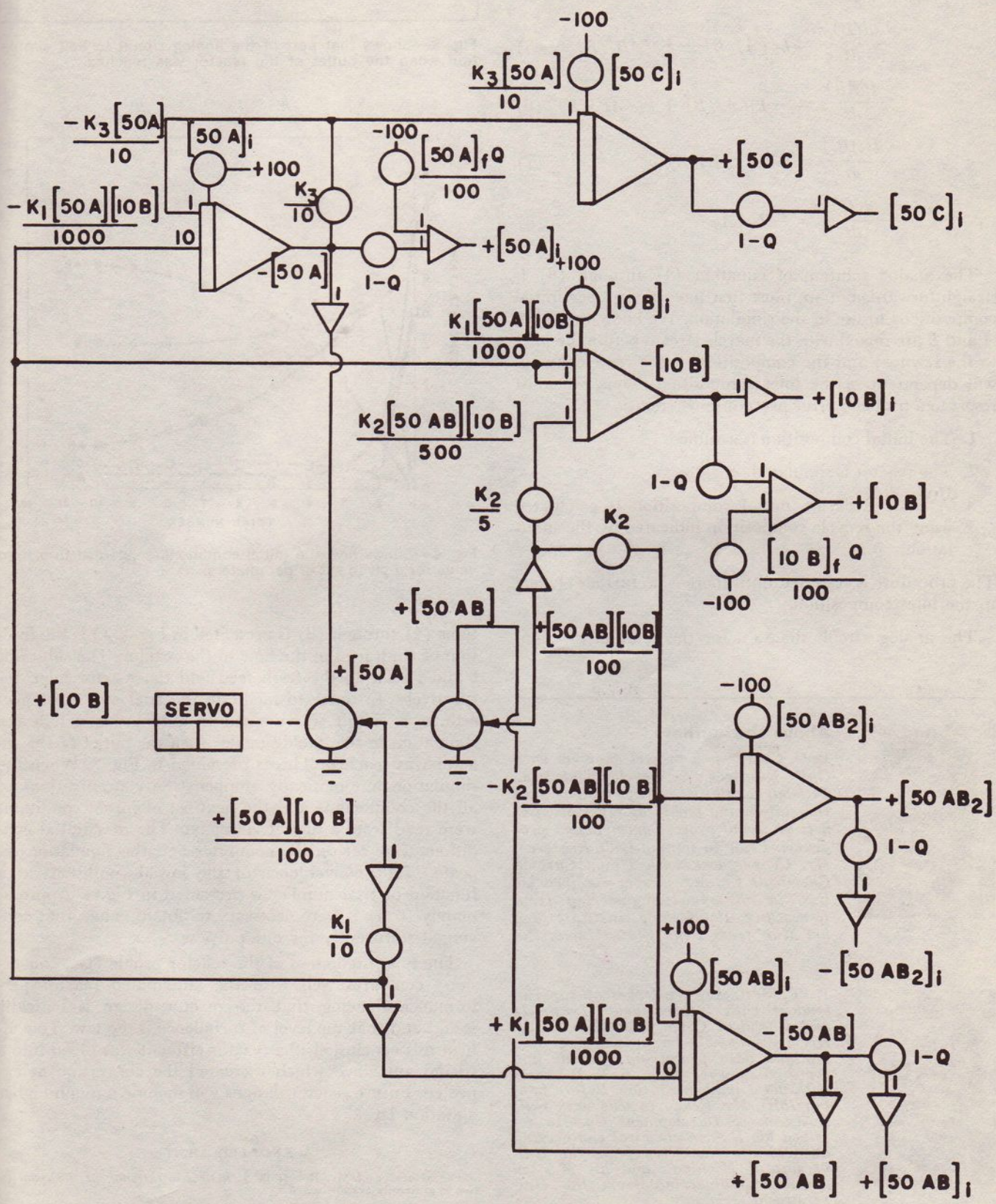

Fig. 2—Shows analog circuit diagram for the simulation of a recirculation reactor.

a function of only the point concentrations. A mathematical model for a plug flow reactor can then be derived easily. Assuming no change in density due to reaction:

$$-\frac{d(A)}{dt} = k_1(A)(B) + k_3(A) \quad (4)$$

$$-\frac{d(B)}{dt} = k_1(A)(B) + k_2(AB)(B) \quad (5)$$

$$-\frac{d(AB)}{dt} = -k_1(A)(B) + k_2(AB)(B) \quad (6)$$

$$-\frac{d(AB_2)}{dt} = -k_2(AB)(B) \quad (7)$$

$$-\frac{d(C)}{dt} = -k_3(A) \quad (8)$$

The analog solution of equation (4) through (8) is straightforward, but we must first have the proper initial compositions to use in the simulation. We know that pure *A* and *B* are mixed with the recycle stream before the inlet to the reactor; and the composition of the recycle stream will depend upon the inlet composition. Thus, we must resort to a trial and error procedure wherein:

1. The initial composition is assumed.
2. The reactor is simulated.
3. A more accurate initial composition is calculated using the recycle composition indicated by the simulation.

The procedure is repeated until there is no further change in the inlet composition.

The analog circuit diagram for the solution of equations (4) through (8) is presented in Fig. 2. Q is the fraction of fresh feed in the flow to the reactor. The subscript f and i refer to the fresh feed and the reactor inlet, respectively. In order to facilitate the trial and error procedure, a circuit was devised to automatically halt the simulation in the "hold" mode when the outlet of the reactor was reached. This is presented in Fig. 3. When the simulation automatically stopped, the concentrations of all the components and the next set of initial conditions were read from a digital voltmeter. The new initial conditions were set on the computer and the simulation repeated. The convergence of the initial conditions as a function of trial number is presented in Fig. 4. Approximately 10 trials were necessary to obtain values that converged sufficiently for our purpose.

The final prediction of the reactor profile (i.e., conversion) compares well with the anticipated reactor performance showing that the reactor design is basically sound and that the level of turbulence is too low. To confirm this conclusion, the reactor effluent was piped into a stirred autoclave which increased the conversion as expected. Future reactor designs will include a much higher agitation level.

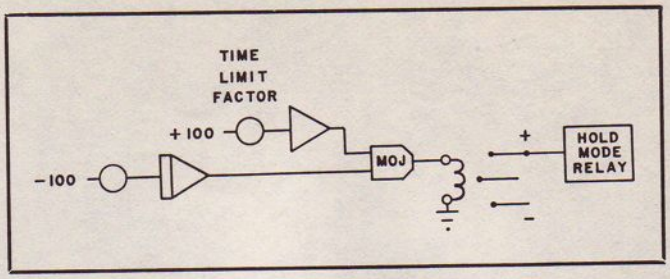

Fig. 3—Shows that part of the analog circuit to halt simulation when the outlet of the reactor was reached.

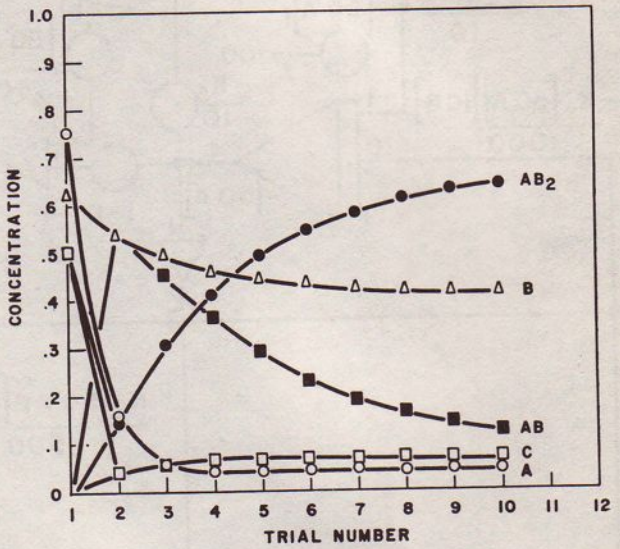

Fig. 4—Shows how the initial conditions converged to a fixed value for a given set of parameters.

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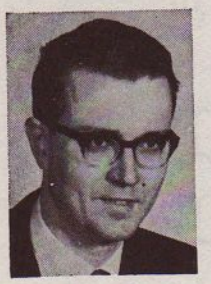
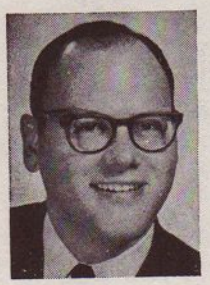
Indexing Terms: Analogs-10, Computers-10, Concentrations-6, Conversion-7, Design-4, Mixing-6, Reactors-9, Simulation-8, Sizing-4.



About the authors

P. G. Cooper *is a project engineer with Gulf Research & Development. Co., Pittsburgh, Pa. His duties include data correlation and technical supervision of petrochemical process development programs. Prior to joining Gulf Research, Mr. Cooper was with Union Carbide Chemicals Co. Mr. Cooper received his B.S. in chemical engineering from Rensselaer Polytechnic Institute and his M.S. from Penn State University.*



E. F. Schagrin *is technical superintendent with International Minerals and Chemical Corp., San Jose, Calif. He is responsible for process engineering and data processing sections and coordinates work from R & D center with plant implementation. Before joining IMC, Mr. Schagrin was with Gulf Research & Development Co. He received his B.S. in chemical engineering and B.S. in chemistry from the University of Michigan and his M.S. in chemical engineering from the University of Delaware.*

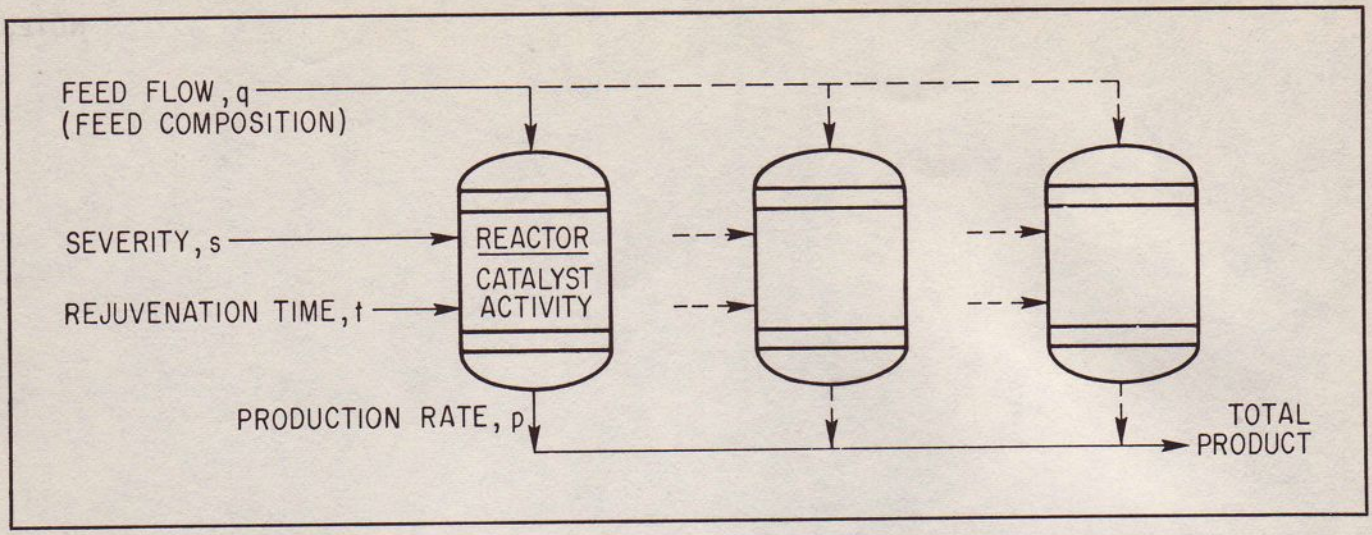


Fig. 1—The simulation program shows the regeneration policy which will maximize total production.

Find Optimum Cat Regeneration Cycle

An analog simulation technique determines the best catalyst regeneration policy. As various processing conditions change, the simulation program modifies the operating guides

Michael D. Harter
Electronics Associates, Inc.
West Long Beach, N. J.

THE BEST CATALYST rejuvenation policy to be applied to a group of continuous reactors is determined as a function of current operating conditions. An analog simulation technique is described which will show the best time at which to begin regeneration and upon which reactor. Return is measured as the total production over the planning interval, considering the productivity of each reactor being lost during its regeneration.

The computational approach is to simulate, at relatively slow speed, the actual plant operation and catalyst activity under the slowly-changing conditions forced by operator varied flow rate and severity. These current running conditions are used as a moving base for the high-speed investigation of alternative regeneration policies, with an oscilloscope providing an operator guide in the form of a predictive display.

The automatic determination of the best reactor to be regenerated and its corresponding regeneration time reduces the dimensionality of the total problem so that the remaining variables can be manipulated by the simulation operator to meet planning needs subject to resource constraints.

The purpose of this article is to demonstrate a flexible and workable method to solve this particular recurring problem in a manner which takes advantage of plant operators experience.

Since the main interest is in the control of solutions to the equations for the model and the investigation of best scheduling policies as influenced by different operating conditions, a very simple plant configuration and reactor description is adopted such as is shown in Fig. 1. More complex plants would not greatly alter the amount of logic required but of course would require additional analog equipment.

EXAMPLE SITUATIONS

Case 1. Assume a crude mechanism such as shown in Equation (1). This represents the formation of the product B from feed A, with degeneration to some unwanted

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \qquad (1)$$

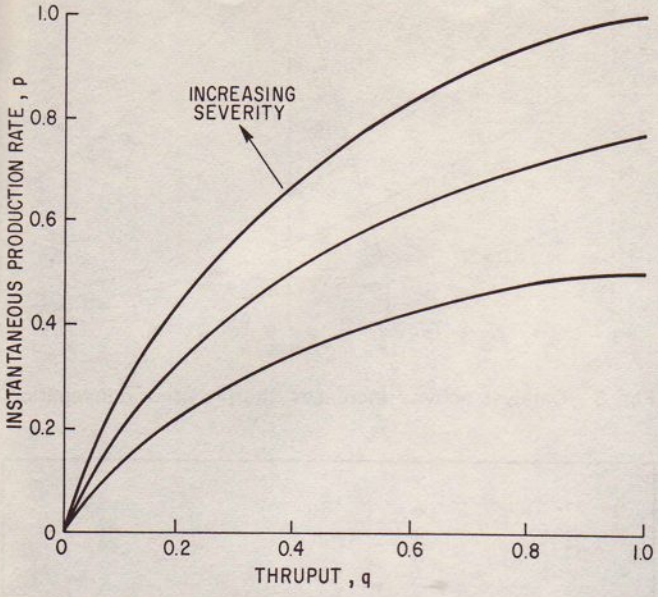


Fig. 2—Thruput and severity can be altered by operator.

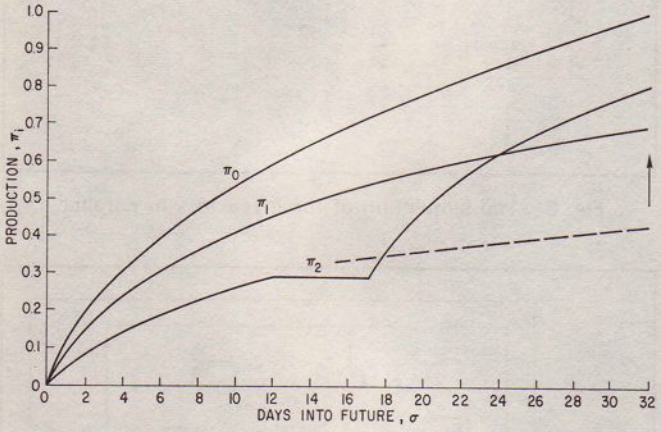


Fig. 3—The No. 2 reactor is rejuvenated after 12 days.

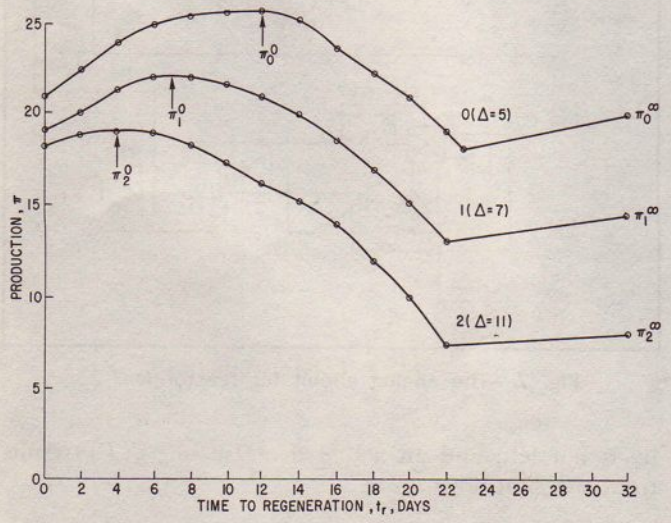


Fig. 4—The peak production for each reactor occurs at different times.

byproduct C. Assuming no B in the feed stream, the steady state solution to the differential equations:

$$dA/dt = (q/v)\ (A_{in} - A) - k_1 A \tag{2}$$

$$dB/dt = (q/v)\,(-B) + k_1 A - k_2 B \tag{3}$$

is given by:

$$A = \frac{A_{in}}{(1 + k_1\Theta)} \tag{4}$$

$$B = \frac{Ak_1\Theta}{(1 + k_2\Theta)} = \frac{(A_{in})\,(k_1\Theta)}{(1 + k_1\Theta)\,(1 + k_2\Theta)} \tag{5}$$

where

$$\Theta = v/q \tag{6}$$

It can be shown that the product concentration B is maximized when:

$$\Theta_{max} = \frac{-(1-k_1)(k_1+k_2) \pm \sqrt{(1-k_1)^2\,(k_1+k_2)^2 - 4k_1k_2\,(1-2k_1)}}{2} \tag{7}$$

In the particular case with $k_1 = 1$, $\Theta_{max} = \sqrt{k_2}$

The reaction rates are assumed to be related to catalyst activity and severity of operation by the following:

$$k_1 = sa \tag{8}$$

$$k_2 = \alpha k_1 = \alpha sa \tag{9}$$

Instantaneous production rate is simply:

$$p = qB \tag{10}$$

Thus, using Equations (5), (7) and (10), the best level of severity may be chosen once production rate is fixed or vice versa.

Case 2. Now consider the following kinetic equation:

$$A \xrightarrow{k} B \tag{11}$$

The steady-state solution to the equation

$$dA/dt = q/v\ (A_{in} - A) - k_1 A \tag{12}$$

is given by

$$B = A_{in} - A = \frac{A_{in}k\Theta}{(1 + k\Theta)} \tag{13}$$

Differentiating the production rate of B with respect to flow and substituting for Θ gives

$$d(qB)/dq = A_{in}\left(\frac{vsa}{q + vsa}\right)^2 \tag{14}$$

It can be seen that there is no supporting relation between flow rate and severity which maximizes production in this case, and the variables (q and s) remain as independent degrees of freedom to the operator .For this reason the mechanism of Equation (11) was used. The instantaneous production rate as a function of flow and severity, is shown in Fig. 2.

A word here about relative time-scales. The speed of response of a reactor to a change in operating conditions—either flow rate or severity—is of the order of

minutes. Catalyst decay time constants are of the order of days and hence the justification for the use of the phrase "instantaneous production rate." To a first approximation therefore we can treat the conversion kinetics as algebra when considered in relation to the planning interval of, say, one month.

Degeneration. Decay is governed by severity of operation and net production rate, the latter term corresponding to a poisonous influence.

It is assumed that catalyst activity decay rate is increased by higher operating severities and is also proportional to the production rate.

$$da/dt = -C\,[sa + p] \tag{15}$$

This latter term corresponds to the deposition of carbon for example or gradual catalyst poisoning.

Rejuvenation. It is assumed that rejuvenation takes place at a fixed rate from the activity level at which rejuvenation was begun up to a standard "clean" level.

$$r = \frac{a^o - a\,(t_r)}{T_r} \tag{16}$$

Since activity decays in an exponential manner and rejuvenation normally takes place at low levels, the rejuvenation interval T_r changes little if r is fixed. Thus the time for which production is lost is approximately inversely proportional to r. During the regeneration, begun at time t_r, catalyst activity is raised from its level at that time up to some maximum level a^o at the rate r. The time taken to regenerate T_r, depends on the time regeneration is started via $a(t_r)$, tending assymptotically to the maximum a^o/r as regeneration is postponed.

PROCESS OBJECTIVE

The approach to the maximization is a simple search over the space (i, j) for each value of a, q, and s. The variable σ is predictive time extending from now to the end of the planning interval T. Note that the base $\tau = o$ is moving. The objective function then is:

$$\max_{(i,\,j)} \pi\,(\tau) = \sum_i \int_\tau^{\tau+T} p_i \left\{ a\,[s\,(\tau), q\,(\tau), t_r, \sigma], s\,(\tau), q\,(\tau), r, t_r \right\} d\sigma \tag{17}$$

with $$\tau < t_r, \sigma < \tau + T$$

and $$o < \tau < T$$

$$t_r = j(T/32), j = 0, 1, 2, \ldots, 32$$

The accumulated product from each reactor over the planning interval for one particular regeneration policy is shown in Fig. 3. Note the plateau in the curve for reactor No. 2 and the improvement in production due to freshened catalyst. These curves are for uniform operating conditions both throughout the interval T and between reactors but for different initial catalyst activities

$$(a_0 = a^o, a_1 = 2a^o/3, a_2 = a^o/3).$$

As regeneration time is varied $\pi_2\,(T)$ will rise and fall. If $(T - T_r) < t_r < T$, the benefit from improved activity is not felt, and an actual decrease in $\pi_2\,(T)$ results from the shut-down.

The influence of regeneration time on production is shown for each reactor in Fig. 4. The decreasing effect on

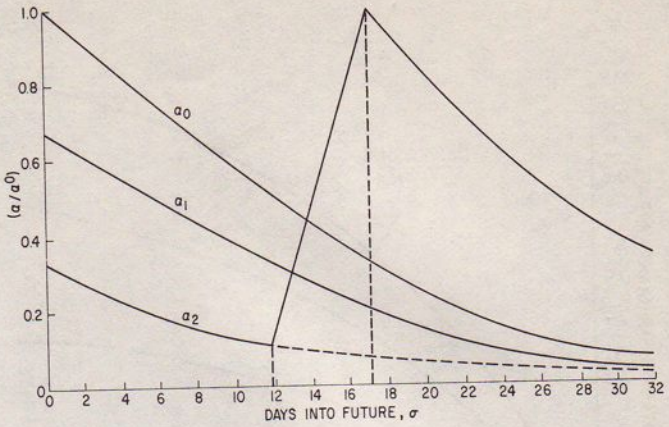


Fig. 5—Catalyst activity increases sharply after rejuvenation.

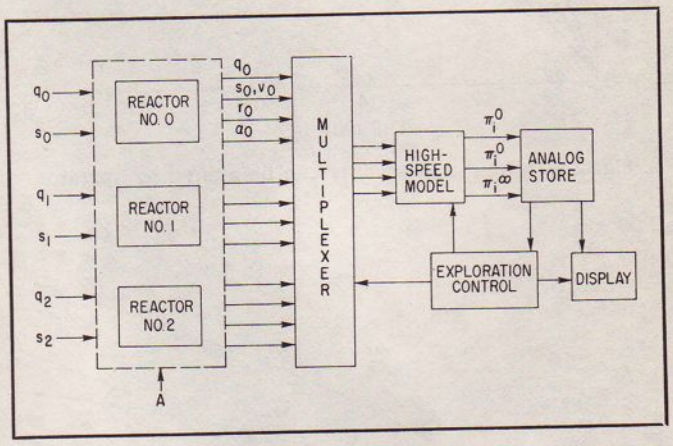


Fig. 6—The simulation of three reactors in parallel.

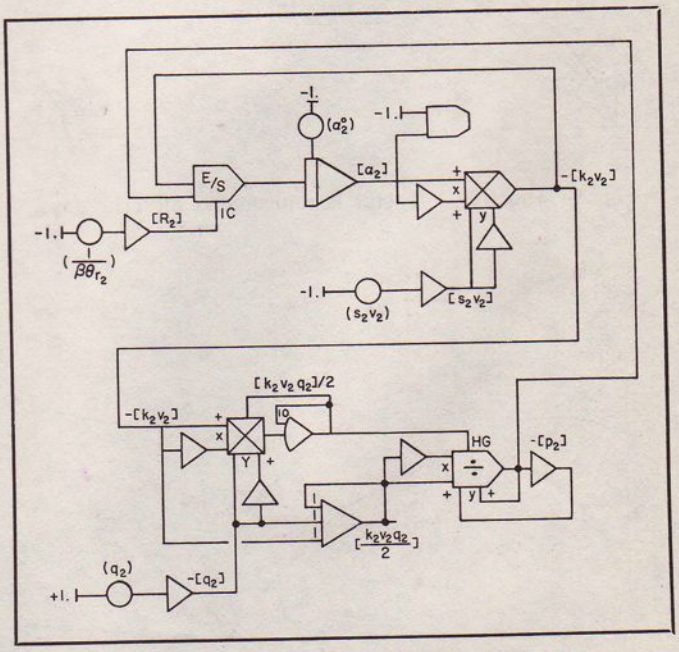


Fig. 7—The analog circuit for reactor No. 2.

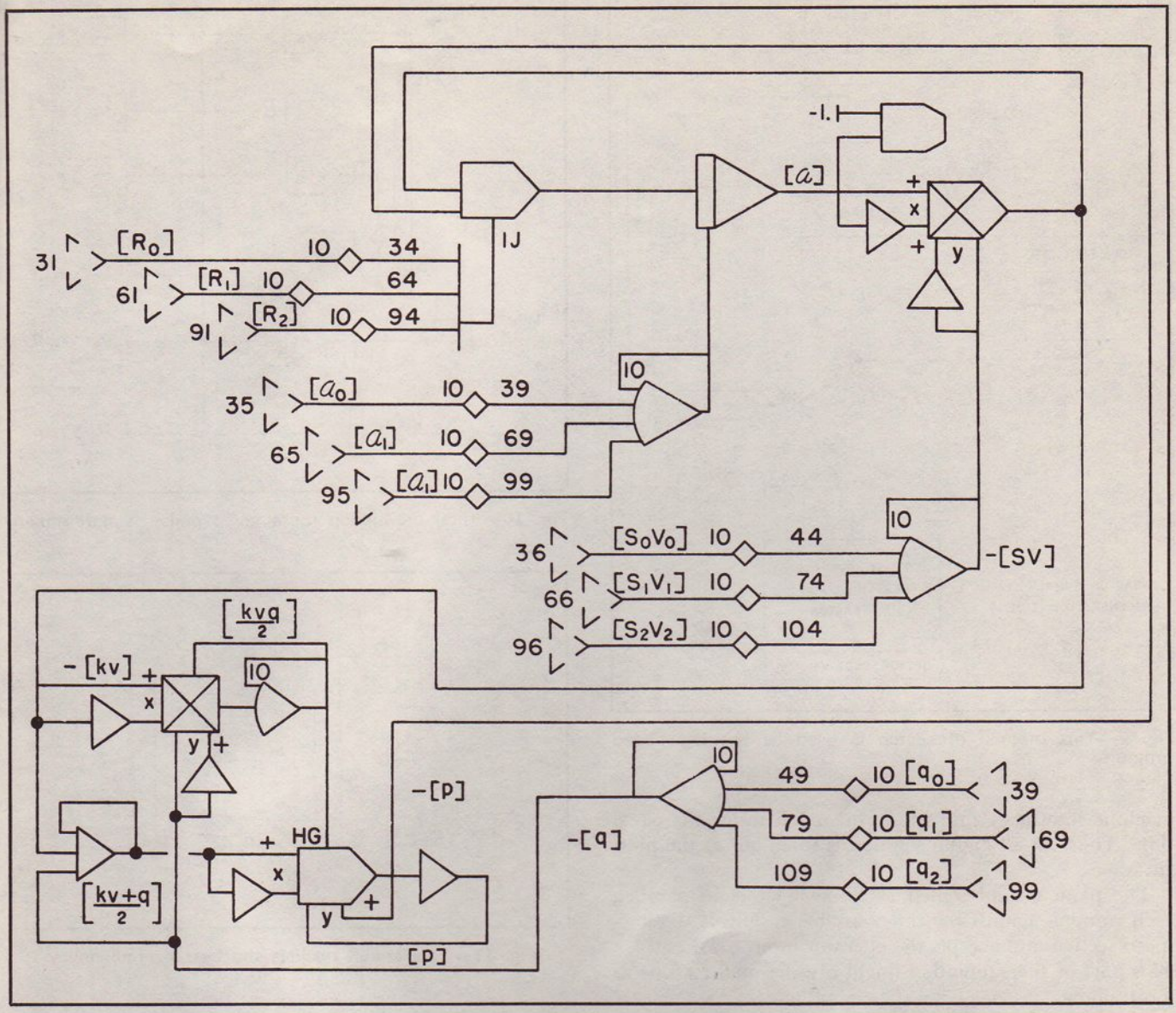


Fig. 8—Production from all three reactors is estimated to determine the best regeneration policy.

the right is due to the shut-down loss just mentioned. Other points to be noticed are that the peaks for each reactor occur at different times and that Δ, the production improvement—the difference between $\pi\ (t_r)$ and $\pi\ (T)$—is greatest for reactor No. 2. The rightmost points $\pi_i\ (T)$ represent production if regeneration is not made within the planning interval. By inspection, the best policy in this case is $P\ (2, 4)$.

About the author

MICHAEL D. HARTER *is a research coordinator for Electronic Associates, Inc., Princeton, N. J., where he studies applications of analog and hybrid computers. Holder of a B.S. degree in physics and mathematics from Leeds University, England, Mr. Harter is doing graduate work at University of Pennsylvania. He worked for Associated Electrical Industries and Esso Petroleum Co. before joining Electronic Associates, Inc. He is a member of ISA, S.I.A.M. and Simulation Councils, Inc.*

For policy $P\ (2, 12)$ and uniform operating conditions, Fig. 5 shows the three catalyst activities, initially $a_o = a^o$, $a_1 = 2a^o/3$ and $a_2 = a^o/3$. The slopes of decay at any time depend on operating conditions. For example, by reducing the severity on a reactor, it is possible to prolong the catalyst "life." The area under the curves, a rough measure of production, is easily seen to be affected by a change in severity, throughput, and regeneration. For constant operating conditions and a given regeneration policy, the passage of time represents a continuous re-definition of the origin of σ.

COMPUTER IMPLEMENTATION

The over-all organization of the simulation for a plant with three reactors in parallel, is shown in Fig. 6.

This approach requires either a hybrid computer or an analog computer with sufficient parallel logic to implement the search control, timing, and best policy selection. The solution requires many integration runs for the differential equations of the models, needs convenient man-

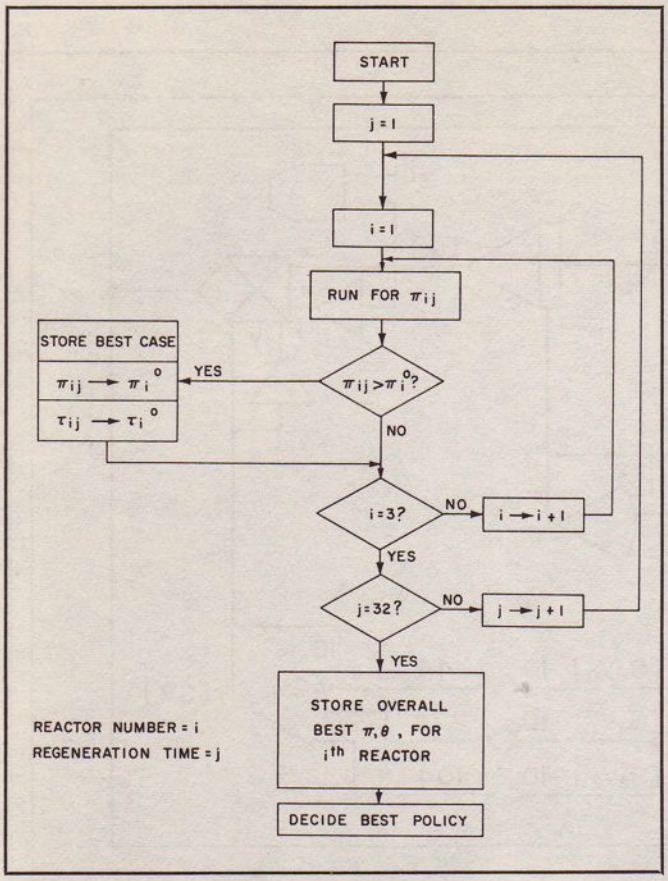


Fig. 9—This method of search is used by the high-speed program.

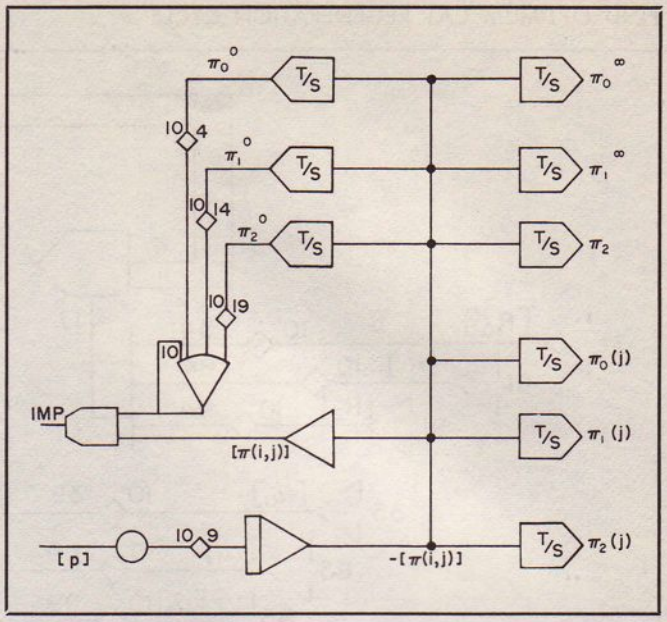


Fig. 10—Total production for a given policy is determined.

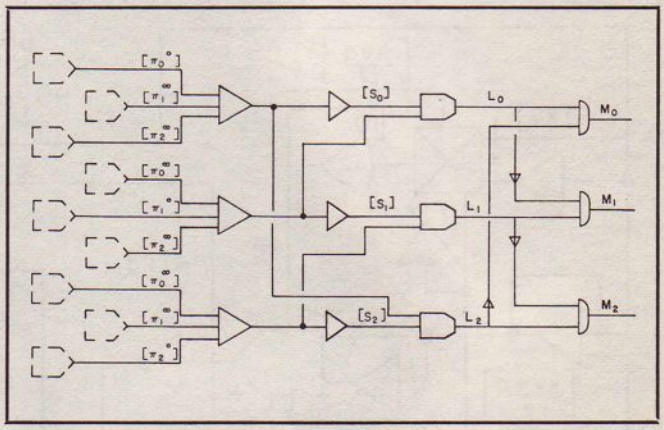


Fig. 11—This circuit decides the best over-all policy.

machine interfaces, and must run much faster than real time. Thus, an all-digital solution is ruled out at the present time.

The plant is represented as three reactors in parallel, each running against the time variable τ. This is the low-speed section and accepts the operator input q_i, s_i and t_{ri}. This part of the simulation might also be used for operator training.

The high-speed section samples conditions in each reactor in turn to determine the best policy at that time. This section runs against the time variable σ, with τ as a moving base. During the search, display of the individual π_i as a functon of t_r is available such as shown in Fig. 4. Following the search, the best policy may be displayed, showing either individual productions (Fig. 3) or individual activities (Fig. 5).

The analog circuit for a single reactor is shown in Fig. 7. Operator inputs are made through the potentiometers as indicated. The rate term to the "*a*" integrator switches between the decay variables—upper connection—and the regeneration variable *r*. Regeneration is initiated through a logic control push-button and is automatically terminated when activity is back to maximum.

The high-speed circuit shown in Fig. 8 is multiplexed between the three reactor models just described. The only basic difference between this and the low-speed circuits is in the control of the regeneration switch. If the reactor currently being copied is in the regeneration mode, then all high-speed exploration runs for that reactor are initiated in that mode also. This is in addition to regeneration as part of the search.

Control for the search mode is shown in Fig. 9. For three reactors and thirty-two days in the planning interval, a total of ninety-six runs are required for the exploration. Including initiallization times an exploration may be completed in 200 milliseconds, an average 2.08 milliseconds per integration. This represents a scale-up of about 10^9 over real time.

The circuit arrangement for computing $\pi_{i,j}$ is shown in Fig. 10. The electronic switch in the input to the production integrator serves as high-speed hold during regeneration. The lower right-hand three track/store units are used merely to display $\pi\ (j)$ during search. The upper right three track/stores sample the production without any regeneration during the planning interval π_i. The left three track/stores pick the peak production for each reactor π_i^0.

When the runs are completed, the circuit shown in Fig. 11 decides the best over-all policy. The logic for this is as follows:

If $S_0 > S_1$ then $L_0 = 1$.

If $S_1 > S_2$ then $L_1 = 1$.

If $S_2 > S_0$ then $L_2 = 1$.

If $M_0 = (L_0)\ (\bar{L}_2) = 1$ then S_0 best.

If $M_1 = (L_1)\ (\bar{L}_0) = 1$ then S_1 best.

If $M_2 = (L_2)\ (\bar{L}_1) = 1$ then S_2 best.

The results from decreasing the regeneration rate 25% are shown in Table 1. A comparison is made against the base case of otherwise uniform operating conditions with an initial catalyst activities distribution of $a_0 = a^o$, $a_1 = 2a^o/3$ and $a_2 = a^o/3$. As expected, the net effect is to decrease the maximum yield from each reactor. The best policy is still obvious although time of regeneration is advanced. One useful application of this information might be to provide quantitative data for a regeneration debottleneck study.

TABLE 1—Sensitivity to Regeneration Rate

	r = 0.75		r = 1 (BASE)	
i	π_i^o	π_i	π_i^o	π_i^∞
0	0.96	0.68	1.0	0.80
1	0.82	0.52	0.86	0.56
2	0.64	0.26	0.72	0.32

TABLE 2—Sensitivity to Severity

	S = 1.5		BASE S = 1.0		S = 0.5	
i	π_i^o	π_i	π_i^o	π_i^∞	π_i^o	π_i
0	1.10	0.75	1.0	0.80	0.80	0.60
1	0.94	0.72	0.86	0.56	0.66	0.40
2	0.82	0.30	0.72	0.32	0.60	0.22
Best Policy						
i	2		2		2	
j	12		10		8	

TABLE 3—Sensitivity to Thruput

	q = 1.5		BASE q = 1.0		q = 0.5	
i	π_i^o	π_i	π_i^o	π_i^∞	π_i^o	π_i
0	1.14	0.78	1.0	0.80	0.76	0.72
1	0.96	0.56	0.86	0.56	0.66	0.44
2	0.82	0.28	0.72	0.32	0.60	0.28
Best Policy						
i	2		2		2	
j	12		10		6	

TABLE 4—Equipment Used

ANALOG

Amplifiers	— 12 Track/Stores
	— 7 Integrators
	— 17 High Gain
	— 7 Summers
	— 4 Electronic Switches
	— 38 Inverters
	85
Multipliers	— 12 (4 as Division)
Pots	— 15
Limiter	— 1
Comparators	— 10
D/A Switches	— 22

LOGIC

And Gates	— 35
Monostables	— 1
Differentiators	— 3
Flip-Flops	— 8
Shift Registers	— 2
Mode Timer	— 1

The corresponding data for a change to severity are shown in Table 2. The best policy under the new conditions (increased severity) is to regenerate reactor No. 2 but postpone for two days the time of regeneration. On the other hand the recommendations with decreased severity is to advance the regeneration time two day. The change is production for this reactor is $(0.4 + 0.1)$ and $(0.4 - 0.12)$ respectively.

Sensitivities to throughput changes are shown in Table 3. The alteration in production for reactor No. 2—still the one to regenerate—is the same as in the case for severity changes, but in the reduced flow instance, an advancement of 4 days in regeneration time is necessary.

Not shown in the table is the influence on π_i^∞: It is, respectively, 0.06; 0.04; and 0.02. This indicates that when reactor No. 2 is shut down, the available feed should be diverted unequally to reactors Nos. 0 and 1, with reactor No. 0 having the larger share. Whether all the available feed should be used and in what precise ratio it ought to be split must be determined at the time when reactor No. 2 is about to be shut down.

All these sensitivity studies were made at a particular value of time τ. By increasing the number of runs at each τ from 96 to 480, the sensitivity trials could be automated. The conditions fed to high-speed circuit would be:

$$\left.\begin{array}{l} a\ (\tau),\ r,\ s\ (\tau),\ q\ (\tau) \\ a\ (\tau),\ r,\ s\ (\tau),\ +\Delta s,\ q\ (\tau) \\ a\ (\tau),\ r,\ s\ (\tau),\ -\Delta s,\ q\ (\tau) \\ a\ (\tau),\ r,\ s\ (\tau),\ q\ (\tau)\ +\Delta q \\ a\ (\tau),\ r,\ s\ (\tau),\ q\ (\tau)\ -\Delta q \end{array}\right\} \text{For all } i,\ j$$

Time to run: 1 second.

The corresponding changes to production and regeneration policy could then be displayed to the operator who may then decide to alter operating conditions as τ evolves.

Another alternative would be to use these influence coefficients as part of some higher-level automatic optimization, say, steepest ascent manipulating s and q.

NOMENCLATURE

A,B,C component concentration	v specific volume
a catalyst activity	α reaction rate ratio
a^o maximum catalyst activity	Δ production improvement
k reaction rate constant	Θ residence time
P regeneration policy	π total production
p production rate	σ predictive time
q flow rate	τ present time
r rejuvenation rate	**Subscripts**
s severity	i reactor index
T planning interval	j day of rejuvenation
t time	r regeneration

Indexing Terms: Analogs-10, Computers-10, Controlling-4, Optimization-4, Output-7, Performance-7, Processing-9, Production-7, Reactors-9, Regeneration-6, Simulation-8, Time-6.

This Distillation Program Generates Its Own Data

This rigorous method incorporates the Chao-Seader correlation and the Redlich-Kwong equation of state to compute the equilibria and enthalpies for multicomponent calculations

Wendell W. Waterman, Vern E. Alden Co., Chicago, and **James P. Frazier,** Natural Gas Pipeline Co. of America, Chicago

THE PROGRAM here presented is useful for hydrocarbon mixtures over a wide range of compositions, temperatures and pressures. It combines two important features:

- Rigorous computation of the number of theoretical plates required for a specified separation.
- Incorporation of the Chao-Seader correlation and the Redlich-Kwong equation of state enabling computation of reliable equilibrium and enthalpy values without introduction of data specific to each problem considered.

PREVIOUS COMPUTER PROGRAMS

Computer programs developed to solve multicomponent distillation problems by rigorous methods may be classed as follows:

Class I—Programs based on the Lewis-Matheson[13] approach in which feed, reflux and the desired separation are specified. The required number of theoretical plates is found by plate to plate calculation, component meshing at the feed plate being obtained by over-all iteration.

Programs developed by McIntire,[16] Maddox and Erbar[15] and Bonner[20] are examples of the Class I group. In their use equilibrium and enthalpy data specific to each problem undertaken must be provided as part of the input data. Plate temperatures are found by computing bubble points below and dew points above the feed.

Class II—Programs based on the Thiele-Geddes[22] approach in which feed, reflux, quantity and state of the distillate, and the number of theoretical plates are specified. Plate to plate computations are made using mol fraction ratios, and product compositions are found by a meshing computation.

Programs reported by Lyster et al,[14] Mills,[17] Newman[18] and Hanson[12] are of the Class II type. Again, enthalpy and equilibrium data must be supplied for each problem. However, in these programs determination of plate temperatures is more difficult. It is accomplished by an iterative process, a temperature profile being assumed to initiate computations. Various special techniques have been used to facilitate convergence.

Class III—Programs based on solving the simultaneous equations which express plate and column material and enthalpy balances. The items specified are the same as for the Thiele-Geddes plate to plate method.

The program developed by Amundson et al[1,2,3] belongs in Class III. Matrix inversion is used for solution of the simultaneous equations. Plate temperatures are determined by iteration as in the Class II programs.

Class IV—Programs in which the progressive change in plate and product compositions from start-up to the attainment of steady state are computed by a relaxation method. Rose, Sweeny and Schrodt[21] have successfully developed this approach.

All these programs are rigorous with respect to material and enthalpy balance computing techniques, but fail to take into account the composition dependency of equilibrium values. Further, although the tedious process of

The method includes a rigorous computation of the number of theoretical plates needed

making plate to plate calculations manually is eliminated, there remains the time consuming work of selecting and preparing equilibrium and enthalpy data for individual problems and the attendant possibility of human error.

Greenstadt, et al[11] described a program of the Class I type in which Newton's method is utilized to solve plate and overall balances as well as the equations for adjusting product distribution to accomplish feed plate meshing. In one method of applying the program the Benedict, Webb, Rubin equation[5] is used in a subroutine to compute equilibrium and enthalpy values. This was the first reported attempt to incorporate a generalized equation of state into a distillation program. It is understood that difficulty in attaining convergence has been experienced with this program.

TABLE 1—Acceptable Components

Non-Hydrocarbons
- Hydrogen
- Nitrogen
- Carbon Dioxide
- Carbon Monoxide
- Hydrogen Sulfide
- Sulfur Dioxide
- Oxygen

Paraffins
- Straight Chain—C_1 through C_7
- iso-Butane
- iso-Pentane
- neo-Pentane
- 2—Methyl Pentane
- 3—Methyl Pentane
- 2, 2—Dimethyl Butane
- 2, 3—Dimethyl Butane

Olefins
- Straight Chain—Double Bond in 1 Position—C_2 through C_7
- 2—Butene—Cis and Trans
- 2—Pentene—Cis and Trans
- 2—Methyl—1—Butene
- 2—Methyl—2—Butene
- 3—Methyl—1—Butene

Diolefins
- Propadiene
- 1, 2—Butadiene
- 1, 3—Butadiene

Cycloparaffins
- Cyclopentane
- Methyl Cyclopentane
- Ethyl Cyclopentane
- Cyclohexane
- Methyl Cyclohexane
- Ethyl Cyclohexane

Aromatics
- Benzene
- Toluene
- Xylenes—Ortho, Meta and Para
- Ethyl Benzene

TABLE 2—Input Specifications

Feed
- Component List (Key Components Designated)
- Mole Fraction of Each Component in Total Feed
- Physical State Alternates
  - (1) Liquid at Bubble Point
  - (2) Vapor at Dew Point
  - (3) Mixed Liquid and Vapor
- Temperature (For Flash Calculation)

Distillate
- Physical State Alternates
  - (1) Vapor
  - (2) Liquid
- Quantities of Light and Heavy Key Components
- Temperature (Starting Assumption)

Bottoms Temperature (Starting Assumption)

Reflux—
- Alternates:
  - (1) Minimum Reflux Computed—Multiplier Specified
  - (2) Reflux Ratio Specified

Column Pressure

After an investigation of alternate methods for predicting K values in hydrocarbon mixtures, Cavett[7] adopted the Chao-Seader correlation[9] together with the Redlich-Kwong equation of state[19] (or alternately for low pressure ranges the Black equation of state[6]) as the preferred method for obtaining thermodynamic properties for use in distillation computations. Cavett developed two programs,[8] one of the Class II and the other of the Class III type in which it is necessary to specify the components in the feed, the reflux and the operating pressure. Equilibrium and enthalpy values are computed as required.

There is an important difference in utility between the Class I and the Class II and III programs. The latter are analytic; that is, they compute performance in a column having a fixed number of theoretical plates. They are well adapted to studies on existing installations, but are inconvenient for design applications since the number of plates required to effect a given separation can be determined only by submitting a series of problems and interpolating among the results. The Class I programs are advantageous for design work since they compute directly the required number of plates. They also determine automatically the optimum point for feed introduction; whereas, with Class II and III programs this must be found by trial and error.

Further the Class II and III programs usually have a maximum number of plates that can be considered. With Class I programs the number of theoretical plates is unlimited.

CHARACTERISTICS OF THIS PROGRAM

The present program is of the Class I type. It is used to compute the number of theoretical plates required to accomplish a given separation by a modified Lewis-Matheson technique. The Chao-Seader and Redlich-Kwong correlations are incorporated together with constants for the acceptable components listed in Table 1. Any 21 of the listed hydrocarbons plus any four of the non-hydrocarbons may be specified in a particular problem. Thermodynamic data needed for rigorous plate to plate calculations are generated by the program for each vapor and liquid stream in the system. Equilibrium values are computed as functions of composition as well as temperature and pressure.

Criteria and equations are included for checking computed feed plate compositions and making the adjustments necessary to secure non-key component meshing. The reflux ratio may be specified or the minimum reflux may be computed and used together with an assigned multiplier.

TABLE 3—Output Data

Column Operating Pressure
Feed Temperature
Feed Vapor: Quantity, Composition and Enthalpy
Feed Liquid: Quantity, Composition and Enthalpy
Top Product: Quantity, Composition and Enthalpy
Bottom Product: Quantity, Composition and Enthalpy
Feed Plate Composition Calculated from Top } for Each Meshing Iteration
Feed Plate Composition Calculated from Bottom } for Each Meshing Iteration
Minimum Reflux
Minimum Reflux Multiplier (Specified)
Reflux Ratio (Specified)
Reflux Quantity and Enthalpy
Reboiler Temperature and Vapor Enthalpy
Reboiler Heat Load
Temperature of Vapor to Condenser
Condenser Outlet Temperature
Condenser Heat Load
Compositions, Temperatures and Enthalpies on Each Plate (If Desired)

The program is written in FORTRAN and has been demonstrated on an IBM 7070-10K computer. It can be readily adapted to other computers that utilize FORTRAN compilers and have adequate storage capacity.

Input specifications are listed in Table 2. It is necessary to specify only the feed, the required separation, the reflux and the column pressure. The feed may be liquid at the bubble point, any vapor-liquid mixture, or vapor at the dew point. Output data are listed in Table 3.

At present the program is set up for one feed and two products. Modifications to accommodate multiple feeds and draw-offs are being developed.

EQUATIONS USED IN PROGRAM

Chao-Seader Correlation.

$$K_i = \frac{y_i}{x_i} = \nu_i^0 \left(\frac{\gamma_i}{\phi_i}\right) \tag{1}$$

$$\log \nu_i^0 = \log \nu_i^{(0)} + \omega_i \log \nu_i^{(1)} \tag{2}$$

$$\log \nu_i^{(0)} = A_0 + A_1/T_r + A_2 T_r + A_3 T_r^2 + A_4 T_r^3 + (A_5 + A_6 T_r + A_7 T_r^2) P_r + (A_8 + A_9 T_r) P_r^2 - \log P_r \tag{3}$$

$$\log \nu_i^{(1)} = -4.23893 + 8.65808\, T_r - 1.22060/T_r - 3.15224\, T_r^3 - 0.025\,(P_r - 0.6) \tag{4}$$

$$\log \gamma_i = \frac{\psi_i\,(\bar{\delta} - \delta_i)^2}{2.303\,RT} \tag{5}$$

Redlich-Kwong Equation

$$z^3 - z^2 - zP\,(B_k^2 P + B_k - A_k^2) - A_k^2 B_k P^2 = 0 \tag{6}$$

$$A_k = \sum_{i=1}^{n} y_i A_{ki},\quad B_k = \sum_{i=1}^{n} y_i B_{ki} \tag{7}$$

The compressibility, z, is used to calculate ϕ_i in the Chao-Seader correlation as follows:

$$\log \phi_i = \frac{(z-1)}{2.303}\frac{B_{ki}}{B_k} - \log (z - B_k P) - \frac{A_k^2}{B_k}\left(2\frac{A_{ki}}{A_k} - \frac{B_{ki}}{B_k}\right)\log\left(1.0 + \frac{B_k P}{z}\right) \tag{8}$$

Enthalpies. Enthalpies of vapor mixtures are computed from ideal gas component enthalpies as follows:

$$H^0 = \sum_{i=1}^{n} y_i H_i^0 \tag{9}$$

$$H^V = H^0 - RT\left[3.454\frac{A_k^2}{B_k}\log\left(1.0 + \frac{B_k P}{z}\right) + 1.0 - z\right] \tag{10}$$

Liquid enthalpies are computed as follows:

$$H_i^L = H_i^0 - \frac{2.303RT^2}{T_c}\left[-\frac{A_1}{T_r^2} + A_2 + T_r\,(2A_3 + 3A_4 T_r) + (A_6 + 2A_7 T_r)\,(P_r) + A_9 P_r^2 + \omega_i\,(8.65808 + \frac{1.22060}{T_r^2} - 9.45672\, T_r^2)\right] - 1.8\,\psi_i\,(\bar{\delta} - \delta_i)^2 \tag{11}$$

$$H^L = \sum_{i=1}^{n} x_i H_i^L \tag{12}$$

Material, Enthalpy and Component Balances. Over the entire column the balances are:

$$F = F^V + F^L = D + W \tag{13}$$

$$H_f^V F^V + H_f^L F^L - q_c + q_r = H_d^V D^V + H_d^L D^L + H_w^L W \tag{14}$$

(Note either $D^V = O$ or $D^L = O$)

$$x_i F^L + y_i F^V = y_i D^V + x_i D^L + x_i W \tag{15}$$

If balances are written around the portion of the tower below the line g-g in Figure 1, the following equations are obtained:

$$L_{n-1} = V_n + W \tag{16}$$

$$H_{n-1}^L L_{n-1} + q_r = H_n^V V_n + H_w^L W \tag{17}$$

$$x_i L_{n-1} = y_i V_n + x_i W \tag{18}$$

Above the line g'-g' the following balances may be written:

$$V_m = L_{m-1} + D^V + D^L \tag{19}$$

$$H_m^V V_m - q_c = H^L{}_{m-1} L_{m-1} + H_d^V D^V + H_d^L D^L \tag{20}$$

$$y_i V_m = x_i L_{m-1} + y_i D^V + x_i D^L \tag{21}$$

The accuracy of the results depends upon the accuracy of the Chao-Seader correlation

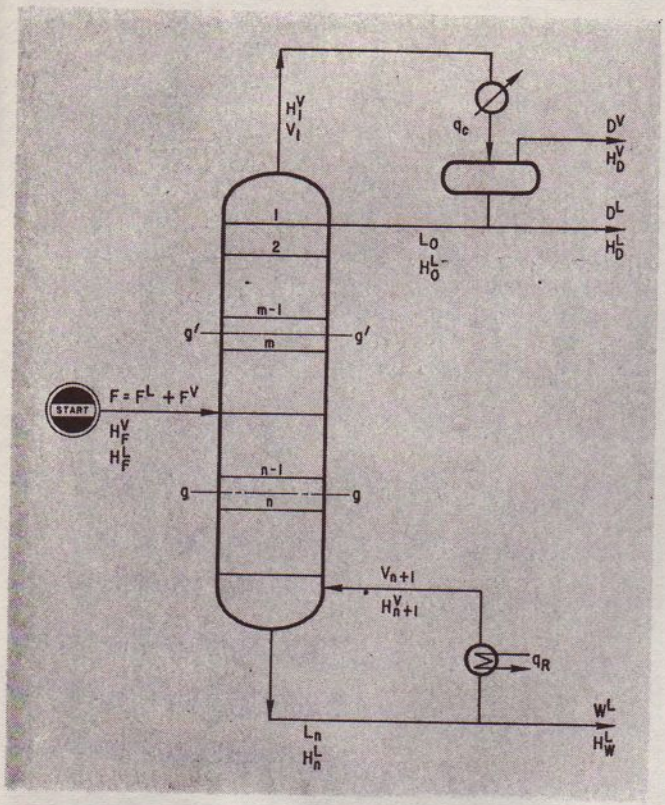


Fig. 1—At present the program is set up for one feed and two products.

Non-Key Component Meshing. The following equation, developed by Edison,[10] is used to compute new assumptions in iterations for meshing non-key components at the feed plate:

$$\Delta_i = 1.5 \left[\frac{x_{fw,i} - x_{fd,i}}{\frac{x_{fw,i}}{W} + \frac{x_{fd,i}}{D}} \right] \qquad (22)$$

This is the relationship employed by Bonner[20] except for the arbitrary 1.5 multiplier which tends to speed convergence.

Minimum Reflux. Minimum reflux is computed by the Bachelor method.[4] Equations and computational techniques used in this operation are not presented here in detail but are available in Bachelor's original paper. The special procedures for subcooled liquid and superheated vapor feeds have not yet been incorporated in the program.

COMPUTING TECHNIQUES

The sequence of computations is shown in Figure 2, the desired separation being specified in terms of heavy and light key components.

The feed is first tested to see if a flash calculation is required. If so, it is computed to determine the split and the composition of the vapor and liquid portions. Next, the bottoms temperature is determined by bubble point calculation and the bottoms enthalpy is computed. The amount of reflux is computed and the overflow established at one point, usually the bottom plate in the column. This permits determination of the quantity of reboil vapor, its composition and enthalpy being available from the bubble point calculation.

From this point on, material and enthalpy plate balances are computed in the conventional manner. After each plate calculation the ratio of key components is checked to see if the feed plate has been reached. Computations of the condensing temperature, top product enthalpy, etc., are performed in a similar manner.

For approximate calculations components heavier than the heavy key are assumed to be entirely in the bottoms and components lighter than the light key are assumed all in the distillate. The number of theoretical plates is computed in a single pass requiring from 7 to 12 minutes depending on the number of components and the number of plates. For most problems this procedure predicts the correct number of theoretical plates and determines accurately condenser and reboiler heat loads.

If greater accuracy is desired the meshing feature of the program may be employed. The computer will adjust the amount of each non-key component in the top and bottom products until the feed plate composition as calculated from the top down agrees with that computed from the bottom up within a specified tolerance. The Edison[10] algorithm used for predicting new assumptions as to distribution of non-key components has been found to converge in 4 to 7 iterations. Meshing satisfactory for most purposes is usually attained in four iterations.

For each distillation problem a large number of bubble and dew point calculations must be made. These are trial and error computations, and to apply the Chao-Seader correlation it is necessary that compositions of both liquid and vapor phase be available. Bubble points are calculated by assuming a temperature, computing a vapor composition based on ideal K values, normalizing and applying the Chao-Seader equation to compute a new vapor composition. If $\Sigma K_i x_i$ does not equal $1.0 \pm$ the specified tolerance a new temperature is assumed and the process is repeated. After the second computation, when two sets of assumed and calculated temperatures are available, a linear fit is used to predict the next assumption. This simple algorithm has been found to converge rapidly and reliably. Similar convergence techniques are used for dew points, and for plate mass and enthalpy balances.

The compressibility, z, is computed by trial and error using Newton's method, the initial assumption being $z = 1.0$. In most problems difficulties due to extraneous

roots arise only at temperatures below the range of reliability for the Chao-Seader correlation. A rigorous analytic solution of the cubic equation has been programmed, but is not normally used because of the increase in computer time.

Accuracy of Computations. The computation methods embodied in the program are completely rigorous and the precision of results depends only on the accuracy of the Chao-Seader correlation and on the tolerances set for convergence routines. Before the program was formulated Chao-Seader K values were compared with experimental data and with values predicted by the Benedict, Webb, Rubin equation for mixtures of light paraffins and nitrogen. The following general observations were made:

- The average deviation of computed K values from experimental values is about 8.0%.
- The Benedict, Webb, Rubin equation predicts equilibrium ratios with slightly better accuracy at higher temperatures than does the Chao-Seader correlation.
- At lower temperatures the Chao-Seader method is slightly more accurate than the Benedict, Webb, Rubin equation.
- The Benedict, Webb, Rubin equation, in numerous instances, will predict very accurately K values of one or two components of a mixture, but be considerably in error on other components. The Chao-Seader method gives more uniform accuracy with respect to all constituents.
- The Chao-Seader correlation gives somewhat poorer predictions for binary and ternary mixtures than for mixtures containing a greater number of components.
- Over its range of applicability deviations from experimental data of K values computed by the Chao-Seader method are of the same order of magnitude as discrepancies among independent determinations by different experimenters.

Of the several K value correlation techniques that have been devised some are not easily adapted to computer applications. Some do not permit determination of equilibrium ratio as a function of composition as well as temperature and pressure. For general use none appear more accurate or versatile than the Chao-Seader correlation.

Program Limitations. The program is limited to ranges of conditions over which the Chao-Seader correlation is valid.[9] Limitations with respect to acceptable components and the number of components handled in a specific problem are described under an earlier section, "Characteristics of This Program."

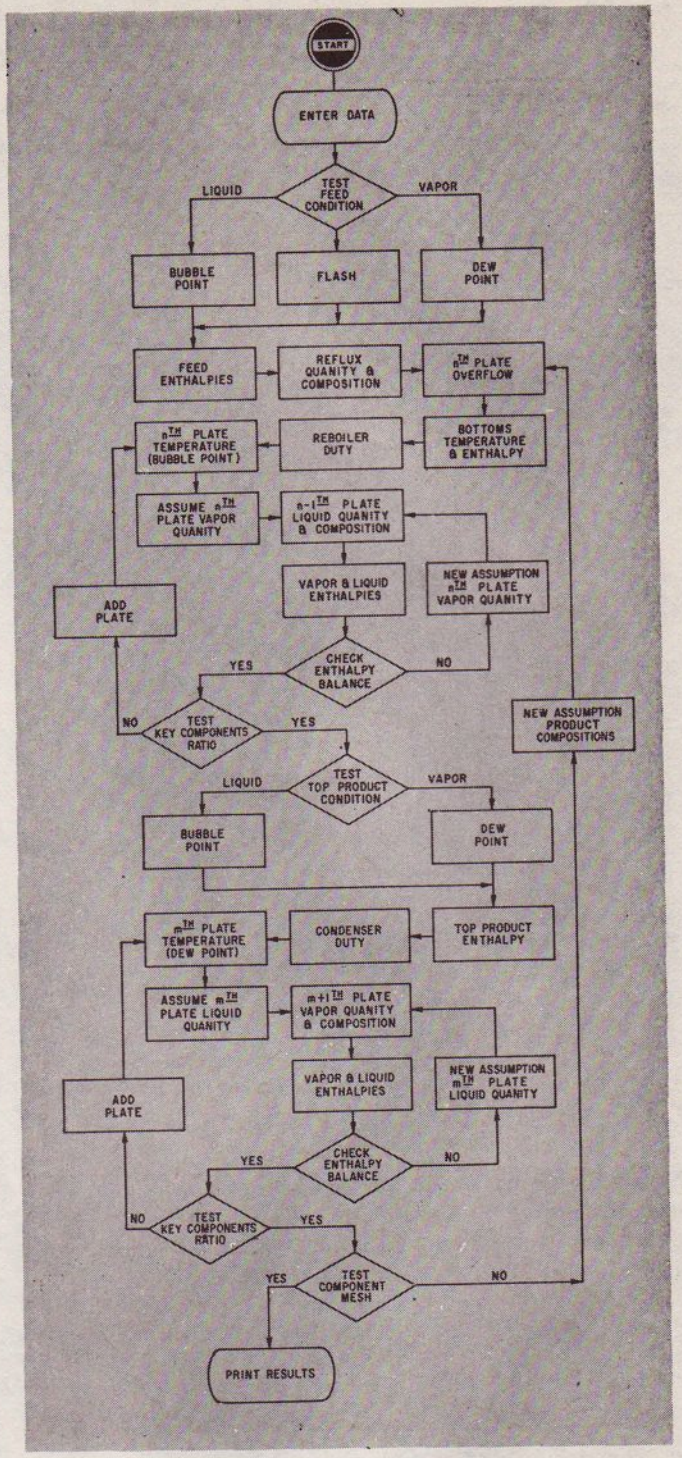


Fig. 2—The program is limited to ranges of conditions over which the Chao-Seader correlation is valid.

Experience. The program has been used to design distillation columns of the following types:

- Natural gasoline stabilizer
- Deethanizer
- Propane separation from heavier hydrocarbons
- Separation of iso and n butanes
- Separation of iso and n pentanes

- Debutanizer
- Depentanizer.

In each application many problems were computed both to test the program and to optimize column designs with respect to reflux ratios and operating pressures.

During development, counters were provided in the program to record the number of iterations in each convergence routine. Various algorithms were tested and only those showing rapid and reliable convergence were retained. With the developed program no convergence failures have been experienced to date.

NOMENCLATURE

$A_0, A_1 \ldots A_9$	coefficients for simple fluids, methane or hydrogen in Eq. (3)
A_{ki}	$[0.4278\, T_{ci}^{2.5}/P_{ci}T^{2.5}]^{0.5}$
B_{ki}	$0.0867\, T_{ci}/P_{ci}T$
D	moles of top product
F	moles of feed = 1.0
H	molal enthalpy
H^0	molal ideal gas enthalpy for mixture
K_i	equilibrium ratio for component i
L	moles of liquid
P	absolute pressure
P_r	reduced pressure $= P/P_{ci}$
P_{ci}	critical pressure of component i
q_c	heat removed in condenser
q_r	heat added in reboiler
R	universal gas constant
T	absolute temperature
T_{ci}	critical temperature of component i
T_r	reduced temperature T/T_{ci}
V	moles of vapor
W	moles of bottom product
x_i	mole fraction of component i in liquid
$x_{fw,i}$	mole fraction of component in feed plate liquor calculated from bottom up
$x_{fd,i}$	mole fraction of component in feed plate liquor calculated from top down
y_i	mole fraction of component i in vapor
z	compressibility factor
γ_i	activity coefficient of component i in liquid solution
Δ_i	adjustment to amount of component i in W for new assumption in meshing iterations
δ_i	solubility parameter of component i (in Chao-Seader equation)
$\bar{\delta}$	$\Sigma x_i \psi_i \delta_i / \Sigma x_i \psi_i$, average solubility parameter of mixture
ν_i^0	fugacity coefficient of pure liquid component i at system conditions
$\nu_i^{(0)}$	fugacity coefficient of simple fluid in liquid state
$\nu_i^{(1)}$	fugacity coefficient correction factor
ϕ_i	fugacity coefficient of component i in vapor mixture
ψ_i	liquid molal volume of component i
ω_i	acentric factor for component i

Superscripts (other than those specifically defined)

L	liquid
V	vapor

Subscripts (other than those specifically defined)

d	top product
f	feed
i	any component
m	number of any plate above feed plate numbering from top down
n	number of any plate below feed plate numbering from top down
w	bottom product

About the authors

WENDELL W. WATERMAN *is director of chemical engineering for Vern E. Alden Co., Chicago, Ill. He holds a B.S. degree from Iowa State University and M.S. and Ph.D. degrees in chemical engineering from University of Iowa. Before joining Alden Co. he was a process engineer for Esso Research and Engineering Co. and in subsequent connections he has supervised process design for plants in petrochemicals, inorganic chemicals and metallurgy. Dr. Waterman is a member of ACS, AIChE and the National Society of Professional Engineers.*

JAMES P. FRAZIER *is a process design engineer for National Gas Pipeline Co. of America, Chicago, Ill. He received a B.S. degree in chemical engineering from Iowa State University and is a member of the National Society of Professional Engineers.*

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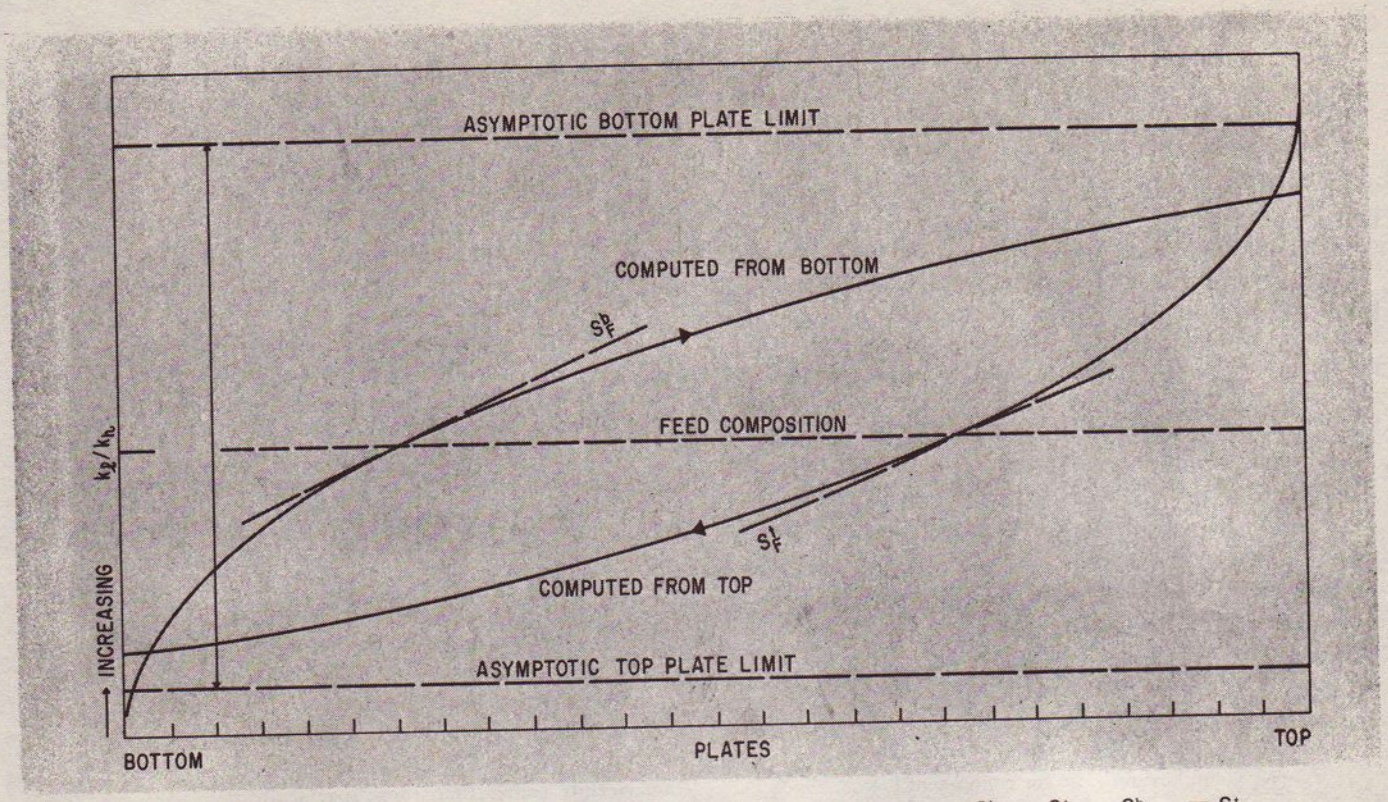

Fig. 1—Key ratio in feed at optimum feed point matches key ratio in column. $S^b_F = S^t_F = S^b_{OPT} = S^t_{OPT}$.

Compute Best Distillation Feed Point

This computer program for multicomponent distillation is modified to give the optimum feed point for many problem situations

Wendell W. Waterman, The Katzman Co., Youngstown, Ohio; **James P. Frazier,** Natural Gas Pipeline Co. of America, Chicago, and **George Martin Brown,** Northwestern University, Evanston, Ill.

MAJOR ADDITIONS AND MODIFICATIONS have been made to a multicomponent distillation computer program[1] which broaden its range of applicability and enable it to cope with various special problems. The original program (now designated Mode I), based on a modified Lewis-Matheson[2] technique, computes the number of theoretical plates required for a specified separation, the feed composition being given and the operating reflux ratio being either specified or determined by application of an assigned multiplier to the minimum reflux ratio computed by the program. Data generation *in situ* is accomplished by use of the Chao-Seader correlation and the Redlich-Kwong equation of state.

The new features include:

- A mode of computation (Mode II) that accepts problems in which the separation attainable with a fixed number of theoretical plates is computed, given the feed composition, reflux ratio, operating pressure, and the over-all split in terms of total moles of distillate and bottoms.

- A mode of computation (Mode III) which accomplishes preliminary determination of required theoretical plates by Mode I followed by meshing iterations under Mode II.

• A mode of computation (Mode IV) similar in essential procedures to Mode I but which determines the optimum plate for introducing the feed in cases where the ratio of key components at the optimum entry point differs appreciably from the key ratio in the feed.

• A mode of computation (Mode V) which accomplishes preliminary determination of required theoretical plates based on optimum feed point location by Mode IV followed by meshing iterations under Mode II.

• A routine for computing the tower operating pressure corresponding to a specified condensing temperature.

• Amplification of the feed analysis routine to enable acceptance of superheated vapor and sub-cooled liquid feeds.

• Storage of all constants used in the Chao-Seader and Redlich-Kwong equations for the entire list of 60 acceptable components in a block data sub-program.

• Major simplification of problem entry techniques.

Mode II. In the previous article,[1] it was explained that the Edison modification[9] of the Bonner equation[10] was used for computing new assumptions with respect to distribution of non-key components in successive meshing iterations. Experience has shown that the Edison modification, involving an arbitrary multiplier applied to the computed adjustment for each component, tends to speed convergence but in certain instances causes excessive swings in early iterations. Consequently, the Bonner equation is now used in its original form.

$$\Delta_i = \left[\frac{X_{fw,i} - X_{fd,i}}{\frac{X_{fw,i}}{W} + \frac{X_{fd,i}}{D}} \right]$$

To initiate a problem, it is the usual practice to enter as the starting assumption for the mole fraction of each light component in the bottoms and each heavy component in the distillate, a very small figure, 1×10^{-20}. Not infrequently, this amount proves too great, and as the computation proceeds from plate to plate, excessive increase in the mole fraction of one or more components may occur.

This "overbuilding" distorts the computation and makes it fruitless to continue without altering the assumed distribution. Occasionally, too, a value predicted by the Bonner equation for either a light or heavy component will be too great and will lead to overbuilding. This is particularly apt to occur in the second meshing iteration.

The program incorporates, both above and below the feed, check routines which compare at each plate the computed mole fraction for each component with the match figure it should agree with (or cross over) at the feed plate. If the match figure is greatly exceeded (some tolerance is allowed), and if the key ratio indicates that more plates must be computed before reaching the feed point, new assumptions are set for distribution of the overbuilding components and computation of the tower section under consideration is restarted. Further, once a value for a component in the distillate (or bottoms) is found to be excessive, this is established (with a tolerance to allow for composition dependency interactions) as a limit so that subsequently no appreciably higher value will be tried even if called for by the meshing formula. Similarly, lower limits are established when values too low for meshing at the feed plate are tried.

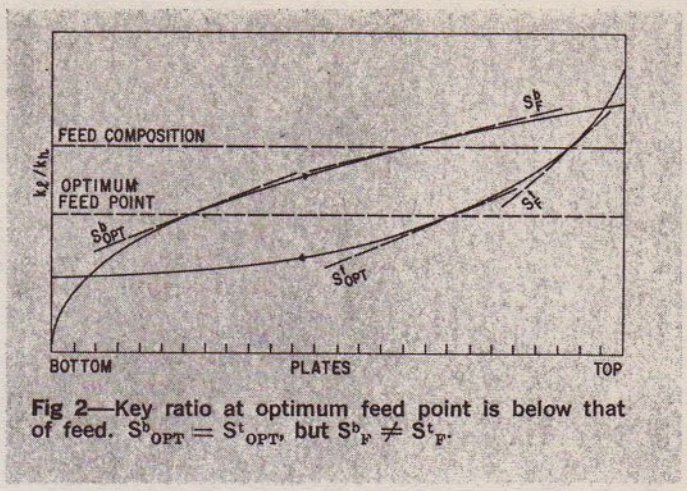

Fig 2—Key ratio at optimum feed point is below that of feed. $S^b_{OPT} = S^t_{OPT}$, but $S^b_F \neq S^t_F$.

The Bonner equation guided by the overbuilding checks and the progressively narrowing limits proves to be a powerful tool in handling meshing problems. It is found that problems involving a fixed number of plates above and below the feed may be fed directly to this routine and solved reliably with rapid convergence. It is necessary, in submitting a problem of this type, to assume an initial split that represents the desired quantities of distillate and bottoms respectively.

This is the method employed in Mode II. The Thiele-Geddes approach[3] has been widely used for solution of problems of this type in other computer programs.[4-8] The present technique offers the advantage that it does not require initial assumptions as to either temperature or composition profiles over the column. In Mode II, key components are not distinguished in the computations and all components are simultaneously meshed at the feed plate.

Mode III. This Mode was developed to cope with an unexpected difficulty encountered in certain problems. In successive meshing iterations under Mode I, the distribution of non-key components in the top and bottom products are adjusted progressively until a pre-determined tolerance is met or until a limiting number of meshing iterations has been run. In most cases the number of theoretical plates is not affected by changes in component distribution from one iteration to the next. However, in certain instances, an oscillation in the number of plates either above or below the feed, though usually not both in a single problem, may occur in the following manner:

Assume that m plates above the feed have been found for the Nth meshing iteration based on a set of assumptions as to amounts of non-key components in, for example, the distillate. For the $N + 1$th iteration new assumptions are computed. Results of the $N + 1$th iteration show $m + 1$ plates required to reach the

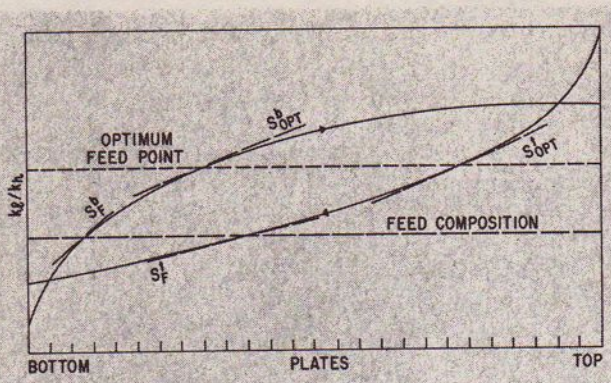

Fig. 3—Key ratio at optimum feed point is above that of feed. $S^b_F \neq S^t_F$.

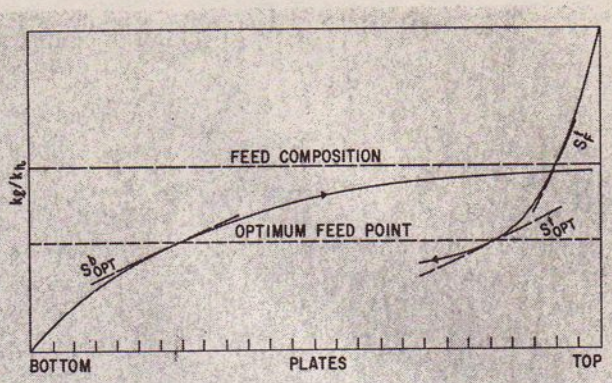

Fig. 4—At low reflux ratio an extremely large number of plates below feed is required to reach feed key ratio.

proper key ratio match point. Further, the proportions of heavy components on the feed plate are found to be excessive since the amounts in the distillate were set for meshing on the mth plate and computations were continued past this point. The $N + 2$ assumptions are then computed on the premise that meshing must be accomplished on the $m + 1$th plate. This calls for reduced amounts of heavy non-key components in the distillate, the amounts being similar to those assumed in the Nth iteration. Upon running the $N + 2$ iteration m plates above the feed are again found and the computed quantities of heavy components on the feed plate are too low. Oscillation in the number of plates will continue until an assigned limiting number of meshing iterations has been reached.

It might appear that this oscillation could be avoided by slightly altering the specified split. However, in cases encountered so far, this was not possible. Increased stringency in the separation merely shifted the oscillation point, so that, for example, instead of oscillating between m and $m + 1$ plates, the computation oscillates between $m + 1$ and $m + 2$ plates.

Integer plate number oscillation occurring in this fashion is due to relative variation in the K values of key components stemming from composition changes. It conclusively demonstrates the necessity in truly rigorous computations of using composition dependent equilibrium values.

Difficulties arising from plate number oscillation might be avoided by determining the fraction of a theoretical plate required for key ratio matching at the feed point. However, another method of coping with the problem has been devised and incorporated in Mode III. This Mode may be used if oscillation is discovered in a problem submitted under Mode I.

In Mode III two iterations are run under Mode I and the larger number of plates found, above, and also below, the feed is accepted and fixed, and operation is transferred to Mode II. This leads, in some cases, to a slightly more complete separation than was originally specified with respect to key components but provides a practicable and rigorous solution to the problem.

Mode III can, of course, be used directly for problems in which no oscillation is either discovered or suspected. It has the advantage, since key designations are dropped after two iterations, of meshing all components at the feed plate and thus more accurately represents actual tower performance than does the Mode I computation.

Mode IV. Problems in which the optimum feed point is displaced from the plate on which the ratio of key components matches that of the feed have been encountered with sufficient frequency to warrant development of a feed point optimizing technique.

For binary systems, the compositions of vapor and liquid leaving the optimum feed plate are directly related to the feed composition. As a first assumption, in multicomponent systems, the ratio of key components in the feed vapor (or liquid) may be taken as equal to the key component ratio in the vapor (or liquid) leaving the feed plate. This criterion gives reasonably good results in many cases. It has been observed to represent roughly the optimum feed point when the relative volatility between the key components is significantly closer to unity than either the relative volatility between the light key and the next lighter component or the relative volatility between the heavy key and the next heavier component. When only one or neither of these conditions exists, the key ratio on the optimum feed plate frequently has been found to be appreciably displaced from the ratio of keys in the feed. Other factors may also affect the location of the optimum feed point.

Plates computed from the top down and from the bottom up are plotted in Fig. 1 on independent ordinates against the key component ratio in the liquid for a typical multicomponent problem in which the feed, the tower pressure and an operating reflux ratio well above the minimum are specified. In the case illustrated, the optimum feed point falls at the point where the key ratio in the vapor from the plate matches that in the feed vapor (or the vapor portion of the feed, or the vapor in equilibrium with a liquid feed). It will be noted that in computing plates from the top down the key ratio falls rapidly at first, then at a diminishing rate. Finally when carried far beyond the key ratio of the feed, the key ratio asymptotically approaches a limit representing a very large number of plates, and has an extremely small change from plate to plate.

A similar, but inverted curve results in the computation of plates from the bottom up, a large change in key ratio is experienced at the beginning and an extremely small change as an asymptotic limit is approached. The spread between the asymptotic limits represents the range of possible solutions to a specific problem. With hydrocarbon mixtures such a range typically exists for any problem in which the operating reflux ratio is well above the minimum. The optimum solution is that which gives the minimum number of total theoretical plates.

When the key ratio on the optimum feed plate matches that of the feed, as illustrated in Fig. 1, the tangent lines to the curves at this key ratio will be parallel. It is apparent that the minimum number of plates for any particular problem will be found at the key ratio where the slopes of the tangent lines to the curves are equal, whether or not this key ratio coincides with that of the feed.

These slopes are designated S^t_{OPT} and S^b_{OPT} in Figs. 1, 2 and 3. Fig. 2 illustrates the case where the key ratio at the optimum feed point is appreciably below that of the feed. Fig. 3 shows the optimum feed point falling at a key ratio higher than that of the feed. It will be noted that in Figs. 2 and 3, the slopes of the tangent lines at the key ratio of the feed S^t_F and S^b_F are unequal and that the sum of top and bottom theoretical plates is greater than at the optimum feed point. In Mode IV, the program computes as much of each plate vs. key ratio curve as may be required to find the point where the slopes are equal and the number of theoretical plates is minimum.

The use of this optimizing technique is facilitated by entering, for the first iteration, small numbers for the assumed mole fractions of heavy components in the distillate and light components in the bottoms since this permits optimization for the first iteration to proceed with minimal chance of overbuilding. However, if needed, the overbuilding routines will operate to enable the computation. Location of the optimum feed plate, as found in the first iteration, is subject to redetermination in subsequent iterations, but such redeterminations are not apt to cause a shift of more than one theoretical plate. After each computation the key ratio on the optimum feed plate is stored and used as the match point for the next meshing iteration.

At reflux ratios close to but above the minimum a number of variations in shape of the plate vs. key ratio curves may occur. At the true minimum reflux ratio only one point of feed introduction gives a solution and the ratio of keys on the feed plate may not coincide with the feed key ratio. Consequently it is possible to encounter problems which, over certain ranges of reflux ratio, have real solutions but which present no solution based on feeding the column on the plate where the key ratio matches that of the feed.

A problem is illustrated in Fig. 4 in which a normal curve exists for top plates but the curve for bottom plates approaches the feed key ratio very slowly. In this case an extremely large number of plates below the feed is indicated when closing on the key ratio of the feed. With the optimizing technique the best solution, representing minimum plates for the separation specified and the reflux ratio considered, is readily found.

An example is presented in Fig. 5 in which a hook exists in the top plate curve making it impossible to reach the feed composition key ratio. The bottom plate curve, however, continues well beyond the key ratio of the feed. In executing the program this condition is detected by a slope inversion test. When inversion is found top plate computations are stopped, bottom plate computations are initiated and the point of parallel slopes is found in the usual manner. A problem of this type cannot be solved by direct convergence on the key ratio of the feed but a range of solutions nevertheless exists and the optimum is determinable by the program. Fig. 6 illustrates the same type of problem but with the hook occurring in the bottom plate curve at a key ratio below that of the feed.

A low reflux ratio problem is illustrated in Fig. 7 which exhibits another variation in the interrelations among plates, meshing and possible feed points. When the problem is introduced in the usual manner with very small amounts assumed for heavies in the distillate and lights in the bottoms the first meshing iteration gives an indicated optimum of the type shown in Fig. 2. However, with new assumptions respecting the distribution of non-key components, in the second iteration the results show hooks in both the top and bottom plate curves with no overlap of key ratios.

In this particular problem, any attempt to distribute non keys to secure meshing at the key ratio where this first set of equal slopes is encountered will result in double hooks with no common key ratio. Despite indications at this point, possible solutions may exist, as shown, the entire range falling between the inversion points of the top and bottom curves respectively.

The optimum feed point is found at the point where the slopes of the inverted curves become equal. The zone of possible solutions may be appreciably less than the full span between low and high invert points since it is limited to points at which complete meshing of all components is possible.

Problems of this type are rarely encountered. When they are, practical considerations usually call for higher reflux ratios. Consequently no attempt has been made to include in the program the capability of optimizing and meshing in this special situation. If such a problem is submitted for solution, the existence of non-overlapping double hooks is detected and the computation terminated. The type of problem presented in Fig. 7 can be resolved, however, by use of the program. Mode II will compute the meshing of all components in this case with key ratios following the curves as shown. However, the number of total plates required and the optimum feed point for a specified separation and given reflux ratio must be determined by trial and error in successive entries of the problem.

Typical curves of plates vs. key ratio at minimum reflux are illustrated in Fig. 8. In this case only a single mesh point is possible at one particular key ratio, which, as indicated above, may be either above or below the key ratio of the feed.

Computation of Column Pressure. In the original program, column pressure was specified and the con-

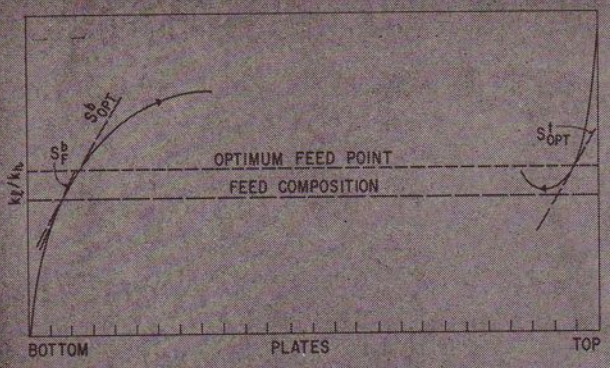

Fig. 5—At low reflux ratio, computation of plates from top down gives a hook in the curve above feed key ratio.

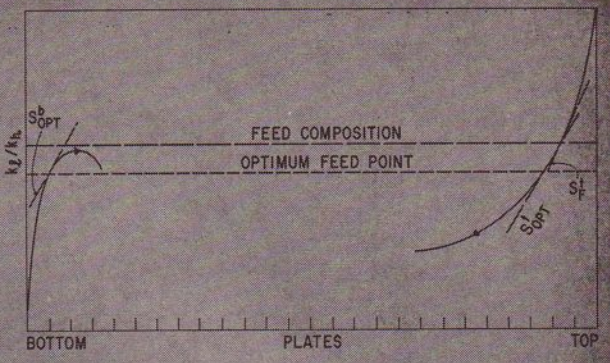

Fig. 6—The hook in the curve can also occur in the computation of plates from the bottom up.

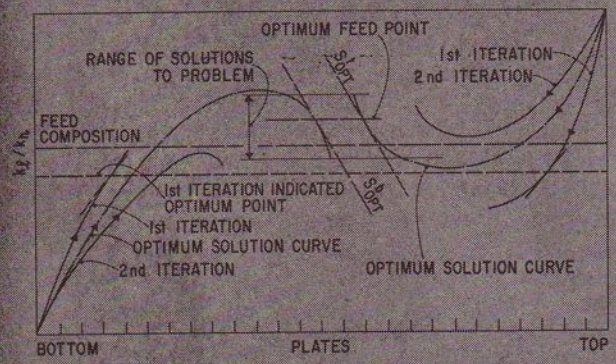

Fig. 7—The second iteration gives hooks in both the top and bottom plate curves with no overlap. Solutions lie beyond the inversion points.

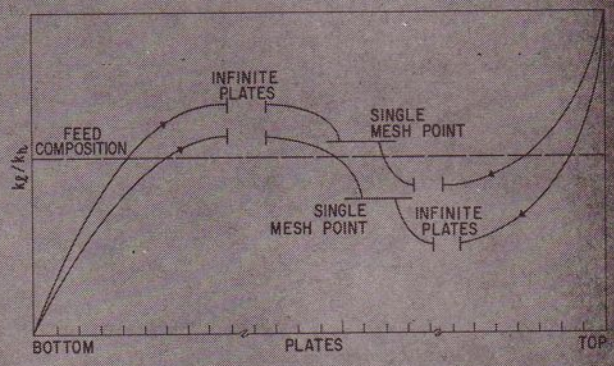

Fig. 8—At minimum reflux, the single mesh point may be at a key ratio either above or below that of the feed.

densing, reboiling and all plate temperatures were computed. In many cases it is desired to specify condensing temperature in order to meet a given cooling water or refrigeration temperature level. The new routine for computing tower pressure entails a determination of the condensing temperature at two assumed pressures and calculation of the tower pressure by interpolation or extrapolation based on an assumed linear relationship between the logarithm of the absolute pressure and the reciprocal of the absolute temperature.

If the condensing temperature is computed on the basis of an initially assumed distribution of components in the distillate, a slight variance may occur when a more precise determination of component distribution is made in meshing iterations. Usually the change is not enough to warrant re-computation of the operating pressure.

Acceptable Feed Conditions. In the original version the program accepted only saturated vapor, mixed liquid and vapor or saturated vapor feeds. If the specified feed temperature was found to correspond to a sub-cooled liquid or a superheated vapor, the specified temperature was ignored and the feed was taken at its saturation temperature. The new version of the program accepts any feed temperature and determines whether this corresponds to liquid, vapor, or a mixture of liquid and vapor. If a superheated vapor or a sub-cooled liquid condition is found, the enthalpy is computed and the feed is introduced at the specified temperature. Enthalpies of liquid, vapor and liquid-vapor mixtures are computed by equations developed by Edmister, et al.[11] The vapor enthalpy equations are applicable to vapor in both the saturated and superheated conditions. The liquid enthalpy equations were developed for the bubble point liquid and have not yet been tested for sub-cooled liquids. In the program these have been used, however, for sub-cooled liquids; so for feeds in this state computed enthalpies must, at this time, be regarded as approximate.

Block Data Storage of Constants. It has been found convenient to store all constants required for the Chao-Seader and Redlich-Kwong equations for the entire list of acceptable components in a block data sub-program. With the original program, it was necessary to submit with each problem a previously prepared card, for each component in the feed, on which appropriate constants were punched. Block data storage eliminates this requirement.

Problem Entry. Problems can now be entered by preparing one card for each component plus two additional cards. On each component card the component number and name, and identifying number are punched together with mole fractions in the feed, distillate and bottoms and an appropriate designation if the component is a light or heavy key. In addition to the component cards, one card is required for problem identification and another for selection among alternate computing modes.

In Modes I, III and IV, with the components listed

in order of decreasing volatility, heavy components in the distillate and light components in the bottoms may be specified as zero or left blank on the problem input cards. If meshing is called for, the program assigns to such components the starting value $1 \times 10.^{-20}$ The split of key components must be specified by entering an amount for the heavy key in the distillate, and for the light key in the bottoms. If for either key the other amount is omitted the program computes it. A starting assumption with respect to split must be provided for distributed components falling between the keys.

The input formats permit entry of any desired set of starting assumptions with respect to distribution of non-key components in the distillate and bottoms. Thus, if reliable approximations are available in advance they may be used to minimize the number of meshing iterations. Further, if a problem has been run for say three meshing iterations, the computed distributions may be entered as input in re-submitting the problem, in which case, meshing iterations are continued without repetition.

In the case of hydrogen in the bottoms the initial assumption of 1×10^{-20} has been found too high in many instances. Any desired value may be entered and this will override the arbitrary assignment. It is the usual practice to enter 1×10^{-30} for hydrogen in the bottoms, particularly if a fairly large number of plates below the feed is anticipated.

A convenient problem input form has been devised consisting of a single 8½ × 11-inch sheet on which all necessary information may be entered. The form includes all required instructions to the key punch operator so that the time of technical personnel required to set up and enter a problem is minimal. Once defined, a problem can ordinarily be entered in 15 to 30 minutes.

Computer Time. Core time has been considerably reduced by numerous minor improvements since the development of the original program. Over the last year, many problems have been run on IBM 7090/94 and Control Data 3400 computers. In this application the speeds of these machines are about equal. A 17-component Hydrotreater Effluent Stabilizer problem with components ranging from hydrogen to decane has been found to require about 2½ minutes when run through five meshing iterations. Satisfactory meshing of all components was achieved. In the IBM 7094 computer the core requirement including that of the processor program and library subroutines is approximately 18 K, 36-bit words.

NOMENCLATURE

D	moles of top product
Δ_i	adjustment to amount of component i in W for new assumption in meshing iterations
K_i	equilibrium ratio for component i, (y_i/x_i)
k_l	moles of light key component in liquid
k_h	moles of heavy key component in liquid
m	number of theoretical plate above feed counting from top down
N	number of meshing iterations
S^b_F	slope of key ratio versus plates below feed curve at key ratio of feed liquid
S^t_F	slope of key ratio versus plates above feed curve at key ratio of feed liquid
S^b_{OPT}	slope of key ratio versus plates below feed curve at optimum feed point
S^t_{OPT}	slope of key ratio versus plates above feed curve at optimum feed point
W	moles of bottom product
x_i	mole fraction at component i in liquid
$x_{fd,i}$	mole fraction of component i in feed plate liquor calculated from top down
$x_{fw,i}$	mole fraction of component i in feed plate liquor calculated from bottom up
y_i	mole fraction of component i in vapor

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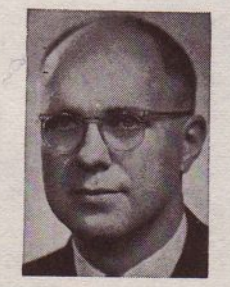
Indexing Terms: Bonner-0, Chao-Seader-0, Columns/Process/-4, Compositions-6, Computing-8, Computers-10, Concentrations-6, Distillation-9, Equations-10, Equilibrium-7, Estimation-4, Input-7, Lewis-Matheson-0, Redlich-Kwong-0, Reflux-6, Separation-9.

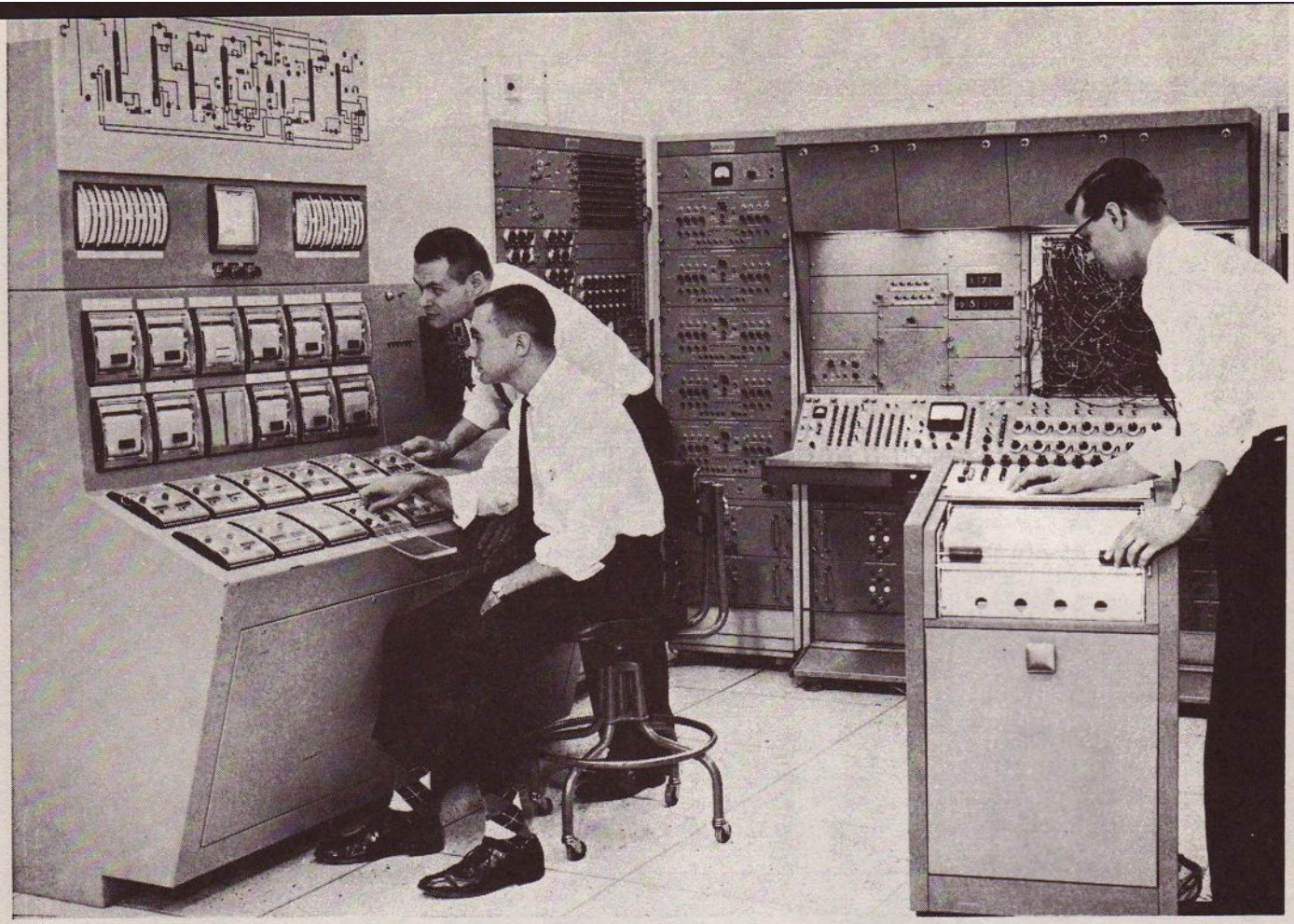
About the authors

WENDELL W. WATERMAN *is vice president of Process Division of The Katzman Co., Youngstown, Ohio. He holds a B.S. degree from Iowa State University and M.S. and Ph.D. degrees in chemical engineering from University of Iowa. He has been a process engineer for Esso Research and Engineering Co. and in subsequent connections he has supervised process design for plants in petrochemicals, inorganic chemicals and metallurgy. Dr. Waterman is a member of ACS, AIChE and the National Society of Professional Engineers.*

JAMES P. FRAZIER *is a process design engineer for National Gas Pipeline Co. of America, Chicago. He received a B.S. degree in chemical engineering from Iowa State University and is a member of the National Society of Professional Engineers.*



GEORGE M. BROWN *is professor of chemical engineering at Northwestern University, Evanston, Ill. Of his chemical engineering degrees, his B.S. degree was from University of Michigan, S.M. from Massachusetts Institute of Technology and Ph.D. from Northwestern University. Dr. Brown has done process design and consulting in separation processes and thermodynamics. He is a member of AIChE, ACS and ASEE.*



Analog Simulation Spells Safe Startups

Analog simulators have long been used in operator training for normal operating conditions. But training for vital startup phase has been largely ignored. Here is how the Humble-Esso organization bridged the gap

R. E. Lieber, Esso Research & Engineering Co., Florham Park, N.J., and **T. R. Herndon,** Humble Oil & Refining Co., Baytown, Texas

IN AN EFFORT to provide experience *before* startup, the techniques of dynamic, realistic simulation have been used in a Esso Research & Engineering Co. training program for experienced operators. These techniques involve simulating operations of a highly integrated section of a new refinery on an analog computer. The goal is to demonstrate major process interactions and their effect on plant operations.

Plant type instruments tied into the computer serve as the "control house." This training program has proved highly successful, as this refinery has been brought on-stream smoothly. Thus, more training sessions of this kind are planned.

Startup simulation is especially useful to an operator on a new, complex, highly heat integrated plant. He has a unique problem because his plant has never before been started up and is inherently more difficult to operate than older plants.

There is benefit in extending such a simulation to cover startup—that is, bringing the plant up to design operating conditions. This would be of value not only in terms of improved operator training, but also in setting optimum startup procedures.

There are big differences between a model developed

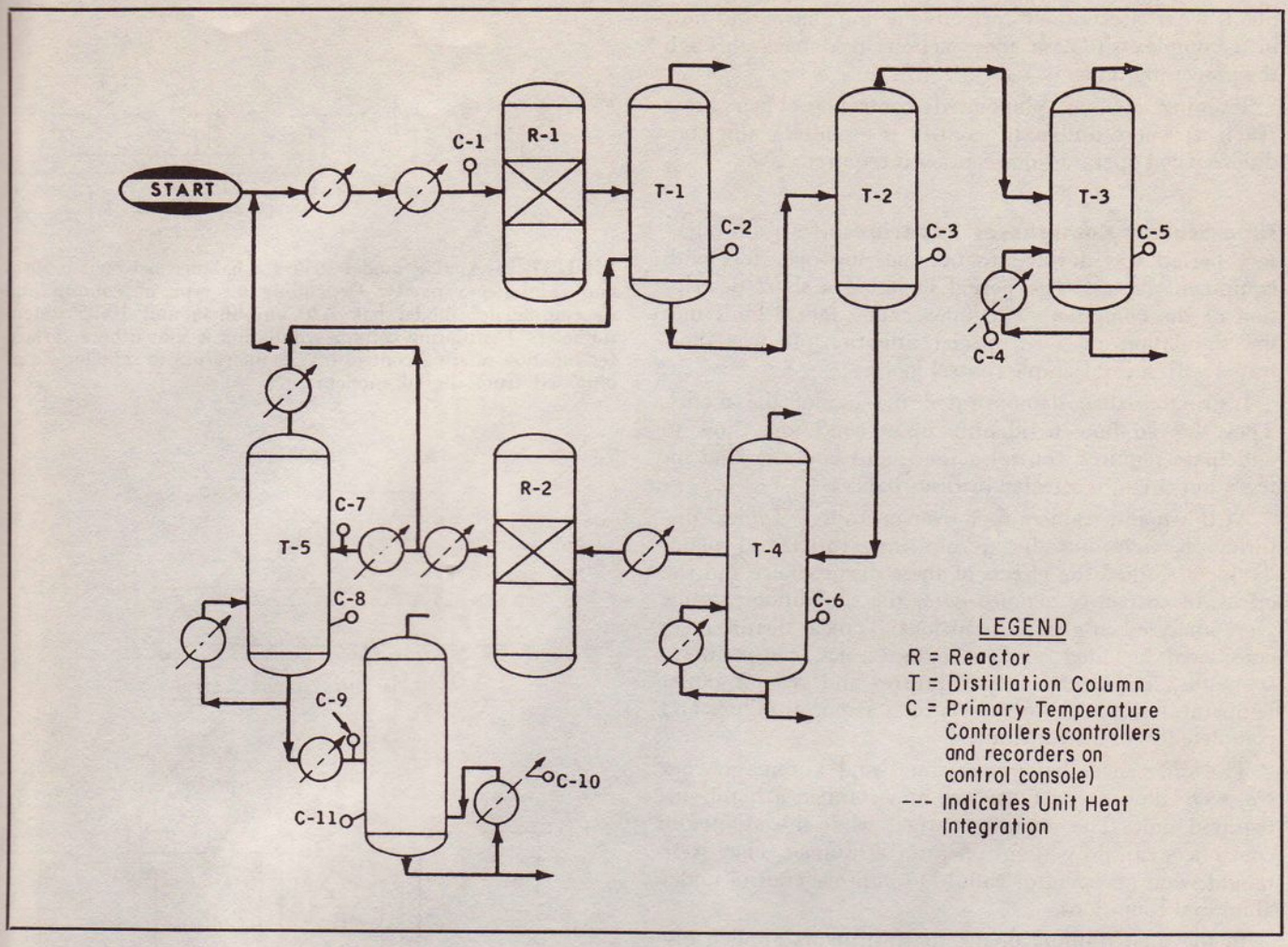


FIGURE 1—This section of the refinery was simulated by the computer and model (Six distillation towers, with preheat exchangers and reboilers, and two reactors). Notes: Unit contains no intermediate tankage. Not shown: Four 15-minute holdups (flow control on outflow); All other associated equipment (condensers, coolers, etc.); Pressure, flow, level controllers.

for normal plant operation and one that simulates startup operations. After describing the normal operation model, we will point out these differences. We will consider what is involved in a plant startup and how this affects the computer model.

Analog Model Adds Realism. The section of the refinery simulated for operator training is shown in Figure 1. Included are six distillation towers, with preheat exchangers and reboilers, and two reactors. For over-all heat economy, 11 exchangers transfer heat from one process stream to another, rather than to cooling water. The plant has no intermediate tankage. The only storage consists of four 15-minute holdup drums with the outflow of each on flow control.

A mathematical model was developed for each major piece of process equipment, describing its steady-state and transient behavior. The complete plant was programed on an analog computer containing about 400 amplifiers and 400 potentiometers. This plant simulation, occupying four standard consoles of analog computing equipment, was then connected to a control console.

The control console has standard plant recorders and electronic controllers. Their input and output voltages are compatible with the computer.

The analog model and control console together simulated the operator's normal plant environment. It also gave him access to similar records and indications that he would have in an actual control house. To use time most efficiently in the 10-day program, simulation was time-scaled, speeding up the process by a factor of 10.

Recorder speeds were stepped up by the same factor. Thus, recorder charts appeared familiar to operators. By taking advantage of the analog computer's time-scaling feature, many dynamic control situations could be investigated in a short time.

Trainees were all experienced operators. So emphasis was on familiarizing them with operating and control characteristics peculiar to the unit. The model gave directional indications of system behavior under upset conditions. It also illustrated the time relationships involved.

Thus, operators got the feel of the instruments. They learned how various disturbances propagate through the plant, what effects their corrective actions have, and how in a complex situation these actions feed back through the processing units.

Training sessions pinpointed control problem areas (such as where automatic control is essential) and conditions when operator intervention is required.

Time-Scaling Compresses Experience. An introductory period was devoted to familiarizing operators with equipment in use. The period included a short description of the computer. The time-scaling factor built into the simulation received special attention. It was illustrated with several simple control loops.

Instructors then demonstrated the use of the model. They showed how to identify upset conditions, how to anticipate required control actions, and how the heat integration circuit is affected by disturbances.

At this point, trainees took over operation. Typical disturbances were introduced into the simulated plant. Trainees studied the effects of these disturbances and the effects of corrective actions. After the simulations, results were analyzed in group discussions. Typical disturbances considered included changes in feed rates, compositions, set-points, feed preheat temperatures and reactor outlet temperatures, and major upsets such as pump failure and complete loss of instrument air.

The differences between manual and automatic control were illustrated. These are important in a highly integrated unit. The trainees learned what the automatic controllers can do without operator assistance. They were taught what an operator can do to improve control under abnormal conditions.

In the final training phase, the instructors applied disturbances which, on the basis of their experience with the model, the operators identified and corrected for.

Simulating Process Units. Even with the large amount of computing equipment used, certain simplifications in the mathematical model were required. Since operator training was the primary purpose, operability limits on some of the equipment were not considered.

For example, it was assumed that the fractionating towers can hydraulically handle the design rates or any applied deviations. Therefore, the model did not include dumping and flooding correlations. Since pressure control is relatively fast and usually good, constant pressure at the design value was assumed for the model.

Control console instruments were mainly recorder-controllers for temperature and differential temperature at points in the fractionator towers, pre-heaters, and elsewhere in the heat integration circuit. Such local instruments as level indicator-controllers on low holdup vessels were not simulated. Other recorders (i.e., flow) were simulated by 8-channel analog recorders.

In deciding how to simulate the dynamic behavior of refinery equipment, the purpose of simulation is very important. For this program, the main concern was to build into the simulation directional indications that familiarize the operators with the idiosyncracies of particular units. Errors up to ± 10 percent were tolerated.

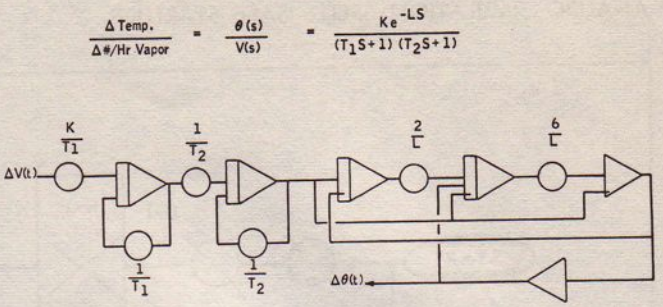


FIGURE 2—Analog model strikes a balance between realism and computer capacity. Depending on type of column and its complexity, model has 7-20 amplifiers and 10-25 potentiometers. Distillation column simulation is shown here. Transfer function relating control tray temperature to reboiler vapor obtained from digital model.

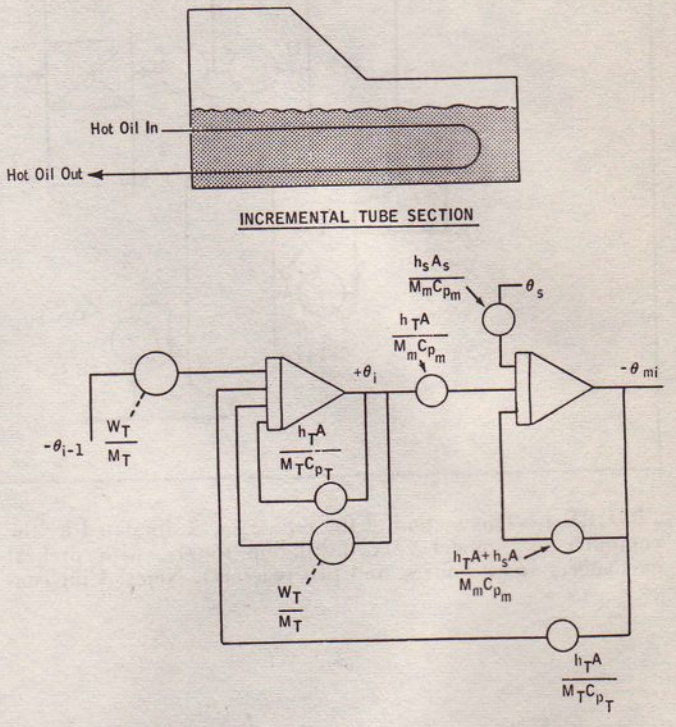


FIGURE 3—Computer model for kettle reboiler simulation (constant shell side temperature).

The model was to represent daily operations. So, extreme excursions from design points would be rare. This allowed certain simplifying assumptions, such as linearized perturbation models, tower control temperatures as functions of composition only and not of pressure, and pseudobinary tower feeds.

To simulate major items of refinery equipment we employed existing rigorous digital models, from which linearized transfer functions, were derived. These transfer functions were then approximated with simpler ones. The simplifying assumptions were based on previous operating experience with similar units. In some cases, actual plant data from a similar unit was used as a check.

Because heat integration affected the reboilers and condensers, distillation columns were isolated from the over-

head and bottom equipment in the calculations. Dynamic plate-to-plate calculations were made digitally, assuming pressure to be constant (but not necessarily uniform across the tower).

The feed was broken down into pseudobinary components.

Linearized transfer functions were obtained to relate product compositions, overhead and bottoms temperatures, and control tray temperatures to such inputs as preheat, reboiler heat, reflux and feed rates, and product withdrawal rates. In simplifying these transfer functions, a balance was struck between program realism and computer capacity. Depending on the type of column and its complexity, the analog model, Figure 2, contained 7 to 20 amplifiers and 10 to 25 potentiometers.

Realistic Reboiler Simulation. Simple heat exchangers such as kettle reboilers with constant shellside temperature and no phase change in the tubes were simulated rigorously. They required 7 amplifiers and 10 potentiometers. For the more complex exchangers, the dynamics were first derived digitally, then approximated by simplified transfer functions.

Each heat exchanger was broken down by tube sections. For each section, heat and material balances were programed to solve for tubeside inlet temperature to the next section θ_T, and shellside vapor generated V.

The analog model for a kettle reboiler, Figure 3, solves the equations:

$$m_M c_M \frac{d\theta_m}{d_t} = h_T A_T (\theta_T - \theta_M) + h_S A_S (\theta_S - \theta_M)$$

$$m_T c_T \frac{d\theta_T}{d_t} = w_T c_T (\theta_{T\,i-1} - \theta_T) + h_T A_T (\theta_M - \theta_T)$$

$$V = \frac{\sum_{j=1}^{n} h_S A_S (\theta_m - \theta_S)}{\lambda}$$

where the subscripts T, S, and M refer to tubeside fluid, shellside fluid, and tube metal; h is heat transfer coefficient, A heat transfer area, Θ temperature, m mass, and c specific heat. λ is the latent heat of vaporization of the shellside fluid (tower bottoms); w_T is the mass flow rate of the tubeside fluid (reactor effluent), and m_T is its holdup mass in the ith section of the exchanger.

Reactor simulation required extensive steady-state calculations. Correlations were first developed relating outlet temperature and conversion to changes in inlet temperature, flow, and concentration. Based on flow rate, holdup, and assumed flow patterns, dynamic behavior was calculated. It was then approximated by such simple transfer functions as a dead time and two time constants. Reactor simulation circuits were similar to those for distillation columns. They required 3 to 6 amplifiers and 4 to 6 potentiometers.

Temperature transmitters were simulated by a first-order lag. The dynamics of transmission lines, valves, 10 to 15-second holdup vessels, and flow controllers were ignored. These responses can be assumed instantaneous relative to the important control aspects of the unit-temperature control and liquid level in 15-minute holdup drums.

Startup Operation. Shortly after the training program was completed, the refinery was brought onstream. Although some of the usual mechanical problems occurred, the plant was smoothly lined out. No problems arose in areas the simulation covered.

Similar analog simulations for operator training are now underway, not only for highly integrated plants, but also for new processes where no previous operating experience exists.

As plants become more complex with higher heat and process integration, the startup phase becomes more critical. With the success of the program just described, we investigated how to simulate actual startup. There are several distinct phases after construction of a new plant is completed. These involve the pre-startup activities such as commissioning utilities, running in oil pumps and compressors, flushing lines, drying furnace refractory and steaming out towers.

After the unit is ready to go, circulation is started by pumping streams into various pieces of equipment.

Levels in drums are established. Heat is added to warm up the equipment and process streams. Inert gases are vented and pressures are built up. The startup progresses as additional equipment is brought into operation in order and the unit begins making product. These streams are initially recycled or sent to slop. The final stage of startup consists of lining out the operating units to bring the products on specification.

Startup Involves Crises. This description of a startup makes it appear a simple operation. Actually, it is a series of small crises. A number of process and mechanical difficulties usually develop. These must be corrected before the next step can be taken.

Thus, the operator must know how to cope with equipment failures occuring at any time in startup. He must be ready for emergency conditions, know how to recognize them, and know what action to take. He must manipulate a large number of process variables either manually or by controller set point adjustments as the unit is brought up. Instruments are normally commissioned as the startup progresses. Still, the operator cannot heavily rely on his controls to correct upset and emergency conditions.

In a complex heat integrated plant, the operators' difficulties are compounded. With heat integration, the startup sequence will usually not follow the processing sequence. This is because the heat source for upstream equipment may not be available until downstream equipment is operable. Thus, pieces of equipment may have to start up simultaneously and be brought up together to maintain heat balance in the unit.

Also, without intermediate tankage between units, levels in surge vessels occupy much operator attention. Thus, the startup of an integrated plant places a heavy load on the operator. This burden is lightened if he

has been through the startup a number of times and is aware of what to expect from action he takes.

The Same Computer Models Do Not Apply. A start-up simulation requires a mathematical model of the time varying behavior of each piece of equipment. However, the two models are vastly different.

Simulation of normal operations involves small excursions about an operating point. Certain variables such as tower pressures and levels in low hold-up vessels can be considered as constant. With this approach, wide use can be made of linearized perturbation models.

During the startup of a plant, flows, temperatures, and pressures undergo many-fold changes. Few variables are constant for a computer model. Since startup is sequential, its simulation undergoes a major change as each piece of equipment is commissioned. Therefore, the main emphasis of a computer model is to account for the heat balance and flow of material as the start-up sequence progresses.

Compositions of product streams do not become significant until the line-out phase. For example, in a pipestill, the initial startup step will involve gas oil circulation. This brings up temperatures in the tower and preheat exchanger train before crude oil is brought into the unit. With the changes in the process variables involved during startup, properties such as gas densities, heat capacities, and thermal conductivities also cannot be assumed as constant. They become dependent variables in a computer model. Thus, perturbation models have little application and many nonlinear computing components are required.

Simulating a Tower. As an example of the differences between the two models, consider a fractionating tower. For normal operation, about the design value, a very adequate model consists of establishing steady-state relationships and using linearized transfer functions to relate tower temperatures and product rates and compositions to input variables. These transfer functions result in simple analog circuitry.

For the startup of a fractionating tower, a computer model must consider warm-up, pressuring and purging. During the pre-startup phase, the tower will have been steamed out and pressured with inerts or light gas. As feed and reboil heat are introduced, hydrocarbons begin condensing on the tower surfaces. This is the principal means of heat transfer during the warm-up. However, the heat transfer coefficients depend strongly on the amount of noncondensible gas present in the tower and this changes as the tower is purged.

Describing the transients of pressure, temperature and the condensed hydrocarbon accumulating in the tower and distillate drum results in nonlinear differential equations such as the following ones for tower pressure.

$$\frac{d}{dt}\frac{P_T}{T_V} = \frac{R}{V}\left[\frac{Q_R - h\left(\frac{P_H}{P_T}\right)A(T_V - T_M)}{\lambda} - (O)\frac{492}{359}\frac{P_T}{T_V}\right]$$

$$\frac{d}{dt}\frac{P_I}{T_V} = -\frac{R}{V}\left[(O)\frac{492}{359}\frac{P_I}{T_V}\right]$$

$$P_H = P_T - P_I$$

where P_T, P_H, and P_I refer to totals, hydrocarbon and inert pressures in the tower; T_V and T_M are vapor and metal temperatures; V is tower volume, R is the gas constant, Q_R is reboiler heat,

$$h\left(\frac{P_H}{P_T}\right)$$

is the heat transfer coefficient as a function of the hydrocarbon composition, λ is latent heat of vaporization and O is the overhead vapor rate.

Similarly, differential equations with dependent coefficients are involved for the vapor and metal temperatures. The analog circuitry for the set of equations describing this operation is considerably more complex than that shown in Figure 2 for a single tower model.

Can the Two Models Be Combined? Since the simulation of normal operation and the startup each require much analog computational equipment, the question of equipment limitations is raised. Obviously, a combination of the two models would be the most effective training tool. Mathematically, this is not difficult. Simulating the operation and startup of a small and single unit is easily done.

However, the value of computer simulation is in its application to complex and integrated processing units from which small portions cannot be isolated. Thus, the nature of the application demands extensive computational facilities. The problem that now remains is the development of solution techniques to permit a practical meshing of the two models.

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About the authors

ROY E. LIEBER *is a systems engineer for Esso Research & Engineering, Florham Park, N. J., where he handles systems analysis, dynamic simulation with computers, and control system consulting. He has a B.S. degree in chemical engineering from New York University (1957). Mr. Lieber also has process and project design experience with Esso R & E, including both analog and digital computer applications. He is a member of the Instrument Society of America.*

THOMAS R. HERNDON *is a staff engineer for Humble Oil & Refining Co., Baytown, Texas, where he does systems studies and consults with and aids others in analog computer research. He holds B.S. degrees in mechanical and electrical engineering from Southern Methodist University. A registered professional engineer in Texas, Mr. Herndon has been with Humble 17 years. He is a past director of Simulation Councils, Inc.*

Train Power Station Operators by Analog

American Oil's Whiting refinery has used analog simulators successfully in a variety of training programs to upgrade operators. Here is their latest innovation, which you may use to increase employe proficiency

L. G. Whitesell and **E. H. Bowles**
American Oil Co., Whiting, Ind.

A RELATIVELY NEW, interesting, fast and efficient method for using an analog model to train refinery power station operators is enjoying success at American Oil Co.'s Whiting refinery. Models are proving useful in many training applications as well as for simulations from which to make operating calculations. (For example see "Train Your Operators by Computer," HP/PR, July 1963, Page 192; and "Try This Analog for Solving Fire-Water Problems," September 1962, page 274).

The latest innovation is a computer-operated working model for power stations. It is set up to fit unusual operating problems at Whiting refinery, but could be applied to any refinery where an analog computer is available. Here's how the system works.

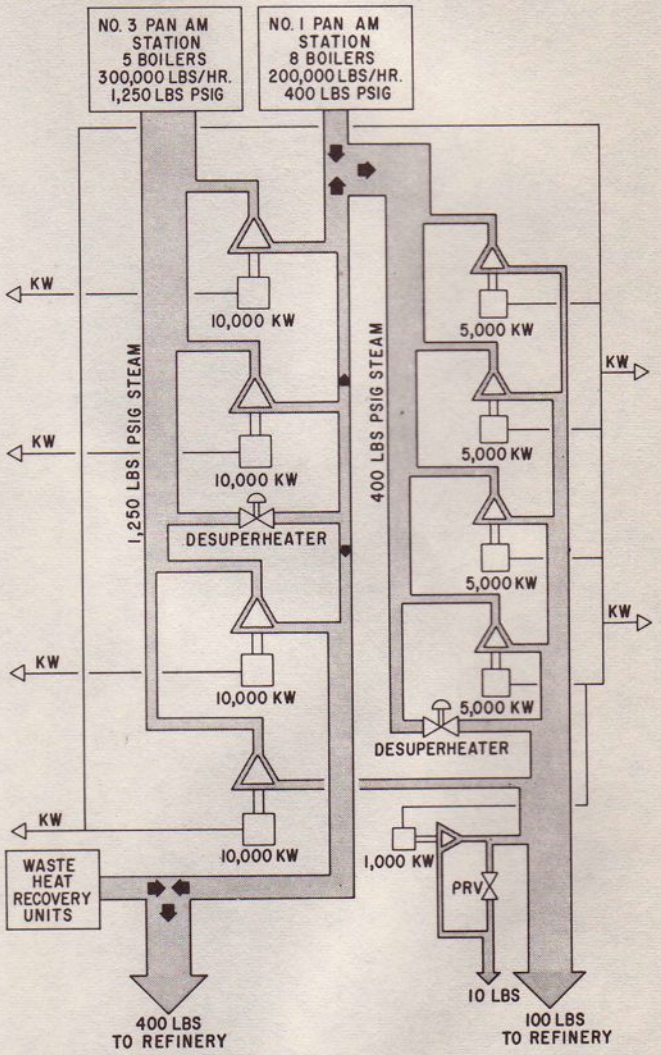


FIGURE 1—These two stations provide all of Whiting refinery's electric power and most process steam. Line widths show relative magnitude of steam flows in various parts of system.

A Complex System to Learn. The two separate, but tightly interconnected, steam and electric power generating stations at the Whiting refinery make up a highly complex system. As electric demand has increased and process steam demand has decreased in recent years, operating problems have steadily grown more difficult.

The efficient training of new men and upgrading of older men's skills has become more important as the steam-electric power balance has grown tighter.

Operators must be able to comprehend the overall system, so they can function smoothly as a "team" to achieve a common operating goal.

The Whiting Power Stations. All electric power and most of the process steam required by the refinery is produced by two stations (see Figure 1). The No. 1 Station produces 400-psi steam which is passed through turbines and converted to 100-psi steam for process use. The No. 3 Station produces 1,250-psi steam, which is

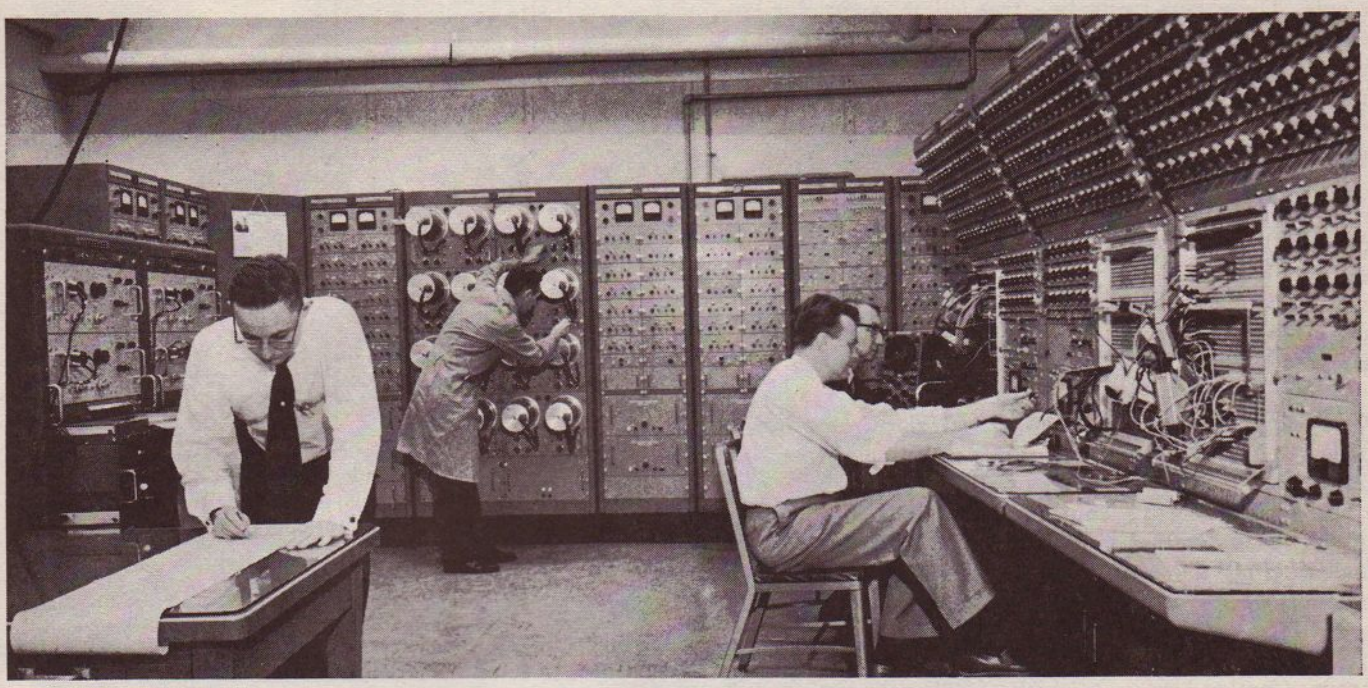


FIGURE 2—The system is controlled by this analog computer, built in a lab near the refinery. It is used exclusively for simulation work.

passed through three turbines to produce 400-psi steam, and through one turbine to produce 100-psi steam. Three small turbines in the No. 1 Station (only one is shown in the figure) use 100-psi steam and provide added operating flexibility in special situations.

Waste heat recovery types of steam generating units are located on refinery process units and beyond the control of the power station operators. These provide half the total refinery demand for 400-psi process steam.

Pressure reducing and desuperheating units parallel each of the two main sets of turbines. They are automatically controlled to maintain a set pressure in the steam system downstream of the reducer. The desuperheaters normally absorb the steam flow variations caused by changes in steam and electric demands.

The line widths in Figure 1 show the relative magnitude of steam flows in the various parts of the system.

Operating Problems. The station operators face two basic classes of problems. One class involves unusual demand changes and equipment failures, when operating conditions are tight and flexibility is limited.

The other involves ability to minimize production of "non-byproduct power" during day-by-day normal operation.

In the past, process steam demand well exceeded that produced by turbines in meeting the electric demand. And, enough steam flowed through the desuperheater units to accommodate any sudden change in demand for either steam or electricity. Individual refinery processing units were small enough that sudden large changes in system load were unlikely.

Today, steam demand barely exceeds that produced by the turbines alone, and the refinery consists of a few large processing units. So, the likelihood of sizeable swings in demand is much greater.

Byproduct Power. Power produced by the turbines when a process requires their exhaust steam is called "byproduct power." In this case the cost of the fuel represented by the latent heat in the steam is charged to the process.

Such byproduct power requires about 3,600 Btu per kilowatt-hour. But if condensing or atmospheric exhaust turbine drives are substituted for the usual electric drives on process units, the "non-byproduct power" thus produced could require as much as 45,000 Btu for every kilowatt-hour.

One can see that minimizing the production of non-byproduct power will save money. Clearly, when the steam-power demand ratio is tight, the reward for optimum day-to-day operation is great. During such a period, much skill is required to handle some types of sudden demand changes, because minimum steam flow is desirable through the desuperheaters.

Development of a Trainer. Several years ago, an intensive operator training program was undertaken by American Oil to improve power station operating techniques. It included both classroom and on-the-job instruction. The results were mostly satisfactory. But new operators required something more than the usual forms of instruction because they lacked the years of experience of older operators. *Simulation* seemed a good answer.

Computer Plus Control Board Equals Training. An analog computer facility designed to simulate refinery process equipment is located in a laboratory near the

refinery. Associated with it is a large control board equipped with commercial recording and control instruments. These can easily be arranged in a graphic-type display of the process simulated on the computer, which is monitored and controlled by the board instruments themselves. This installation, used to train operators for refinery process units, is also used to train power station operators.

The power-station trainer features a graphic instrument display which follows, as closely as possible, the physical layout of equipment in the two stations. Recorders and indicators are provided for all important steam flows, steam pressures, and electric power demands. Figure 2 shows the electronic analog computer used to simulate the system.

Control Board Setup. Figure 3 demonstrates how a boiler, a turbine-generator, and a desuperheater are represented on the control board. The trainee has control knobs for starting up, shutting down, and trimming the outputs of individual boilers. Switches adjacent to these knobs permit the operator to switch from automatic to manual control of boiler firing. He can also choose low or high speed draft fan operation.

Wherever possible, the simulator has been tailored to produce system responses which "feel" real to the experienced operator. The knobs controlling turbine governor adjustment, for changing the relative loadings on the turbine-generators, present the same action and "feel" as their counterparts in the actual stations.

Even system frequency has been made to respond realistically to load changes and machine adjustments. Behind the board, compressed air is vented noisily whenever header pressures exceed the settings on pressure relief valves.

A small panel out of sight of the trainee is used by the instructor to vary the electric loads on feeder groups, change the demands for steam, and cause the failure of selected station and refinery equipment.

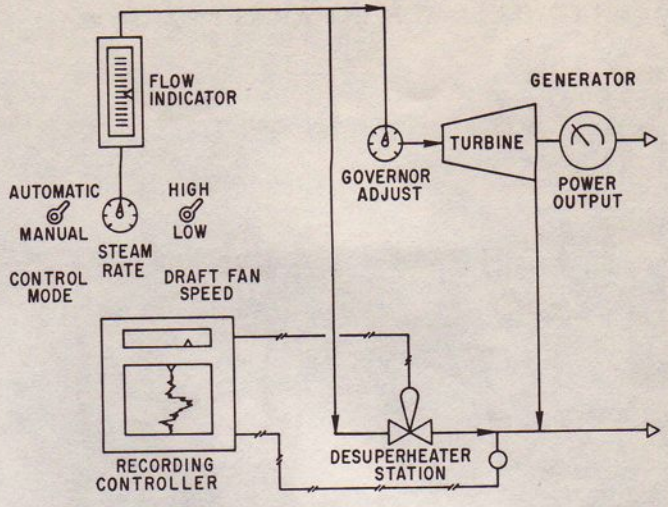


FIGURE 3—Here is how a boiler, turbine generator and desuperheater are represented on the simulator's control board. Trainees can start-up, shut-down, and trim outputs of each boiler.

The Training Program. Training on the analog simulator is conducted in two phases. Both are under the direction of an experienced shift supervisor.

In the first phase, one boiler room operator and one turbine room operator are together familiarized with the simulator panel. Then they are given a standard set of typical operating problems to solve. Situations they must handle include **1.** Emergency loss of a boiler under several conditions. **2.** Loss of a turbo-generator. **3.** Unexpected shutdown of a major refinery process unit. **4.** Minimizing of non-byproduct power generation during a period of tight steampower balance.

This session lasts eight hours. The second phase is much like the first. However, the operators bring their own problems, questions, and experiences to the training session. All current trainees have completed phase one, and several have completed phase two.

Results and Conclusions. Because the program is still under way, the full results of this training technique have not yet been evaluated. However, there are many gratifying indications that the program is working out well.

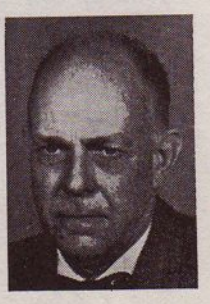
Analog simulator training does not eliminate the need for classroom and on-the-job instruction, nor does it detract from the value of many years of experience. But it does provide a quicker, clearer means of getting a complex operating problem across to an inexperienced operator.

The performance of the trainees and the questions they ask reveal the weaknesses and gaps in their understanding and previous training that were not apparent before. These weaknesses point up areas in the conventional training program which need to be reinforced.

Finally, turbine room and boiler room operators are becoming more conscious of one another's problems. It is apparent that a better informed, more thoroughly rounded-out crew is being developed. ##

About the authors

LOWELL G. WHITESELL *is a research supervisor in the Research and Development Department, American Oil Co., Whiting, Ind. A graduate of Purdue University, with B.S. and M.S. degrees in electrical engineering, he joined American in 1950. He is engaged in solving engineering problems involving analog simulation, and also consults on electronic aspects of instrumentation and control. He is a member of AIEE, Eta Kappa Nu, Tau Beta Pi and Sigma Xi.*



E. H. BOWLES *is a superintendent at American Oil's Whiting refinery, where he has spent 29 years in the Utilities Division. He also has seven years experience with Ingersoll-Rand in sales engineering. Mr. Bowles is in charge of the boiler house, air compressor house and utility distribution at the plant, and handles statistical studies involving power station operations and equipment. He has a B.S. degree in mechanical engineering from New York University.*

Minimum Reflux Figured an Easier Way

David L. Ripps
American Cyanamid Co., Wayne, N.J.

To CALCULATE minimum reflux ratio by the Underwood method, it is necessary to solve the following equation[1] for Θ:

$$U(\Theta) = \sum_{i=1}^{I} \frac{\alpha_i x_i}{\alpha_i - \Theta} - (1 + p) = 0 \qquad (1)$$

where α_i = relative volatility of component i
x_i = mole fraction of component i in the feed
p = thermal condition of the feed
I = number of components

Equation 1 is highly non-linear with a singularity at each value of $\Theta = \alpha_i$. The roots of interest lie in the open interval between adjacent pairs of α's. Because of the strongly non-linear character of Equation 1 a direct application of the standard methods of iteration (viz., Newton, false-position, etc.) often fails to converge or requires an excessive number of cycles to reach a root. We will now develop a specific method for solving Equation 1 in a reasonably efficient manner.

In this discussion it will be convenient to number the components so that the α's are in ascending order.

$$\alpha_1 < \alpha_2 < \ldots < \alpha_I \qquad (2)$$

Let us suppose that we wish to find a root, say the one in the interval

$$\alpha_r < \Theta < \alpha_{r+1}$$

Presuming for the moment that the root lies close to α_r we may rewrite Equation 1 as

$$\frac{\alpha_r x_r}{\alpha_r - \Theta} = \phi_r(\Theta) \qquad (3)$$

where

$$\phi_r(\Theta) = \frac{\alpha_r x_r}{\alpha_r - \Theta} - U(\Theta) \qquad (4)$$

Equation 3 may be solved for Θ by treating ϕ_r as a constant. Since ϕ_r is actually a function of Θ, the solution must be iterative. Then

$$(\Theta_c)_n = \alpha_r \left(1 - \frac{x_r}{\phi_r(\Theta)_n}\right) \qquad (5)$$

where
$(\Theta)_n$ = guessed value of Θ at cycle n of the iteration
$(\Theta_c)_n$ = computed value of Θ at cycle n of the iteration

Expanding Equation 5 in first-order Taylor series gives

$$(\Theta_c)_{n+1} - (\Theta_c)_n = \frac{d\Theta_c}{d\Theta}\left[(\Theta)_{n+1} - (\Theta)_n\right]$$

A solution on the next cycle would require

$$(\Theta_c)_{n+1} = (\Theta)_{n+1}$$

Combining the foregoing two equations and solving for the next cycle

$$(\Theta)_{n+1} = (\Theta)_n + \frac{(\Theta_c)_n - (\Theta)_n}{1 - (d\Theta_c/d\Theta)} \qquad (6)$$

For efficient solution we will use the previous two cycles in order to evaluate the derivatives.

$$\frac{d\Theta_c}{d\Theta} = \frac{(\Theta_c)_n - (\Theta_c)_{n-1}}{(\Theta)_n - (\Theta)_{n-1}}; \; n = 2, 3, \ldots \qquad (7)$$

To start the procedure we will take Θ as the mid-point between α_r and α_{r+1}.

$$(\Theta)_1 = 0.5\,(\alpha_r + \alpha_{r+1}) \qquad (8)$$

We assumed originally that the root in the interval between α_r and α_{r+1} is closer to α_r than to α_{r+1}. Evaluating the function at $(\Theta)_1$ provides a test of this assumption. If $U(\Theta)_1$ is positive the assumption is correct and we may proceed. If that function is negative, however, the root is closer to α_{r+1} and we should replace r by $r+1$ in subsequent parts of the iteration.

To continue we use Equation 5 as a direct iteration to give the second starting point. Thus

$$(\Theta)_2 = (\Theta_c)_1$$

Thereafter we will use the modified Newton given by Equations 6 and 7.

Example Problems.

Example 1: Benzene — Toluene — Xylene.[2]

$x_1 = 0.1$ $\quad x_2 = 0.3$ $\quad x_3 = 0.6$
$\alpha_1 = 0.4$ $\quad \alpha_2 = 1.0$ $\quad \alpha_3 = 2.45$
$p = -1$
Desired: Root in interval $1.0 < \Theta < 2.45$

Cycle	θ	U (θ)	$\phi_2(\theta)$	θ_c
1	1.725	1.5836	−1.9974	1.1502
2	1.15020	−0.9198	−1.0776	1.2784
3	1.25501	6.9517×10^{-3}	−1.1834	1.2535
4	1.25380	2.8228×10^{-5}	−1.1821	1.2538

Example 2. Four component system.

$\alpha_1 = 0.3$ $\quad \alpha_2 = 1.0$ $\quad \alpha_3 = 1.3$ $\quad \alpha_4 = 3.3$
$p = -1$

Desired: Root in interval $1.0 < \Theta < 1.3$
Tolerance on $\Theta \pm 0.00001$

Case	x_1	x_2	x_3	x_4	θ	r	Cycles to converge
1	0.05	0.10	0.75	0.10	1.02705	2	4
2	0.05	0.10	0.20	0.65	1.05060	2	4
3	0.25	0.25	0.25	0.25	1.11967	2	4
4	0.10	0.40	0.40	0.10	1.12767	2	4
5	0.65	0.20	0.10	0.05	1.19071	3	4
6	0.10	0.75	0.10	0.05	1.25504	3	4

LITERATURE CITED

[1] Robinson, C. S., and Gilliland, E. R., "Elements of Fractional Distillation," McGraw-Hill Book Co., Inc., 1950, p. 356.
[2] Ibid., p. 358.

Indexing Terms: Computations-4,7, Design-4, Distillation-8,9, Engineering-4, Equations-10, Iteration-6, Refluxing-9, Separation-8,9, Underwood-0.

TABLE 1—Input Data

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0   11    1    0   14   12F    0    1    3    0    5    1
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2   51    1    1   29    1     1   33    1    1   47    3
2     677.00      11          0.0
0   14   19    0   11    1     0    1    1    2   43    1
2   34    5    2   51    2     2   20    1    2   25    1
1   29    1    1   38    1     1   47    1    0    0    0
3      70.00       9          0.0
0   14   46    0   11    1     0    1    1    0   10    1
1   31    1    1   45    1     1   47    1    1   20    2
1   34    4    0    0    0     0    0    0    0    0    0
4     986.00      12          0.0
0   14   16    0   11    1     0    1    1    2   43    1
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2   25    1    1   29    1     1   38    1    1   47    1
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1   31    1    1   38    1     1   47    2    0    0    0
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```

```
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20    127.00      11          0.0
0   14   14    0    1    1     0   11    1    2   34    4
2   51    6    2   20    3     2   43    1    2   25    1
1   32    1    1   38    1     1   47    2    0    0    0
21    630.50      14          0.0
0   14   30    0    2    2     0    1    1    0   11    1
2   25    1    2   51   12     2   20    4    2   34   30
2   21    1    2   25    2     2   43    1    1   31    1
1   47    4    1   38    1     0    0    0    0    0    0
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0   14   19    0    2    1     0    1    1    0   11    1
2   43    2    2   34    4     2   51    3    2   20    2
1   32    1    1   38    1     1   47    3    0    0    0
23     20.00       8          0.0
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0   14    5    0    5    1     0    4    2    0    0    0
37   1258.50       3          0.0
0   14    8    0    5    1     0    4    1    0    0    0
38   1938.00       3          0.0
0   14   27    0    5    1     0    4    2    0    0    0
39    952.00       3          0.0
0   14   13    0    5    1     0    4    2    0    0    0
40    197.00       3          0.0
0   14    4    0    5    1     0    4    2    0    0    0
41    447.00       3          0.0
0   14   13    0    5    1     0    4    1    0    0    0
42    505.00       1          0.0
0   14    8    0    0    0     0    0    0    0    0    0
11
2     7.92      10
1   25   26   27    2   14   37   35   34   13    0    0
3     9.01      18
1   25   26   28   29   30   31   33    3   15   40   41
39   38   36   35   34   13    0    0    0    0    0    0
4     7.58      12
1   25   26   28   29    4   16   38   36   35   34   13
5    10.00       6
1   25    5   17   34   13    0    0    0    0    0    0
6    10.00      10
1   25   26   28    6   18   36   35   34   13    0    0
7    10.00      10
1   25   26   27    7   19   37   35   34   13    0    0
8    10.00      16
1   25   26   28   29   30    8   20   40   41   39   38
36   35   34   13    0    0    0    0    0    0    0    0
9     7.97       4
1    9   21   13    0    0    0    0    0    0    0    0
10    10.00      17
1   25   26   28   29   30   31   32   10   22   42   39
38   36   35   34   13    0    0    0    0    0    0    0
11    1.99      17
1   25   26   28   29   30   31   32   20   23   42   39
38   36   35   34   13    0    0    0    0    0    0    0
12     0.0      17
1   25   26   28   29   30   31   33   12   24   41   39
38   36   35   34   13    0    0    0    0    0    0    0
```

Design Best Cooling Water System

This computer program helps design an economical cooling water system. It gives the overall installed cost of the piping and can be used for sizing the pump

Jogindra P. Kohli*
Union Carbide Corp., Tonawanda, N.Y.

THIS COMPUTER PROGRAM is based on the installed cost of the piping for a cooling water system at a given location. For given allowable pump head, pipe routing and maximum and minimum velocity limits; it designs the most economical piping system. The program can also be used for sizing the pump, calculating head losses in an existing system, and computing the cost of a given system. Typical results from the computer program are presented.

Optimum Design. What is a most economical design? It is the design which satisfies all the required conditions and costs the least.

For a cooling water system, the required conditions to be satisfied are (1) flow, (2) maximum velocity, (3) available head. Flow through a pipe is equal to its area times the maximum velocity and therefore two of the three requirements can be satisfied by calculating the minimum diameter of pipe for required flow and maximum velocity. The system thus designed is the best design if it can satisfy the third requirement of available head, but usually it does not. Therefore, some lines in the system are to be increased in size (within the range of minimum velocity) such that available head loss conditions are satisfied.

Which lines should be increased? The answer can make the difference between the best and the worst design. If the lines that are increased cost the least, the design is the most economical design. It is not an easy job to find which lines cost the least to increase (especially in a large system). For example, a line of a relatively smaller diameter with two valves may cost more to increase in size than a larger diameter line of some length but without the valves. This is where the computer can be used to the greatest advantage.

The design of a cooling water system (or a water supply system) involves a trial and error procedure. In the normal procedure, the lines are sized approximately for the given flow and the friction head loss is calculated. This friction loss is added to the various other head losses (equipment head loss, cooling tower head, etc.) and checked against the available pump head. If the head loss calculated for the system is more than available pump head, some line sizes in the system are increased and friction head loss recalculated. The procedure is repeated until the total head loss through the system becomes less than the available head.

* Present address: State University of New York at Buffalo, Amherst, N.Y.

TABLE 2—Results of Cooling Water Piping Design Program

CIRCUIT NO.	HEADLOSS(FT.)
2	87.0
3	87.3
4	85.4
5	78.7
6	87.6
7	82.3
8	86.2
9	65.3
10	82.3
11	71.3
12	81.5

ALLOWABLE PUMP HEAD = 108.0 COOLING TOWER HEAD = 20.00

INSTALLED COST OF THE WHOLE SYSTEM IN DOLLARS = 29076.93

DESIGN DATA USED IN THE PROGRAM
MAXIMUM ALLOWABLE DESIGN VELOCITY FLOW 45 GPM AND MORE = 12.00 FT./SEC.
MAXIMUM ALLOWABLE DESIGN VELOCITY FLOW LESS THAN 45 GPM = 10.00 FT./SEC.
AVERAGE LABOR RATE FOR INSTALLED COST CALCULATIONS = 7.00 $/MANHOUR

INSTALLED COST UNDER GROUND PIPING IN DOLLARS = 21366.98
INSTALLED COST ABOVE GROUND PIPING IN DOLLARS = 7709.94
INSTALLED COST OF THE WHOLE SYSTEM IN DOLLARS = 29076.93

TABLE 3—Head Loss Through the Circuits

BRANCH NO.	FLOW G.P.M.	DIA INCHES	HEADLOSS FEET	INSTALLED COST DOLLARS	ABOVE GROUND COST(DOLLARS)	UNDERGROUND COST(DOLLARS)
1	4552.00	14.000	16.56	5206.33	1733.68	3472.66
2	877.00	6.000	8.58	507.09	261.87	245.22
3	70.00	3.000	1.74	419.18	112.58	306.60
4	986.00	6.000	11.61	523.96	306.67	217.29
5	80.00	2.000	9.85	181.88	52.08	129.80
6	645.00	6.000	4.02	430.19	287.38	142.81
7	381.50	4.000	5.86	366.18	228.42	137.76
8	127.00	4.000	0.82	263.95	175.47	88.48
9	630.50	6.000	7.43	926.74	459.62	467.12
10	485.00	6.000	2.48	631.94	269.81	362.13
11	20.00	1.000	17.62	104.50	42.04	62.46
12	250.00	4.000	4.23	375.10	220.53	154.57
13	4552.00	14.000	12.47	3411.08	693.73	2717.35
14	877.00	6.000	11.67	724.66	306.67	417.99
15	70.00	3.000	3.44	413.63	128.29	285.34
16	986.00	8.000	3.39	690.46	368.11	322.35
17	80.00	2.500	8.55	210.87	63.89	146.98
18	645.00	6.000	12.01	448.73	287.30	161.43
19	381.50	4.000	4.84	233.49	109.81	123.68
20	127.00	4.000	2.74	355.84	211.04	144.80
21	630.50	6.000	10.44	983.18	587.93	395.25
22	485.00	6.000	6.90	594.93	325.90	269.03
23	20.00	1.500	4.78	129.54	74.01	55.53
24	250.00	3.000	17.76	519.29	403.13	116.16
25	3921.50	14.000	5.95	2199.54	0.0	2199.54
26	3841.50	16.000	2.38	657.21	0.0	657.21
27	1258.50	10.000	1.98	543.84	0.0	543.84
28	2583.00	14.000	1.45	594.12	0.0	594.12
29	1938.00	12.000	2.16	662.38	0.0	662.38
30	952.00	10.000	0.75	274.15	0.0	274.15
31	825.00	10.000	0.80	405.60	0.0	405.60
32	505.00	6.000	1.85	179.70	0.0	179.70
33	320.00	6.000	0.97	190.81	0.0	190.81
34	3921.50	16.000	2.21	1300.17	0.0	1300.17
35	3841.50	14.000	5.58	1160.48	0.0	1160.48
36	2583.00	14.000	1.86	503.70	0.0	503.70
37	1258.50	10.000	1.31	289.51	0.0	289.51
38	1938.00	12.000	2.26	798.39	0.0	798.39
39	952.00	8.000	2.65	300.03	0.0	300.03
40	197.00	4.000	1.74	91.87	0.0	91.87
41	447.00	6.000	1.51	198.32	0.0	198.32
42	505.00	6.000	0.27	74.48	0.0	74.48

Types of Problems. For a given value of allowable pump head, a defined routing, given flow and limiting velocities the program designs the cooling water system for least cost and calculates the total installed cost of the system. The program can design a number of systems for different head values for the same data and thus can be used in selecting a pump, such that the combination of pump cost (installed cost plus operating cost for certain number of years) and the system cost is least. The program can handle a system up to 30 circuits (each circuit having not more than 48 lines) and up to 120 lines (each line having not more than 16 fittings). The program can calculate the head losses in an already sized system, and it can also compute the cost of such a system.

Method of Analysis. The procedure consists of four basic steps:

- Initial sizing of the system
- Determining the head losses in the circuits and comparing them with the available head
- Determining the most economical line to be increased in size and repeating operations one to three until head losses in all the circuits are less than the available head
- Computing the cost of the system thus designed and printing out of the results.

Initial Sizing of the System. Initially all the lines are sized to satisfy flow requirements with maximum velocity.

$$\text{Area} = \text{Flow}/\text{Velocity}$$

$$\pi D^2/4 = (144\ (0.1337)Q)/(60\ AMV)$$

where

D = pipe diameter, in.

Q = flow through line, gpm

AMV = allowable maximum velocity, ft./sec.

Then

$$D = 12\sqrt{0.1337\ Q/47.1\ AMV} \qquad (1)$$

The lines thus sized are the minimum sizes for given maximum velocity conditions.

Head Loss Through the Circuits. After lines are sized, head loss through each line is calculated by means of the following two equations:

For length of pipe (Hazen Williams Formula),

$$HL = (0.002083)\ (QL)\ (QF)^{1.85}/(PDC)^{4.8655} \qquad (2)$$

Where

HL = friction head loss, ft.

QL = length of pipe, ft.

QF = flow through pipe, gpm

PDC = pipe diameter, in.

For fittings in the pipe,

$$HF = (0.00259)\ (K)\ (QN)\ (QF)^2/(PDC)^4 \qquad (3)$$

Where

HF = friction head loss, ft.

K = constant for different fittings

QN = number of fittings

The head losses through circuits are calculated by adding equipment head losses to the line head losses. These circuit head losses are compared with the available head (pump head-static head). The circuits, with head loss greater than available head, are used to determine the most economical line to be increased in size to reduce the head.

The assumptions are:

- Labor rate is assumed to be a uniform average rate for a particular location.
- Value of *"C-100"* is used for old piping at 60° F in calculating head loss in piping by William and Hazen formula.
- Values of *"K"* for fittings, in calculating head loss by $KV^2/2g$, are used as per "Hydraulics" by Schoder and Dawson.

Most Economical Line. Pipe sizes are increased one at a time, and each time a most economical line is chosen. Selection of the most economical line is done in the following way:

Costs of all the lines that occur in the circuits requiring head loss reduction are calculated. All these lines are increased in diameter to their next size and their new costs are calculated. The difference in the two costs for each line gives us the amount of money it will cost to in-

crease that particular line by one size. The same operation is repeated for head loss calculations and difference in two head losses gives us the amount of head loss reduction due to increase in that line size. This is the actual head loss reduction.

Effective head loss reduction is obtained by multiplying actual head loss reduction by a factor that depends upon the effectiveness of the increase of size of the line to the whole system. The factor known as the effectiveness factor is obtained for each line. To calculate the effectiveness factor for the line, the number of times each line occurs in the circuits requiring head loss is found. If the difference between the circuit head loss and available head is more than the head loss reduction due to increase in size of line, the value of factor is one for that circuit. Otherwise it is the ratio of the difference of circuit head loss and available head to the head loss reduction due to increase in line size. If the line does not occur in a circuit requiring head loss, its effectiveness factor is zero. All the factors for all the circuits are summed for each line. This gives the value of the effectiveness factor for each line.

Thus, cost per foot of head for each line is obtained by dividing the amount it costs to increase that line one size by the effective head reduction due to that increase in size. These costs are compared for all the lines and only the line with the least cost per foot of head is chosen. That line is checked for minimum velocity requirements. If it satisfies, this is the most economical line size to increase. If not, the line with the next higher cost is chosen.

The above chosen line is increased in size and head losses recalculated. The procedure is repeated until all the circuits satisfy the head loss requirements. This is the optimum design.

When all design requirements are satisfied, the program calculates the cost of all the lines and prints out the line sizes, head loss, cost of each line, head loss through each circuit, and the cost of the over-all system.

Computer Program. The computer program has been written for IBM/360 computer which has a storage capacity of 64,000 locations in the core storage. The program consists of a main program and five subroutines and requires 49,282 locations. Input data is read from the cards and the output is on a paper printer. The program took about two months to write and, apart from designing an optimum system, it has reduced the actual design time from 3 days to about 25 minutes.

Input to the program consists of two types:

- Constants. These are the cost values and allowable minimum and maximum velocities. They can be updated from time to time, but not necessarily for each program.
- Regular input data for the program. These consist of description of lines through the use of code numbers already assigned for various fittings, the description of circuits and their lines.

The input and output shall not be described in detail; however, the printout of an example problem is presented. The whole thing is self-explanatory except for input data that uses already assigned code numbers for the description of the fittings in the line.

Example Problem. A cooling water system for a plant at Mims, Fla., was designed by the computer program. The cooling water system consists of 42 lines and 11 circuits. The available pump head is 108 feet and static head is 20 feet. The program took about 25 minutes to design the system. The input data and the results of the program are presented in the accompanying tables.

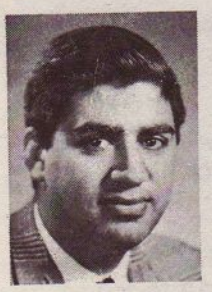
The program does the optimum sizing of the system based on installed cost. The results of the example problem show that the various circuits are very nearly balanced and are very close to the allowable limit. Eight out of 11 circuits are within 10 percent of the allowable value. Also, the lines are sized such that the system cost is the least. This is the most significant aspect of the program, for in sizing the line the program takes into account every fitting present in the line and optimizes the over-all cost.

Advantages of the Program.

- Initial selection of the pump for a given system. A routing of piping can be run for various allowable heads and the cost of the systems can help in selection of the pump.
- Design of the system
- Calculation of the cost of the systems.

The program can be further extended to prepare the field and fabrication bill of materials, purchase requisitions, and isometric drawings. Using the same input data, all of the above items can be obtained. Work is presently being done in the above field and very soon the program shall be able to prepare the field and fabrication bill of materials.

The program makes full use of the advantages offered by the computer over the hand calculations. It saves in the computational time as well as in the cost of system. It completely eliminates the guess work that is usually involved in the sizing of a system by hand calculations.



About the author

JOGINDRA P. KOHLI *is with the Department of Computer Science for State University of New York at Buffalo, Amherst, N. Y. At the time of this report he was with Union Carbide Computer Center in Tonawanda, N. Y., where his work included design implementation and evaluation of engineering projects on computers. He holds a B. Tech. degree with honors from the Indian Institute of Technology Kharagpur and a M.S. degree from the University of Rhode Island. He is a licensed professional engineer of New York State.*

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Simplified Utility Loop Balancing

Utility distribution systems require periodic checks on flow and pressure drops in the loop mains. This method reduces the calculation time from days to minutes

B. West and **A. J. Newton**
Polymer Corp., Ltd., Sarnia, Canada

UTILITY DISTRIBUTION SYSTEMS for refineries and chemical plants are becoming larger and more complex. Usually these systems are looped, so that the utility supply to any unit is not dependent on one path through the system. As a result, complicated piping networks are built up.

A major plant expansion will normally include a study of the utility distribution systems, to determine the effect of the load increase, and to indicate where expansion is required. These studies when performed by hand are very time consuming and prone to error because of the large number of repetitive steps involved.

The repetitive nature of the calculations naturally leads to the use of a computer method of evaluation. Computer programs 2, 3, 6, 7, 8 have been written to solve this type of problem.

The following is a description of the network analysis program developed at Polymer Corp.

Information Required. It is decided to examine one of the plant utility distribution systems. The object of the study is to determine the effectiveness of the system under present and future loads. The effectiveness might be determined by comparing required pressures at various points in the system to the predicted pressures. It could also be determined by comparing the predicted fluid velocity in the pipes to the maximum allowable fluid velocity.

This information can be provided by determining the flows and pressure drops in the pipes of the system. The procedure used to find the correct flows is relatively simple but tedious to solve by hand. The calculation procedure can be broken up into steps.

1. **Collect Data.** Pipe diameters, pipe equivalent lengths (i.e. including length for fittings.), system configuration and average fluid properties.

2. **Estimate Flows in the Network.** The flow rate of fluid in all the pipes in the system is estimated. The only criterion for this estimate is that the chosen flows must be consistent with the over-all mass balance. It is preferable, however, to make reasonable estimates, as this will reduce the length of the calculation.

3. **Calculate the Pressure Drop in the Pipes.** Any standard pressure drop calculation is used. In the computer program, the Polymer standard procedure is used.

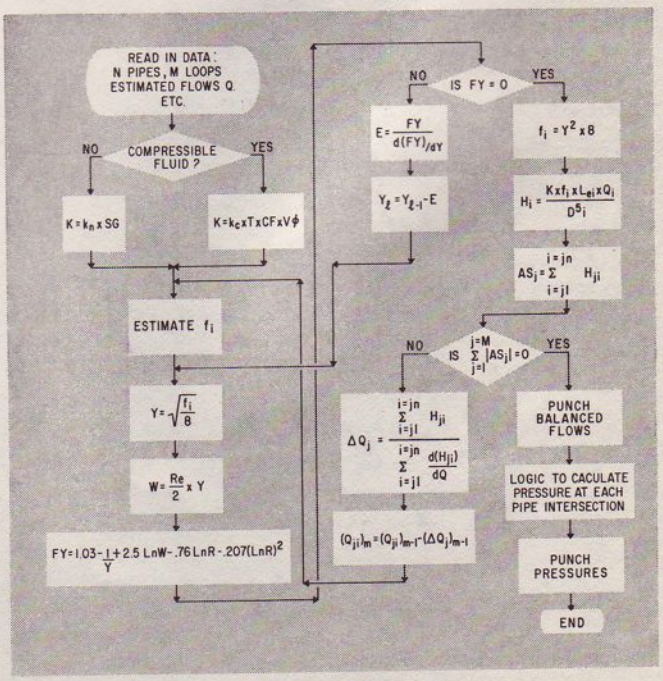


Fig. 1—Simplified computer flow diagram.

4. Check to Find if the Loops Balance. Each loop is examined individually. The algebraic sum of the pressure drops in the loop pipes is found. If this is zero, the loop is in balance. If this sum is not zero, an adjustment must be made to correct the flow rates in the loop, to give balance. Each loop is checked and corrections made to the estimated flows if necessary.

5. Return to Step 3. Steps 3 and 4 are repeated until all the loops in the system balance.

The above procedure is applicable to both hand or computer solution. Hand calculations make use of various approximations because a detailed calculation would take too long. Computer solutions may be made rigorous by reducing the number of approximations.

BASIS FOR COMPUTER CALCULATIONS

The relationships used for pressure drop calculations in our program are simplified and reflect certain assumptions stated below. The degree of sophistication used to calculate the pressure drops is very much dependent upon the individuals' needs. For our requirements we have found the flow formulas presented here to be adequate.

The assumptions inherent in the following theory are:

- Isothermal flow for compressible fluids,
- Fluid properties are for the average temperature and pressure of the fluid in the system,
- The pipes are rough, and
- Datum temperature is 50° F.

The basic relationships used for analyzing the loops are the equations for flow of fluids in pipes.

Pressure Drop Equations

Noncompressible Fluids. The relationship between inlet and outlet pressures is

$$p_1 - p_2 = \left(\frac{fL_e}{D}\right)\left(\frac{G^2}{Zg\rho}\right) 12 \qquad (1)$$

$$\text{or } p_1 - p_2 = k_n\,(S.G.)\,f\,L_e\left(\frac{Q^2}{D^5}\right) \qquad (2)$$

Compressible Fluids.

$$p_1^2 - p_2^2 = \frac{G^2 p_2}{g\rho_2}\left[\frac{fL_e}{D}\,(12) + ln\left(\frac{p_1}{p_2}\right)\right] \qquad (3)$$

$$p_1^2 - p_2^2 = k_c T\,(CF)(VO)\,f\left(\frac{L_e}{D^5}\right) Q^2 \qquad (4)$$

Equation 2 and 4 can be put in the form:

$$H_i = Kf_i\,(Le_i)\left(\frac{Q_i^2}{D_i^5}\right) \qquad (5)$$

The value of K will be constant for a given system.

Equation 5 is the general equation used in the computer program to calculate pressure drops in the pipes.

Friction Factor. In Equation 5 all the terms except f, the friction factor, are input data predetermined for the system under study. The friction factors can be read off a chart if the calculation is done by hand. The computer solution requires an analytical expression for friction factor. An expression developed by Dukler[4] from Moody's friction factor chart and used in the program is shown:

$$\frac{1}{\sqrt{\frac{f^1}{2}}} = 1.03 + 5.76 \log\left(\frac{Re}{2}\sqrt{\frac{f^1}{2}}\right) - 1.75 \log R - 1.10\,(\log R)^2 \qquad (6)$$

where $$R = Re\left(\frac{K^1}{D}\right)\sqrt{\frac{f^1}{2}}$$

Substituting the following into Equation 6.

$$f = 4f^1$$

$$Y = \sqrt{\frac{f^1}{2}} = \sqrt{\frac{f}{8}}$$

$$W = \frac{Re}{2}\sqrt{\frac{f}{8}} = \frac{Re}{2}\,(Y)$$

gives:

$$\frac{1}{Y} = 1.03 + 5.76 \log W - 1.75 \log R - 1.10\,(\log R)^2$$

or

$$FY = 1.03 - \frac{1}{Y} + 2.5\,ln\,W - 0.76\,ln\,R - 0.207\,(ln\,R)^2 \qquad (7)$$

The correct estimate of f gives $FY = O$.

To solve Equation 7, a value of Y is chosen and FY calculated. If FY is not zero, a correction is made to the initial value of Y. This correction is found by application of the Newton-Ralphson technique.[1]

Where $$Y_l = Y_{l-1} - E$$

and

$$E = \frac{FY}{\frac{d(FY)}{dY}} = \frac{1.03 - \left(\frac{1}{Y}\right) + 2.50\,(ln\,W) - 0.76\,(ln\,R) - 0.207\,(ln\,R)^2}{\frac{1}{Y^2} + \frac{1.74}{Y} - \frac{0.414}{Y}\,(ln\,R)} \qquad (8)$$

This procedure is repeated until FY is zero then f is found from Y.

Balancing Loop Flows. The pressure drops in all the pipes are calculated based on the initial estimates of flow

For long pipes (+ 200 ft) or low velocities $ln\left(\frac{p_1}{p_2}\right)$ approaches zero.

rates. The algebraic sum of the pressure drops is found for each closed path or loop taking the clockwise flows as positive (this is the Hardy-Cross convention). If the estimated flow rates are correct, this sum will be zero for all the loops. If this sum is not zero, an adjustment must be made to the estimated flows. The adjustment is made according to the Hardy-Cross[5] formula which is a special application of the Newton-Ralphson technique.

$$\text{Algebraic Sum} = AS_j = \sum_{i=j1}^{i=jn} H_{ji} = \sum_{i=j1}^{i=jn} \left[\frac{Kf_{ji}\, Le_{ji}\, Q_{ji}^2}{D_{ji}^5} \right] \tag{9}$$

If AS is not equal to zero a correction is made to the estimated flows in the loop, j.

$$\left[Q_{ji} \right]_m = \left[Q_{ji} \right]_{m-1} - \left[\Delta Q_j \right]_{m-1}$$

where

$$\Delta Q_j = \frac{\sum_{i=j1}^{i=jn} H_{ji}}{\sum_{i=j1}^{i=jn} \frac{dH_{ji}}{dQ}} = \frac{\sum_{i=j1}^{i=jn} \left[Kf_{ji}\, Le_{ji}\, Q_{ji}^2 / D_{ji}^5 \right]}{2 \sum_{i=j1}^{i=jn} \left[Kf_{ji}\, Le_{ji}\, Q_{ji} / D_{ji}^5 \right]} \tag{10}$$

The new estimated flows are used to recalculate the pressure drops and the procedure continues until the loops are balanced.

i.e. until

$$\sum_{j=1}^{j=m} | AS_j | = O$$

Tolerances on the Iterative Procedures. Iterative techniques are used to determine the friction factors and the correct flows in the network. The criterion for finding the correct value is that a test variable (FY and $\Sigma\ AS_j$) should become zero. An optimum tolerance is required on the convergence test of these variables. A balance must be struck between the accuracy of the results and the computing time.

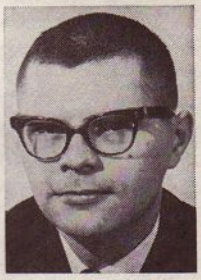
Friction Factor Calculation. Two different tolerances are used on the test variable FY. Initially a tolerance of $\pm$ 0.1 is used and if the flow rates are changed by less than 5 percent from the flows in the previous iteration, a new friction factor is not calculated. When the flows are almost balanced the friction factor criterion is tightened. The tolerance becomes $\pm$ 0.001 and a new friction factor is calculated for each change of flow rate.

Flow Balancing Criterion. Ideally, when the loops are in balance the values of AS in each loop equals zero. To attain this value would require considerable computing time. The criterion used to decide whether the flow rates need further modification is to sum the absolute values of the deviations from zero of each loop, and if this exceeds a desired value, a further change is made to the flow rates. This desired value is best determined anew for each system, taking into account the computing time available and the desired accuracy of the results.

Absolute Pressure Calculations. The pressure drops in each main in the network are now known. For completeness, it is necessary to calculate the absolute pressure at the end of each pipe.

About the authors

B. WEST *is a process engineer with Polymer Corp. Ltd., Sarnia, Ont., Canada. His work involves responsibility for process design, quality control, plant efficiency control and evaluation in the Styrene Department with particular responsibility towards the Litol unit under construction. Mr. West holds a B.Sc. (Tech) in chemical engineering from Manchester University, England. He joined Polymer after graduation as a process engineer in the Utilities Department, was transferred to the Butadiene Department, and now to the Styrene Department. He is a graduate of the Institution of Chemical Engineers, London, and is a registered engineer in Ontario.*



A. J. NEWTON *is a process engineer with Polymer Corp. Ltd., Sarnia, Ont., Canada. His work involves process design, quality control and other technical assistance in the Styrene Department. Mr. Newton holds a B.Sc. degree in chemical engineering from the University of Saskatchewan. Prior to his present assignment, he was a process engineer in the company's Utilities Department. He is a member of the Association of Professional Engineers of the Province of Ontario, the Engineering Institute of Canada, the Chemical Institute of Canada, and the Association of the Chemical Profession of Ontario.*

The following systematic approach is used. The loops are treated in turn. Loop one contains the input (or the highest pressure input if there are several inputs) to the system, at which point the pressure is known. All the pressures are calculated around loop one. The next loop in numerical order is then considered. A pipe is found which is common to a previous loop or enters an intersection common to a previous loop. This search provides a point of known pressure from which the other pressures around the loop may be determined. All the loops are examined to give all the pressures throughout the system. It is important to number the loops in such a way that they have mains or intersections in common with lower numbered loops. This is necessary to ensure that each loop has a starting point where the pressure has already been found.

Fig. 1 shows a simplified flow diagram of the computer program.

Experience With the Program. The program described here has been used extensively by the Utilities Department of Polymer Corp. for evaluating proposed changes to the steam and water distribution systems. The program has been checked by comparing the results obtained with the actual system. A good agreement has been obtained.

The great reduction in calculating time has enabled more varied modifications to be studied for each expansion.

A sample problem follows which shows the preparation and computing times for the problem and for typical utility problems. For the example shown, the computer gives the result in about 15 minutes; whereas the hand

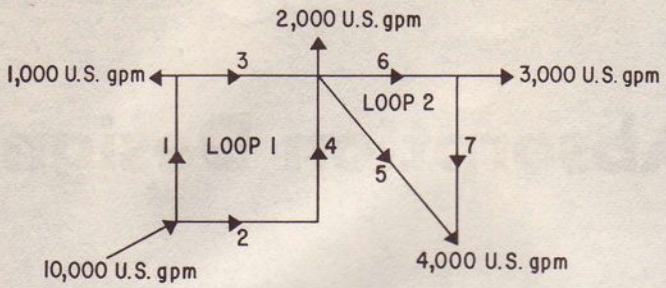


Fig. 2—Sample problem.

TABLE 1—Input Data for the Sample Problem

Main Number	Diam. (in.)	Eq. Lgth. (ft.)	Est. Flow USgpm
1	12	1000	5000
2	10	600	—5000
3	10	500	4000
4	10	1200	—5000
5	10	1500	—3000
6	10	200	4000
7	10	1000	1000

TABLE 2—Computer Calculated Values of Flow and Pressure in Each Loop Main

Main Number	Balanced Flow, USgpm	Outlet Pressure, psia
1	5934	68.2
2	—4065	80.7
3	4934	34.6
4	—4065	34.6
5	—2235	16.4
6	4764	24.1
7	1764	16.4

calculation would take at least one hour. The advantages of the computer are greatly increased as the size of the system is increased. One hour's computing time replaces two weeks or more required for hand calculations on the big utility systems.

Sample Problem. Determine the flow rates and pressures in the network shown on Fig. 2.

Table 1 gives the main numbers in the loop and tabulates the diameter of the main, the equivalent length, and the estimated flow in USgpm.

Table 2 is the computer calculated flow in each main and the outlet pressure.

The time taken to complete the problem was as follows:

Function	Time
Prepare data	10 minutes
Punch data	2 minutes
Computer solution	3 minutes
	15 minutes

Hand vs Computer Calculation Time. A steam distribution system consists of 29 mains and 7 loops.

A typical computing time for this system based on a reasonably accurate initial estimate is 30 minutes.

The service water distribution system consists of 41 mains and 10 loops.

A typical computing time is 15 minutes.

No specific times of calculation by hand are available, but several days of continuous work were required to produce results of comparable accuracy.

A recent paper[8] gives an excellent description of a much more rigorous method of solution to complex pipe system problems. The method has obvious attractions for use in systems where the fluid conditions and properties are subject to considerable change. The simple procedure presented here, appears sufficiently accurate for fluids at steady conditions.

ACKNOWLEDGMENT

The Polymer Corp. Management is duly acknowledged for the permission to publish this article.

NOMENCLATURE

AS	Algebraic sum of pressure drops in a loop
CF	Compressibility factor of fluid
D	Diameter of pipe, inches
f	Weisbach-Darcy friction factor
f^1	Fanning friction factor
FY	Friction factor test variable
g	Newtons-law conversion factor, ft.-lbs. mass/lb. force-sec.^{2}
G	Mass velocity, lbs. mass/ft.^{2} sec.
H	Pressure drop in pipe, lbs. force/in.^{2} (lbs.-force^2/in.^{4}) (units for compressible fluids)
k_n	Constant for noncompressible fluids, lbs. force in.^{5} min.^{2}/ft.^{3} USG^2
k_c	Constant for compressible fluids, lb. force^2 in.^{5} hr.^{2}/ft.^{8} °R lb. mass
K	Constant for system and fluid
K^1	Absolute roughness magnitude
Le	Equivalent length of pipe, ft.
M	Total number of loops
N	Total number of pipes
p_1	Inlet pressure, lbs. force/ft.^{2}
p_2	Outlet pressure, lbs. force/ft.^{2}
Q	Volume or mass flow rate, USgpm or (lbs. mass/hr.)
Re	Reynolds no.
$S.G.$	Specific gravity of fluid at flow temperature
T	Absolute temperature, (°R)
VO	Specific volume of gas at standard temp. and press. (ft.^{3}/lb. mass)
ρ	Fluid density at flow temperature, lbs. mass/ft.^{3}
ΔQ	Flow correction factor, USgpm or (lbs. mass/hr.)
E	Friction factor correction factor

SUBSCRIPTS

i	Pipe number
j	Loop number
m	Over-all iteration number
l	Friction factor iteration number
jn	Number of pipes in loop j.

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Figure Optimum Absorption Design

The minimum cost to recover solute can be determined graphically from the computer data plotted here

J. C. Kim and M. C. Molstad
University of Pennsylvania, Philadelphia

THE MINIMUM UNIT COST of recovered solute is obtained by the proper selection of absorber height and operating conditions. The relationship of these optimum conditions is presented graphically. To use the method, it is necessary to evaluate the quantity $C_5\ \Theta\ r\ m\ G_M/C_3\ H_{OG}\ (K_D - 1)$. An example is solved showing the use of water to recover acetone vapor at minimum unit cost from an air stream.

Governing Equations. Equations giving the total annual cost of treating a gas stream entering an absorber have long been available[1] and have more recently been put into somewhat modified form.[2,3] The total cost includes:

- the fixed cost of the absorber, to which has been added for convenience one-half of this fixed cost to cover the energy required to overcome gas pressure drop
- the value of the unrecovered solute taken at the market cost of its replacement
- the cost of recovery of the solute in the stripper operation.

The cost to be minimized is the total annual cost of recovering one pound mole per hour of solute vapor fed to the absorber in the gas stream, i.e. $C_T/G_M S\ (Y_1 - Y_2)$. The solute content is assumed to be small enough so that the total molal gas flow rate, G_M, can be considered constant in the absorption column. The expression for the foregoing cost is

$$\frac{C_T}{G_M S\ (y_1 - y_2)} = \frac{C_T}{G_M S y_1\ (1 - 1/Y)}$$

$$= \frac{C_3 Z}{G_M y_1\ (1 - 1/Y)} + \frac{C_4 \Theta}{(Y - 1)}$$

$$+ C_5 \Theta \left(\frac{r\ \{ 1 - [(K_D G_M/L_M)\ (y_1)\ (1 - 1/Y)] \}}{(K_D - 1)\ (G_M/L_M)\ (y_1)\ (1 - 1/Y)} + 1 \right) \quad (1)$$

where Z is the height of absorption tower given by

$$Z = H_{OG} \frac{ln\ \{ [1 - (mG_M/L_M)]\ Y + (mG_M/L_M) \}}{1 - (mG_M/L_M)} \quad (2)$$

Equation (1) is partially differentiated with respect to the absorption factor, and the resultant equation is set equal to zero. The final expression, from which the optimum absorption factor is computed for the foregoing case, then becomes:

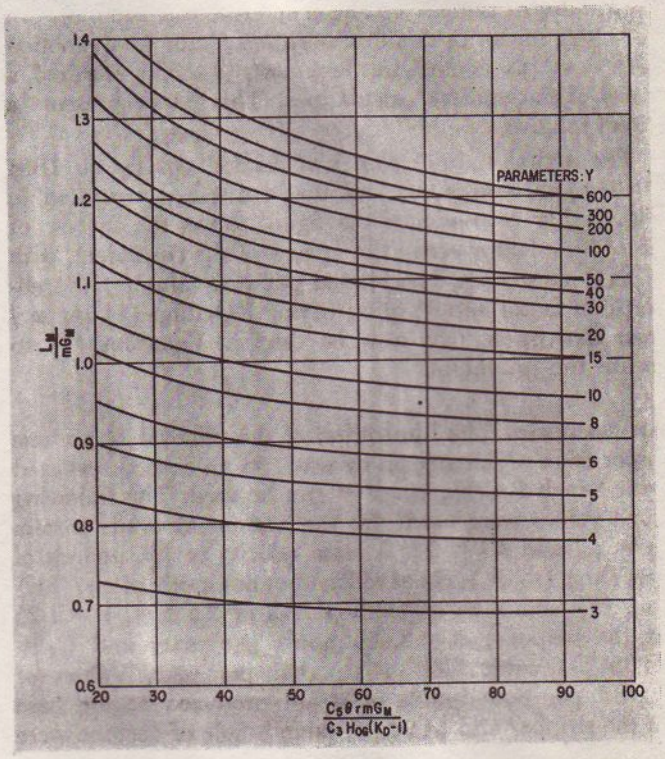

Fig. 1—A digital computer was used to establish these curves.

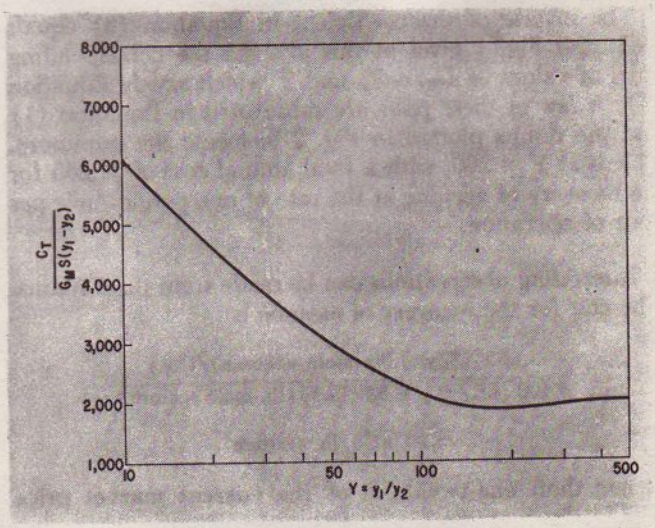

Fig. 2—Results are plotted to show the minimum design.

$$(L_M/mG_M)\,[(L_M/mG_M) - 1] =$$

$$[C_3H_{OG}\,(K_D - 1)\,/C_5\,\Theta rmG_M]\left(\frac{1 - Y}{[1 - (mG_M/L_M)]\,Y + (mG_M/L_M)} + \frac{ln\,\{[1 - (mG_M/L_M)]\,Y + (mG_M/L_M)\}}{1 - (mG_M/L_M)}\right) \qquad (3)$$

A Direct Solution. All the quantities in the coefficient, the first term on the right side of Equation (3), are given or known in an absorption operation. The remaining terms are explicit functions of the absorption factor L_M/mG_M and Y, the ratio of the inlet and exit solute concentrations in the gas stream. Therefore this equation can be solved for an optimum absorption factor as a function of Y and the coefficient. Previously this has required a series of cut-and-try calculations. This paper presents a direct solution.

The actual computation was carried out by an IBM 7040 digital computer, and the results are presented in Fig. 1. For convenience the figure shows the inverse of absorption factor versus the inverse of the coefficient, with Y as a parameter. The related pairs of values of the absorption factor and Y, all satisfying Equation (3) for any lean absorption, may now be used in Equation (1) to locate the minimum.

An Example. The illustration of the removal of acetone vapor from an air stream by water in an absorber packed with 1-inch Raschig rings[1,2,3] can be used. The following same values were used: for the acetone-air-water system $m = 2.7$ and $K_D = 23$; a mass velocity of 735 pounds of gas/(hr.) (sq. ft.), equal to 25.4 pounds moles of air/(hr.) (sq. ft.) and a corresponding H_{OG} of 2.5 feet; $r = 1.25$ in the stripper; $\Theta = 8{,}400$ hours per year; and $C_3 =$ \$4.35 per cubic foot of absorber per year. Values of \$0.018 per pound-mole of steam produced at the base of the stripper and \$4.90 per pound-mole of acetone were used as today's costs. The value of 0.02 taken for y_1 was chosen to be less than the flammability limit of acetone-air mixtures.

The inverse of the coefficient in Equation (3) equals 54.1, and Fig. 1 gives at this abscissa the corresponding pairs of values of L_M/mG_M and Y which satisfy Equation (3). A few of these pairs are substituted in Equation (1) and the results plotted in Fig. 2 to locate the minimum. This is at $Y = 200$, with a total annual cost of \$1,865 for the recovery of acetone at the rate of one pound-mole per hour of operation.

Interesting observations can be made from these results. The cost for the recovery of acetone is

$$\frac{1{,}865\ (\$/yr.)/lb.\text{-mole acetone})/(hr.)}{8{,}400\ (hr./yr.)\ \times\ 58\ (lb.)/(lb.\text{-mole acetone})}$$

$$= \$0.0038/lb.\ acetone$$

or less than one-twentieth of the current market price used in the example.

The values for the three cost terms in Equation (1) at optimum conditions are \$430, \$205 and \$1,230, respectively. At $L_M/mG_M = 1.22$ the height of the absorber is 20 transfer units or 50 feet. When $Y = 200$, 99.5 percent recovery of the entering acetone is obtained. (The final recommended design would undoubtedly be for a shorter tower, where the incremental return on the added investment would be the minimum acceptable.)

The assumed values of m and G_M give a water mass velocity of 1,510 pounds water/(hr.)(sq.ft.), which is found to, at or near a loading condition,[4] although the pressure drop is only 0.8 inches of water per foot of tower packing. Therefore the calculation should be repeated with a lower G_M.

For any problem the first cost term is affected by the values taken for H_{OG} and C_3. In the absence of experimental data the published H_{OG} values for the dilute ammonia-water system could serve as a guide.[5] The value of C_3 would be taken from current costs of absorption equipment.[6,7,8,9]

Thus the optimization of an absorption operation is determined by evaluating the various terms in the dimensionless quantity $C_5\Theta rmG_M/C_3H_{OG}\,(K_D - 1)$. For any value of this quantity the height of the absorber and its operating conditions for minimum unit cost of a recovered solute can be readily determined.

Nomenclature

C_3	Annual cost of power and fixed charges per volume of absorption column, \$/(cu. ft.) (year)
C_4	Cost of solute, taken at current market, \$/lb.-mole.
C_5	Total cost of stripping operation, expressed as \$/lb.-mole of vapor produced at the base at the stripper; includes fixed charges, cost of cooling water, and cost of steam
C_T	Total annual costs, \$/yr.
G_M	Molal gas velocity through absorber, lb.-mole/(hr.) (sq. ft.)
H_{OG}	Height per transfer unit, ft.; assumed constant
K_D	Slope of the equilibrium curve ($y = K_Dx$) in the stripping column; assumed constant
L_M	Molal absorbent velocity through absorber, lb.-mole/(hr.) (sq. ft.)
m	Slope of the equilibrium curve ($y = mx$) in the absorption column; assumed constant
mG_M/L_M	Absorption factor
r	Ratio of actual to minimum reflux ratios in the stripping column
s	Absorber cross-sectional area, sq. ft.
x	Mole fraction of solute in the solvent
y_1, y_2	Mole fraction of solute in the gas stream at the inlet and exit of the absorber, respectively
Y	y_1/y_2
Θ	Hours of operation per year

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Best Approach to Compressor Performance

When a centrifugal compressor is specified for nonideal gases and the manufacturer's data is based on air, how do you predict design and off-design performance? This calculation procedure solves the problem

Stephen A. Shain
Shell Development Co., Emeryville, Calif.

THE SPECIFICATION of a centrifugal compressor and prediction of design and off-design performance are parts of a problem that continually arise in process design studies. To make these calculations less difficult, a computer program was written which handles very general situations including multistage compression, inter- and intra-stage leakage, multicomponent gas streams, departures from perfect gas behavior, intercooling when necessary, and allowances for manufacturers' data on the basis of air to permit design for hydrocarbons and other vapors.

The equations used for the individual compression stages of the compressor are summarized in the sections which follow. The assumptions and limitations implied in the general efficiency and head coefficient correlations used, are discussed. The equations given are more general than those usually appearing in the literature.[1, 4, 6, 8, 9, 12]

COMPRESSOR PERFORMANCE EQUATIONS

Outlet Temperature and Pressure. The temperature and pressure at the outlet of the compression stage are related to the hydraulic efficiency (polytropic efficiency) and head coefficient by the following set of equations:

$$T_2 = T_1 + \frac{(0.0012854)}{(60)^2 C_p}\left[\frac{1}{\varepsilon} + \left(\frac{\partial \ln Z}{\partial \ln T}\right)_p\right]\frac{\pi^2 D^2 N^2 \Psi}{2g_c} \tag{1}$$

$$P_2 = P_1\left(\frac{T_2}{T_1}\right)^m \tag{2}$$

where

$$m = \frac{1}{\frac{ZR}{MC_p}\left[\frac{1}{\varepsilon} + \left(\frac{\partial \ln Z}{\partial \ln T}\right)_p\right]} \tag{3}$$

The efficiency and head coefficient* are defined by

$$\varepsilon = \frac{(0.0012854)\, W_p}{H_2 - H_1} \tag{4}$$

$$\Psi = \frac{2\,(60)^2\, g_c\, W_p}{\pi^2 D^2 N^2} \tag{5}$$

where the polytropic head, W_P, is defined

$$Wp \equiv (144)\int \frac{dP}{\rho} \quad \text{(Polytropic path)} \tag{6}$$

The properties appearing in Equations (1) and (3) are to be averaged over the compression path. The temperature equation, Equation (1), requires an efficiency which is an appropriate average over the path of the compression, but the pressure equation is only valid for a constant efficiency path.

Dimensionsless Numbers. Dimensional analysis of the compressible fluid flow equations[7] indicate those variables and groups of variables which are important in specifying the performance of a centrifugal compression stage. Applicable equations are the equation of of continuity, the momentum equation, the energy balance, and the equation of state. These equations must be solved subject to specified boundary conditions.

The solution to the equations is controlled by the magnitude of the following dimensionless groups:

The Grashof number

$$N_{Gr} \equiv \frac{g\beta\Delta T L^3}{\nu^2} \tag{7}$$

The Reynolds number

$$N_{Re} \equiv \frac{UL}{\nu} \tag{8}$$

The Prandtl number

$$N_{Pr} \equiv \frac{C_p \mu}{\lambda} \tag{9}$$

The Eckert number

$$N_{Ek} \equiv \frac{(0.0012854)\, U^2}{g_c\, C_p\, \Delta T} \tag{10}$$

If the reference temperature, ΔT, in the energy balance equation is taken to be the absolute temperature, T, the Eckert number is related to the Mach number

$$N_{Ek} = \frac{(k-1)\, N_{Ma}}{\left[1 + \left(\frac{\partial \ln Z}{\partial \ln T}\right)_p\right]^2} \tag{11}$$

* The definition of the head coefficient, Equation (5), involves a factor of 2 which is omitted in some sources.

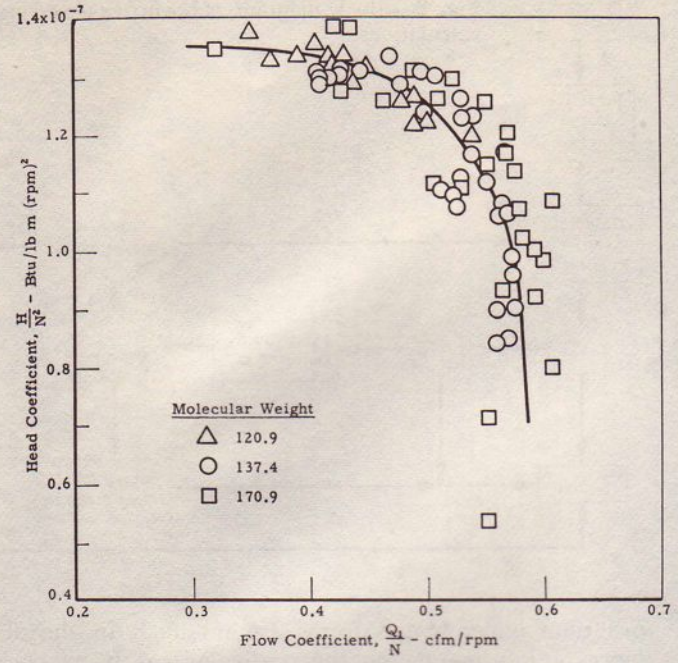

Fig. 1—Head correlations for a variety of speeds.

In the above list of dimensionless groups, the Eckert number (Equation 10), may be replaced by

The Mach number

$$N_{Ma} \equiv \frac{U}{V_s} \tag{12}$$

The speed of sound, appearing in the denominator of Equation (12), is the speed at which a small amplitude disturbance will propogate through the gas in the absence of absorption losses, i.e., for an adiabatic reversible or isentropic process. The speed of sound is given by the relation:

$$V_s = \sqrt{144\, g_c \left(\frac{\partial P}{\partial \rho}\right)_s} \tag{12a}$$

The relations of thermodynamics may be used to transform this equation to a form which allows direct use of the equation of state:

$$V_s = \sqrt{144\, g_c\, k \left(\frac{\partial P}{\partial \rho}\right)_T} \tag{12b}$$

The final relationship for the speed of sound in a nonideal gas is:

$$V_s = \sqrt{\frac{144\, g_c\, kZRT}{M\left[1 - \left(\frac{\partial \ln Z}{\partial \ln P}\right)_T\right]}} \tag{12c}$$

The calculation makes use of Equation (12c) evaluated at the inlet of a compression stage.

In the computer program, the characteristic velocity *(U)* is taken to be the impeller tip speed. In addition to the above groups, the equation of state and the boundary conditions are implicit in determining the solution.

Two compression stages will have the same solution in terms of appropriate dimensionless variables provided certain side conditions are satisfied. First of all, the boundary conditions in the two situations must be identical. Second, both compression stages must be geometrically similar, that is, the ratios of all dimensions must be identical, and third, the equation of state for the two gases undergoing compression must be identical.

Thermodynamic Variables. Solutions to gas motion equations are generally given in values of gas thermodynamic properties as functions of spatial variables in the impeller and diffuser. However, the solutions of interest are certain functions of these thermodynamic variables rather than their complete spatial variation. In particular, the solution may be thought of as the ratio of useful work to the total work or total enthalpy rise, and the ratio of useful work or pressure head to the kinetic head of the impeller. This first variable is the polytropic head divided by the actual work input and is referred to as the hydraulic efficiency. The second variable is the head coefficient. These variables have been previously defined by Equations (4) and (5). These ratios will depend on the boundary conditions and in particular on the ratio of the fluid velocity to the tip velocity of the impeller. This ratio is the volumetric flow coefficient (ϕ)

$$\phi \equiv \frac{Q}{\pi DNA} \tag{13}$$

and the formal relations for the efficiency and head coefficient and the flow coefficients are:

$$\varepsilon = \varepsilon\,(\phi; N_{Gr}, N_{Re}, N_{Pr}, N_{Ma};\ \text{equation of state parameters, geometric variables})$$

$$\Psi = \Psi\,(\phi; N_{Gr}, N_{Re}, N_{Pn}, N_{Ma};\ \text{equation of state parameters, geometric variables})$$

The volumetric flow used in defining the flow coefficient may be an inlet flow, an outlet flow, or any average of inlet or outlet flows. Several alternate approaches have been reported in the literature.[2,3,4,9,11] Better correlations appear to result from a use of intermediate flows, but correlations in this form are not always available from the manufacturers. The example given is based on inlet volumetric flows.

For impellers which are geometrically similar, the area *(A)* is uniquely related to the impeller diameter *(D)*. However, the value of *A* has been left free so that it may be adjusted to improve the efficiency and head coefficient correlations or to put them in a convenient form, particularly if geometric similitude is not maintained. For example, the flow coefficient may be interpreted as the ratio of the volumetric flow to the manufacturers' design volumetric flow if a nominal area *(A)* is taken to be

$$A = \frac{Q\ (\text{design point})}{\pi DN} \tag{14}$$

This form is often convenient since the manufacturers' correlations are commonly in terms of percentage flows relative to the design point, i.e., Equation (14) fixes $\phi = 1$ at the design point. A similar definition of a nominal diameter *(D)* may be obtained from Equation (5) for $\Psi = 1$ at the design point.

Efficiency and Head Coefficient Correlation. When the heat loss to the surroundings is negligibly small, the Prandtl number may be dropped from the solution.[7] If the Reynolds number is large ($N_{Re}^2 >> N_{Gr}$), natural convection is no longer of importance; thus the Grashof number may be eliminated from the solution.[7] If the Mach number is smaller than 1, that is, if the speed of sound is not exceeded, at all points along the compression path the performance of the compression stage is insensitive to the Mach number.[9,12,13] For Reynolds numbers greater than 100,000, as is usual, the results are insensitive to the Reynolds number.[2,3,6]

The mechanical design of different impellers for a given frame or frames is not generally based on the principle of geometric similitude. Impellers for the same frame designed for varying volumetric flow capacities will typically have the same impeller diameter with a varying channel width or area of flow. The assumption of geometric similitude is then not strictly applicable. An assumption implied in the example calculation is that a single correlation for head coefficient and for efficiency applies for all of the impellers available in the computation. This assumption will be strictly valid only if the impellers are geometrically similar. However, it is necessary to make this assumption in many cases since more detailed information on the performance of the individual impellers is not always available.

The form of the correlations which is suggested for use reduces to:

$$\varepsilon = \varepsilon\,(\phi)$$
$$\Psi = \Psi\,(\phi) \qquad (15)$$

An example correlation of head coefficient as a function of volume coefficient is presented based on the data of C. A. Macaluso[4] for a single stage compressor. Since the actual physical dimensions of the compressor were not included as part of the data, the results are correlated only in terms of ratios of the appropriate quantities. That is, the head coefficient is replaced by the dimensional ratio (in enthalpy units)

$$\Psi \sim \frac{H}{N^2} \qquad \left[\frac{\text{Btu/lb mass}}{(\text{rpm})^2}\right] \qquad (16)$$

and the volume coefficient (based on suction volume) is replaced by the dimensional ratio

$$\phi \sim \frac{Q_1}{N}\,\frac{cmf}{rpm} \qquad (17)$$

The results for a variety of speeds ranging from 5,400 rpm to 8,250 rpm and volumetric flows of 2,000 cfm to 4,500 cfm are presented in Figure 1. While there is scatter of the results, a single correlation can be presented with an accuracy of 5-10 percent. A point of particular interest is that the results are for compression of different gases (molecular weights of 120.9, 137.4, and 170.9). The surge limit or minimum value of the volumetric flow coefficient and the choking limit or maximum value of the volumetric flow coefficient are reduced to single values of the volumetric flow coefficient when presented on the basis of Figure 1.

The above results and others from the literature[9,11] suggest that correlations for both head coefficient and efficiency as functions of volumetric flow coefficient may be used for a variety of nonideal gases provided the appropriate dimensionless forms are retained. In the absence of information on the particular gas being compressed, manufacturers' information based on air can be used in the computation even though exact similitude would not be obtained.

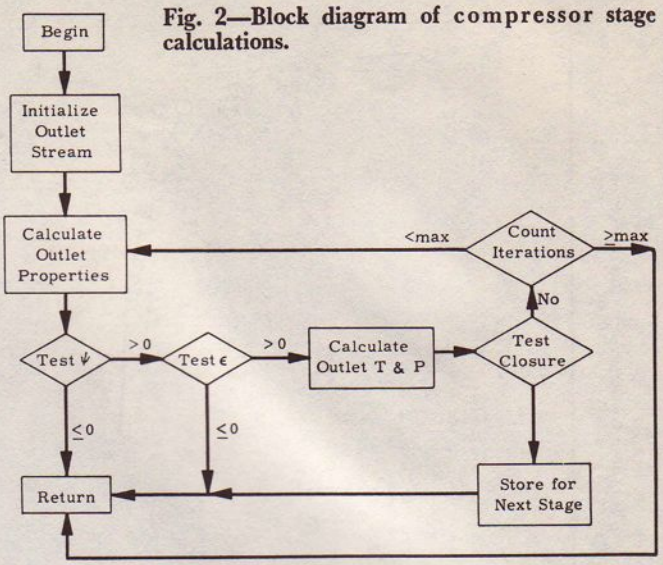

Fig. 2—Block diagram of compressor stage calculations.

Compressor Performance Calculations. The performance calculation for a compressor or series of compressors is accomplished on a wheel-by-wheel basis. The performance of each impeller or compression stage is considered in sequence by application of the general set of performance equations, Equations (1), (2), and (3). These equations allow calculation of the temperature and pressure at the outlet of a compression stage provided that the efficiency and head coefficient are known.

The specific definitions of the coefficients and dimensionless groups used have been presented as Equations (4) and (5). The efficiency and head coefficient are represented as functions of a single variable, the volumetric flow coefficient, Equation (15). The correlation of efficiency and head coefficient with volumetric flow coefficient is often a satisfactory representation of the performance of not only a specific impeller, but also of other impellers of similar design but which are scaled for use at different volumetric flows. This correlation of efficiency and head coefficient provides a convenient condensation of information on the performance of a compression stage for a variety of operating conditions.

There are limitations inherent in this approach, and some of these have been discussed above. The calculation procedure is sufficiently flexible so that additional information, when available, can be included.

Outline of Program Logic. The program logic may be schematically outlined as follows:

1. Read in input data.
2. Calculate recycle (leakage) flows.

[If the compressor calculations are incorporated with other process calculations, recycle flows (not necessarily leakage, as in this example) may depend on the compressor discharge conditions. In that case an over-all material balance may require iterative application of the entire compressor calculation.]

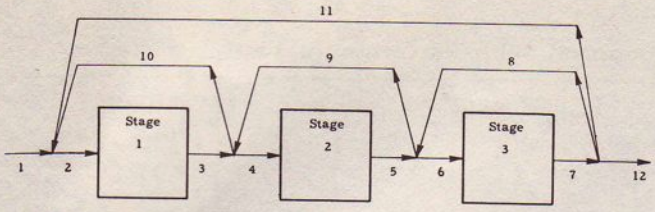

Fig. 3—Flow diagram for a three-stage compressor.

3. Calculate physical properties for the suction.
4. Initialize stage discharge physical properties.
5. Calculate appropriate average flow coefficient.
6. Calculate head coefficient and efficiency.
7. Calculate new discharge temperature and pressure.
8. Compare current and previous discharge temperature. If closure to within a specified tolerance is not achieved, return to (5). If closure is achieved, calculate the next stage starting with (4). After the last stage, continue with (9).
9. Print out final results.

Figure 2 is a simplified diagram of the subroutine which calculates the performance of a single stage.

Use of the Computer Program. The input data required by the program can be divided into the following categories:

Component data—consisting of a specification for vapor components in the form appropriate to the subroutines which calculate the compressibility factor, Z, and other physical properties required for the computations.

The equation of state used in the example is based on a modified version of the Martin and Hou equation of state[5,10]

$$p = \frac{RT}{(v-b)} + \frac{A_2 + B_2T + C_2e^{-KT/T_c}}{(v-b)^2} + \frac{A_3 + B_3T + C_3e^{-KT/T_c}}{(v-b)^3} + \frac{A_4}{(v-b)^4} + \frac{B_5T}{(v-b)^5}$$

Impeller correlation data—specifying a correlation of efficiency and head coefficient of the impeller or impellers with the volumetric flow coefficient. (The correlation may be based on inlet flow, outlet flow, or any average of inlet and outlet flows from a compression stage. Variations in the efficiency and head coefficient with Mach number and Reynolds number may be included, if desired.)

Compressor sizing data—consisting of a list of impeller scale parameters or physical dimensions to be used in the correlations for efficiency and head coefficient. (These usually are a characteristic impeller area and diameter, but other variables which reflect the capacity of the impeller may be used.)

Stream data—consisting of a specification of the inlet stream temperature, pressure, and molar flows for each component.

Miscellaneous specifications—including the rotational speed for each frame, and several bounds and increments which must be specified.

The output from the program is a reiteration of the input data and a statement of the calculated properties for the inlet stream, i.e., the density and the volumetric flow. A listing of parameters and properties for the outlet stream of each compression stage is presented. These include the stream number, the frame number and impeller number, the nominal diameter and area for the impeller, the rotational speed, the temperature, pressure, density, molecular weight, the volumetric flow, and arithmetic average value of the specific heat ratio, the value of the exponent which defines the compression path (given by Equation 3), the value of the average flow coefficient, the Mach number, Reynolds number, head coefficient, efficiency, the head and horsepower. When a stage consists of intercooling, the temperature and pressure of the stream is presented, and, if phase separation occurs, molar flows of both the vapor and the liquid stream are presented.

In addition to the calculated properties, a warning flag, FLAG, is indicated for each compression stage. Values of FLAG are used to indicate the course of the computation and signal any difficulties which may have been encountered during the computation. The warnings which may be indicated by FLAG are:

- The Mach number exceeds the critical Mach number.
- The average value of the flow coefficient is less than a minimum value.
- The average value of the flow coefficient is larger than a maximum value.
- The number of iterations for the calculation at this stage has exceeded the maximum number of iterations, i.e., the calculation has failed to converge.
- The calculated head coefficient is negative (may result from inappropriate extrapolation of correlation).
- The calculated efficiency is negative (as in head coefficient above).
- Intercooling has resulted in condensation.
- The temperature has exceeded the maximum allowable temperature.

Example Calculation. An example is presented on the application of the above procedure using a large scale digital computer. Calculations are made for a three-stage propylene refrigeration compressor. The shape of the head-capacity and the efficiency-capacity relations was taken to be the same for all three wheels, with the flow coefficient based on inlet flows. The head-capacity relation for the second stage was used as supplied by the manufacturer. The shape of the curves for the first and third stages differ by 2-5 percent at the extremes in the range of 60-140 percent design capacity. An efficiency-capacity relation was not available for the wheels in this machine. The manufacturer was able to supply an efficiency-capacity curve for a similar machine at a specific speed which was close to the design condition at the second stage. This curve was used to calculate

Table 1—Example Calculations Compared With Performance Test

Flow[a] Lb.-Mole/Hr.	RPM	SUCTION Temp., °F	SUCTION Press., psia	SUCTION cfm[b]	DISCHARGE (3rd Stage) Temp., °F	DISCHARGE (3rd Stage) Press., psia	DISCHARGE (3rd Stage) cfm	DISCHARGE (3rd Stage) Brake, hp[c]	PERFORMANCE TEST Press., psia	PERFORMANCE TEST Brake, hp
3250	8950	78	80	3563	231	312	1093	2949	308	2820
3500	8950	78	80	3837	225	304	1197	3025	298	2870
3750	8950	78	80	4111	218	292	1325	3078	286	2930
4000	8950	78	80	4385	211	276	1487	3107	268	2980

[a]–100 Percent Propylene. [b]–For feed flow, temperature, and pressure. [c]–1.02 x Compression hp.

an efficiency-capacity relation for the range in capacity of from 60-140 percent of the design points. Again, the wheels may differ by approximately 5 percent at the extremes of the range. The flows in the recycle (leakage) streams were taken as 1.5 percent at each stage and 6.5 percent from the discharge of stage 3 to the suction of stage 1. Figure 3 is a schematic diagram indicating the interstage flow, stream 12, and the intrastage flows, streams 8, 9, and 10.

The results of the computations are summarized in Table 1 and are compared with a performance test.

The discharge pressures of 312-276 psia and power requirements of 2949-3107 hp are somewhat above the 275-200 psia and 2,400-2800 hp ranges from the original design specifications. However, the calculated values are close to those from the actual performance tests for this machine. The calculated discharge pressures (third stage) are within 1-3 percent of the pressures actually achieved with even closer agreement for the brake horsepower. The agreement is excellent considering that manufacturers' head and efficiency data for air has been used to calculate performance for propylene under conditions where it is a nonideal gas.

Why This Approach? The approach presented here is intended as a thermodynamically consistent method for performance calculations when nonideal gas phases are important. It is hoped that the presentation will encourage publication of further experimental results which will allow evaluation of this approach and outline more clearly its limitations. The author would like to emphasize to those concerned with design, manufacture, and performance of such compressors that methods and computer capabilities for evaluation of thermodynamic properties of fluids are becoming generally available and should extend the usefulness of many design methods. The physical properties programs[10] used here have been made available to the Physical Properties Project Subcommittee of the American Institute of Chemical Engineers.

About the author

DR. S. A. SHAIN *is a chemical engineer with Shell Development Co., Emeryville, Calif. He is engaged in a variety of activities relating to fundamental understanding and model simulation of physical and chemical processes. Dr. Shain holds a B.S. degree from M.I.T. and a Ph.D. degree from the University of California (Berkeley). He is a member of AIChE and ACS.*

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NOMENCLATURE

A	nominal area, sq. ft.
C_p	heat capacity at constant pressure, Btu/lb. mass-°R
D	nominal diameter, ft.
g	local acceleration of gravity, ft./sec. sq.
g_c	gravitational constant, 32.16 lb. mass-ft./lb. force-sec. sq.
H	enthalpy, Btu/lb. mass
k	heat capacity ratio, C_p/C_v
L	characteristic dimension, ft.
m	exponent, defined by Equation (3)
M	molecular weight, lb. mass/lb. mole
N	rotational speed, rpm
N_{Ek}	Eckert number, defined by Equation (10)
N_{Gr}	Grashof number, defined by Equation (7)
N_{Ma}	Mach number, defined by Equation (12)
N_{Pr}	Prandtl number, defined by Equation (9)
N_{Re}	Reynolds number, defined by Equation (8)
P	pressure, psia
Q	volumetric flow, cmf
R	gas constant, equal to 1.987 Btu/lb. mole-°R, or 10.73 psia-cu. ft./lb. mole-°R
S	entropy, Btu/lb. mass-°R
T	temperature, °R
U	characteristic velocity, ft./sec.
V_s	velocity of sound, ft./sec.
W_p	polytropic head, ft.-lb. force/lb. mass
Z	compressibility factor

Greek Symbols

β	coefficient of thermal expansion, vol fract/°R
ε	polytropic efficiency, defined by Equation (4)
λ	thermal conductivity, Btu/sec.-ft.-°R
μ	viscosity, lb. mass/ft.-sec.
ν	kinematic viscosity, sq. ft./sec.
π	constant, equal to 3.14159
ρ	density, lb. mass/cu. ft.
ϕ	volumetric flow coefficient, defined by Equation (13)
Ψ	polytropic head coefficient, defined by Equation (5)

Subscripts

1	refers to compression stage inlet
2	refers to compression stage outlet

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