HYBRID SIMULATION OF A CONTROL SYSTEM FOR A TUBULAR CHEMICAL REACTOR*

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INTRODUCTION

This Study describes the simulation on the EAI HYDAC® 2400 HYbrid Digital-Analog Computer of a control system for a tubular chemical reactor. Specifically, it describes the transient simulation of the reactor itself, its product separator, and its control system (Figure 1 shows a block diagram of the physical system simulated); the study calls for the solution of distributed parameter reactor equations, which can be accomplished best by a hybrid computer having the mathematical capability of function storage.

Although the chemical process industries (CPI) have made extensive use of the analog computer alone in the past to solve complex design, control, and data analysis problems, the simulation of distributed parameter systems impose a heavy burden on the computing capability of the hardware usually available. In most instances, for example, the capacity of a normal computer facility (say 100 - 200 amplifiers) rarely is challenged by problems requiring the simulation of linear and non-linear ordinary differential equations.

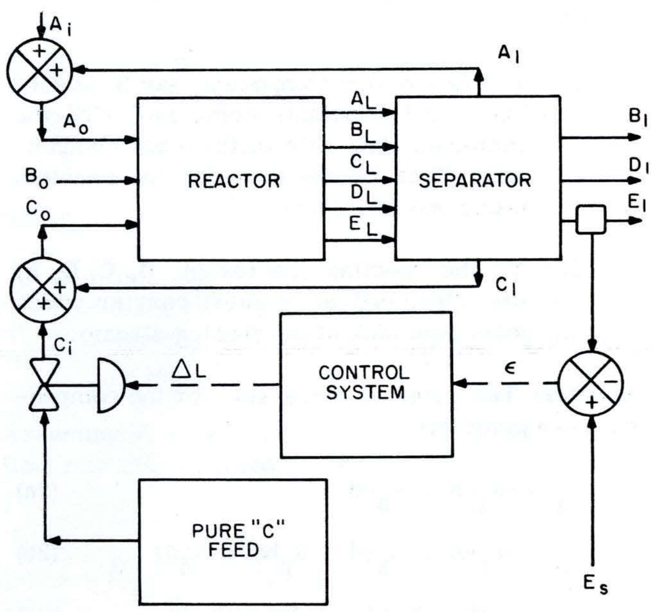

Figure 1: Block Diagram of Physical System

However, mathematical models involving several partial differential equations (PDE)...models of fixed bed transients, tubular reactors, etc....frequently tax this computing capacity, and the available hardware definitely becomes the limiting factor in such cases, usually requiring simplification of the equations, the overall system model, or both, and some compromise of the simulation accuracy. These excessive hardware requirements for the solution of PDE's are due to the transformation of each PDE into a set of ordinary differential equations (ODE), each of which must be solved simultaneously (i.e., in parallel). This requires the implementation by means of analog components of a large number of almost identical computing circuits, a requirement which is usually sufficient to exhaust the equipment complement of even the most fully supplied laboratory.

This situation has been changed by using a different mathematical formulation of the equations which requires a function memory capability. Hybrid computers, coupling analog speed with digital memory and accuracy have satisfied this requirement and thus enable system analysts to utilize the maximum problem solving capability of their computing facilities. In addition, they have provided simple means for implementing logical operations, transport delays, and the transient simulation of stage-wise processes...processes which are, themselves, hybrid in nature.

The purpose of this Study is to illustrate the solution of a typical chemical process problem on the HYDAC 2400 Hybrid Computing System, consisting of an EAI 231R-V General Purpose Analog Computer, a DOS-350 Digital Operations System, and a

*EAI Application Study: 6.4.1h describes the development of a Tubular Reactor Control System program using serial memory capability. This study describes a more sophisticated approach using function memory capability and a completely integrated hybrid computer.

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DCS-375 Digital Computing System. The problem described is the simulation of a tubular reactor (represented by 2 PDE's), its separator, and a control system. Problem definition, organization, programming, and hardware requirements are presented in detail.

OBJECTIVES

The objectives of this simulation are typical of those encountered in many CPI simulations. They are:

(1) To define the physical system mathematically,

(2) To propose a control system to maintain a constant output product flow rate, and

(3) To determine controller settings for the proposed control system.

PHYSICAL SYSTEM*

The complete system under study, shown schematically in Figure 1, consists of a tubular reactor, a separator, and a control loop. The kinetics of the system are:

$$A + B \underset{k_1}{\overset{k_3}{\rightleftarrows}} C + D \qquad (1A)$$

$$C + B \underset{k_2}{\overset{k_4}{\rightleftarrows}} E + D \qquad (1B)$$

where component E, the desired product, is formed by feeding A, B, and C to the reactor. Component D is a waste product which is discarded.

The reactor effluent is fed to a separator, which ideally separates the effluent into five pure product streams, A_1 ---- E_1. Unreacted A and C are recycled and combined with make-up feeds, A_i and C_i, to obtain reactor feed rates, A_o and C_o. Component B is returned to tankage on leaving the separator. It is supplied in excess to the reactor at a constant feed-rate, B_o. Excessive amounts of B are used to maintain favorable reactor behavior.

Disturbances (step changes and noise such as valve chatter or low frequency sinusoids) enter the system through the make-up feed stream, A_i, and cause variations in product flow, E_1. The purpose of the control loop is to operate on the flow error, ϵ, using a control system to vary the feed rate of component C. Since B is present in excess, variations in C (note reaction 1B) have a direct effect on product formation. The control system selected is a conventional three-mode controller.

It has been assumed that the separator is 100% efficient and that its dynamics can be represented by a first-order lag. Sensor and valve dynamics associated with the control loop are assumed negligible and the valve-position-versus-flow relationship is considered to be linear.

MATHEMATICAL MODEL

Assumptions: The assumptions used to establish the mathematical model of the problem are as follows:

1. The velocity through the reactor, V, is constant.
2. The process is isothermal with the consequence that the rate of reaction is dependent only on composition.
3. The density of the reaction mixture, ρ, and the average molecular weight of the reaction mixture, m, are constant, independent of composition.
4. The reactor is of the plug-flow type; i.e., there is no axial diffusion.

The first assumption can be justified, even though the flow rates of A, B, and C at the inlet to the reactor vary, if one of the following conditions exists:

1. The flow of one component, say B, is very high (and constant) compared with the combined flow rate of the other components. This is the case for the problem under consideration.
2. All the reacting species (A, B, C, D, E) are dissolved in an inert carrier which forms the bulk of the flowing stream.

Kinetics: The rates of conversion for the components are given by:

$$r_a = -k_1ab + k_3cd \qquad (2a)$$

$$r_b = -k_1ab + k_3cd - k_2bc + k_4de \qquad (2b)$$

$$r_c = k_1ab - k_3cd - k_2bc + k_4de \qquad (2c)$$

This system was patterned after the one described in Reference (1).

$$r_d = k_1 ab - k_3 cd + k_2 bc - k_4 de \quad (2d)$$

$$r_e = k_2 bc - k_4 de \quad (2e)$$

where $a \ldots e$ = concentrations of components A, ...E, lb moles/ft^3

$r_a, \ldots, r_e$ = rates of formation, lb moles/(ft^3) (sec)

$k_1, \ldots, k_4$ = reaction rate constants, (ft^3)/(lb mole) (sec)

Only two of these equations are required, since r_b, r_c, and r_d can be stoichiometricly related to r_a and r_e,

$$r_b = r_a - r_e \quad (3a)$$

$$r_c = -r_a - r_e \quad (3b)$$

$$r_d = -r_b \quad (3c)$$

Integrating these equations yields

$$b = b_o + a - a_o - e \quad (4a)$$

$$c = c_o + a_o - a - e \quad (4b)$$

$$d = b - b_o \quad (4c)$$

The initial concentration, d_o, is zero and is omitted from equation 4c.

Reactor Equations: The concentration dependence of components A and E with respect to time and position is expressed by two partial differential equations:

$$\frac{\partial a}{\partial t} + V \frac{\partial a}{\partial x} = r_a \quad (5a)$$

$$\frac{\partial e}{\partial t} + V \frac{\partial e}{\partial x} = r_e \quad (5b)$$

where

t = time, sec

x = distance from entrance of reactor, ft.

V = velocity of mixture through the reactor, ft/sec

Assuming V, ρ, and m are constant, z (total molar) flow rate also is constant; therefore,

$$z = \frac{\rho V \gamma}{m} = A + B + C + D + E$$
$$\frac{F\rho}{m} = \text{CONSTANT} \quad (6)$$

where

A----E = the flow rates of each component, moles/sec

γ = cross-sectional (or flow) area, ft^2

F = volumetric flow rate, ft^3/sec

ρ = fluid density, lbs/ft^3

m = fluid molecular weight, lbs/lb mole

Since A = Fa and B = Fb, equations 4 and 5 can be rewritten in terms of flow rates to obtain

$$\frac{\partial A}{\partial t} + V \frac{\partial A}{\partial x} = -k_1 \frac{AB}{F} + k_3 \frac{CD}{F} \quad (7a)$$

$$\frac{\partial E}{\partial t} + V \frac{\partial E}{\partial x} = k_2 \frac{BC}{F} - k_4 \frac{DE}{F} \quad (7b)$$

$$B = B_o - A_o + A - E \quad (7c)$$

$$C = C_o + A_o - A - E \quad (7d)$$

$$D = B_o - B \quad (7e)$$

Separator Equations: The separator equations, which are first-order lags, are, in transfer function notation,

$$\frac{A_1}{A_L} = \frac{C_1}{C_L} = \frac{E_1}{E_L} = \frac{1}{\tau S + 1} \quad (8)$$

where

S = Laplace operator, sec^{-1}

τ = separator time constant, sec

The subscripts "L" and "1" denote reactor and separator effluent concentrations, respectively.

Separator equations were not written for components B and D since their effluent concentrations are not required in the simulation.

Control System: The classical transfer function for a 3-mode controller is

$$\frac{\Delta 1}{\epsilon} = K_c \left(\frac{\tau_D S + 1}{\alpha \tau_D S + 1} \right) \left(\frac{\tau_r S + 1}{\tau_r S + \frac{1}{K_r}} \right) \quad (9)$$

where

τ_D = derivative time constant, sec

τ_r = reset time constant, sec

γ = derivative gain, dim

K_r = reset gain, dim

K_c = controller gain, sec/lb mole

$\Delta 1$ = change in percent of valve opening, dim

The controller gain includes the gain of the valve, sensor, valve positioner, etc. The constants K_c, τ_r, and τ_D are settings available to plant operators whose determination is one of the objectives of this study.

The error signal, ϵ, is

$$\epsilon = E_s - E_1 \tag{10}$$

where E_s, the set point, is the desired product flow rate.

Feed and Recycle Equations: Based on the linear valve assumption (as shown in Figure 2), the make-up feed, C_i, of "C" is

$$C_i = C_s + \left(\frac{C_m}{100}\right) \Delta 1 \tag{11}$$

where

C_s = design flow rate of make-up feed, moles/sec

C_m = maximum flow rate of make-up feed, moles/sec

The make-up feed rate, A_i, of component "A" is

$$A_i = A_s + f \tag{12}$$

where

A_s = design flow rate of make-up feed, moles/sec

f = disturbance introduced into the system, moles/sec

The disturbance can take two forms: a step change,

$$f = K \tag{13}$$

or a sinusord,

$$f = K \sin \omega t \tag{14}$$

where

K = magnitude of the disturbance, moles/sec

ω = frequency of the disturbance, rad/sec

Equations 11 thru 14 can be combined with recycle flows, A_1 and C_1, to obtain reactor feed equations.

$$A_o = A_1 + A_s + f \tag{15a}$$

$$C_o = C_1 + C_s + \left(\frac{C_m}{100}\right)\Delta 1 \tag{15b}$$

Recall the feed rate, B_o, of component "B" is fixed.

Method of Characteristics: The partial differential equations can be reduced to ordinary differential equations by the method of characteristics (2). Consider the first order partial differential equation

$$\frac{\partial F}{\partial t} + V(x, t)\frac{\partial F}{\partial x} = g(F, x, t) \tag{16}$$

which is of the same form as equations 7a and 7b. The solution is wanted for $t>0$ and $0<x<L$, where L represents the length of the reactor.

Throughout this general discussion, F will be used to describe the flows (A,...,E) in the mathematical model.

The method of characteristics requires that integration be performed along lines in the space-time domain, defined by

$$\frac{dx}{dt} = V(x, t) \tag{17}$$

To find the equivalent of equation 16, write the total derivative of F

$$dF = \frac{\partial F}{\partial t}dt + \frac{\partial F}{\partial x}dx$$

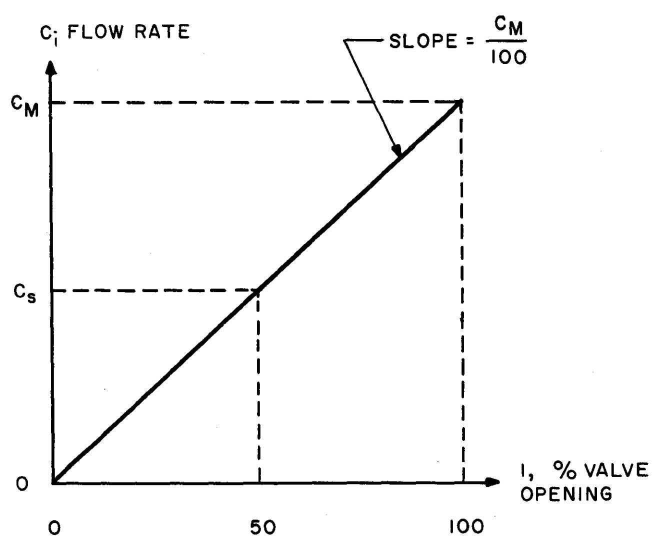

Figure 2: Value Characteristic Curve

to obtain

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial x}\frac{dx}{dt} = \frac{\partial F}{\partial t} + V\frac{\partial F}{\partial x} = g\,(F,x,t) \qquad (18a)$$

or

$$V\frac{dF}{dx} = \frac{\partial F}{\partial t} + V\frac{\partial F}{\partial x} = g\,(F,x,t) \qquad (18b)$$

This equation is an ordinary differential equation and can be solved directly by an analog computer. For the problem under consideration, V is constant which means that the characteristics consist of straight lines having a slope of V, as shown in Figure 3. The initial condition, F (0, t), is given by the problem, and for the tubular reactor, this represents the variation in the flow of components at the inlet to the reactor. Since the conditions at the outlet of the reactor are desired, the procedure based on the method of characteristics is to integrate equation 19b on the computer until x = L, or $t = \frac{L}{V}$

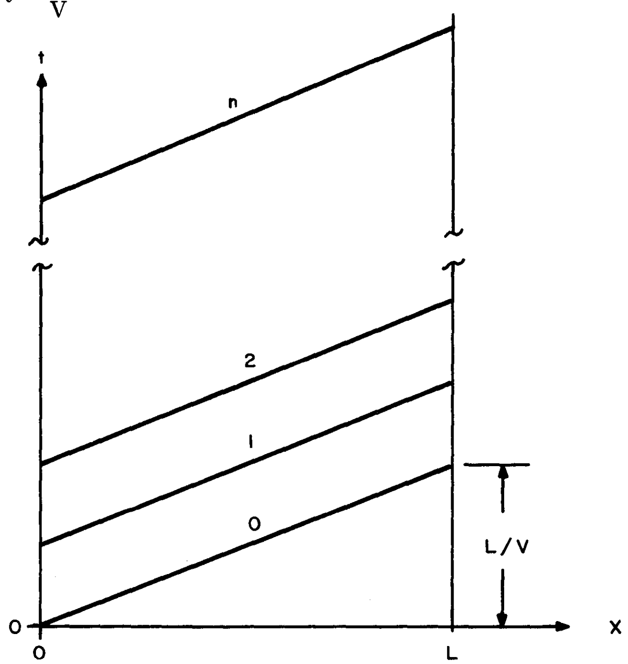

Figure 3: Characteristic Lines in the Space-Time Domain

For example, if F (0, t_o) represents the condition at the reactor inlet at time t_o, the integrator which generates F would be reset to F (0, t_o), and then allowed to integrate until x = L, at which time the integrator would produce the values of F at the outlet of the reactor τ seconds later, i.e., F (L, $t_o + \tau$).

Since the characteristic curves for the problem under investigation are straight lines having a slope of V, the residence time in the reactor is a constant (which also is the computation time, L/V).

High speed computation techniques will be used to allow a large number of characteristic lines in the space-time domain to be "scanned" in order to obtain a semi-continuous solution.

Computational Model: The reactor-separator system is presumed to be operating at its design point when a disturbance is introduced into the system. Therefore, good scaling practice dictates that equations be rewritten in perturbation form. Defining

$$\Delta A_L = A_L - A_{Ls} \qquad (19a)$$

$$\Delta C_L = C_L - C_{Ls} \qquad (19b)$$

$$\Delta E_L = E_L - E_{Ls} \qquad (19c)$$

$$\Delta A_1 = A_1 - A_{1s} \qquad (19d)$$

$$\Delta C_1 = C_1 - C_{1s} \qquad (19e)$$

$$\Delta E_1 = E_1 - E_s = -\epsilon \qquad (19f)$$

yields the following separator-feed equations

$$\frac{\Delta A_1}{\Delta A_L} = \frac{\Delta C_1}{\Delta C_L} = \frac{-\epsilon}{\Delta E_L} = \frac{1}{\tau S + 1} \qquad (20a)$$

$$A_o = \bar{A}_s + \Delta A_1 + f \qquad (20b)$$

$$C_o = \bar{C}_s + \Delta C_1 + \left(\frac{C_m}{100}\right)^{\Delta 1} \qquad (20c)$$

where

$\bar{A}_S$ and $\bar{C}_S$ denote $A_s + A_{1s}$ and $C_s + C_{1s}$, respectively.

The non-linearities in the reactor equations make perturbation variables impractical; however, their form lends itself to solution by the method of characteristics. Applying this technique (see equation 18b) yields

$$\frac{-dA}{dy} = k_1 AB - k_3 CD \qquad (21a)$$

$$\frac{-dE}{dy} = k_4 DE - k_2 BC \qquad (21b)$$

where

$$y = \frac{\gamma x}{F^2} = \frac{x}{VF}$$

The above equations, solved in conjunction with the three algebraic equations (equations 7c thru 7e) defining B, C, and D in terms of A and E, are the computational model of the reactor.

The controller equation (equation 9) requires no modification since it is already in perturbation form. However, it should be noted that $\Delta 1$ is limited $(o \leq 1 = 1_s + \Delta 1 \leq 100)$.

As mentioned before, a high-speed computational procedure is required to allow the reactor outlet product flows to be obtained in a semi-continuous manner.

METHOD OF SIMULATION

High Speed Computing Techniques: Referring to the description of the Method of Characteristics and to Figure 4, if integration along the characteristic line is speeded up so that it occurs in a small interval of time, Δ (including reset), the value of F at the end of this interval would be $F(L, t_0 + \Delta)$. If this value is delayed by $\frac{L}{V} - \Delta$ seconds and then introduced into the simulation, real-time simulation of $F(L, t_0 + \frac{L}{V})$ is accomplished. In the HYDAC 2400 system, the obvious means for storage is to use the digital computer (DCS 375) memory.

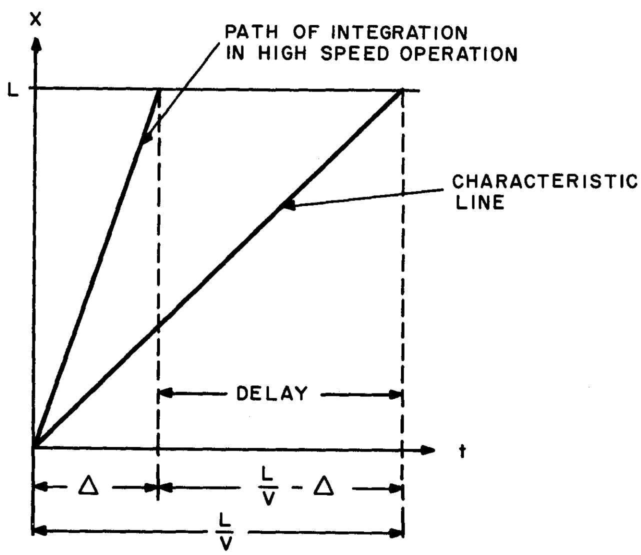

Figure 4: Diagram of High-Speed Computing Technique

The benefit of high-speed computation results from the fact that over the time inerval L/V, a large number of computations (namely $L/V\Delta$) can be made instead of just one computation being performed in real-time. This number can be as high as several hundred in a practical case. It has to be chosen equal to the number of memory words available in the delay simulator(3) divided by the number of data points to be stored. In the present case, 150 memory words were used for each flow rate variable of interest.

Computational Assignments: Table 1 indicates the computational assignment of each part of the HYDAC 2400 System. Note that the analog computer operates in two speeds. It simulates the separator, controller, and feed equations in real-time while using high-speed repetitive operation to solve the reactor equations.

Table 1: Computation Assignments in the HYDAC 2400 System

Unit	Function
231-R (Analog)	High-speed solution of Equa. (21) for simulating tubular reactor.
	Real-time simulation of separator and controller.
	Problem control including: 1. Control of repetitive operation 2. Control of DOS modes
DOS-350	Control of information between DOS and System 375 through use of digital-analog and analog-digital converters.
SYSTEM 375 (Digital)	Storage of data for the delay required to simulate the tubular reactor.

The computer circuits to be described are based on the requirement that three of the flow rates of components (A, C, and E) are to be simulated in real-time. This can be seen from Figure 1 in which the reactor outlet flows of only these components affect the inlet flows (i.e., A and C are recycled and E is used to adjust the supply of fresh C). This means that the delay simulator in the digital part of the computer must be able to handle three channels of information.

The retention time in the reactor, (L/V), is to be 3.0 sec. If the operate period is 12 ms and the reset period is 8 ms, then the combined period, Δ, is 20 ms. The number of storage locations in the DCS 375 computer for each variable (A, C, and E) is 3000/20 or 150.

Problem Control Assignment: Since an investigation of this kind requires continual modification of both forcing functions (f) and parameters (controller settings), and continuous function readout, etc., problem control has been assigned to the analog computer. Its mode of operation controls both the DOS-350 System and DCS 375 computer.

COMPUTER PROGRAMMING

Analog Computer Programming: The scaling, programming, and problem check-out of the analog portion of this study is straightforward and will not be discussed at this time. However, a table of scaled voltage equations is shown in Table 2 for information purposes, and Appendix A contains circuit diagrams, pot sheets, etc.

Referring to the computer diagram, track-store units 12, 13, 17, 18, 22, and 23 monitor the flows of A, C, and E and stored ΔA_L^*, ΔC_L^*, and ΔE_L^*, the terminal flow rates. This occurred during the operate period (which was 12 ms) of the high-speed repetitive operation (HSRO) cycle when y=1. It was implemented using the logic signal from an electronic comparator (ECOO). The terminal values were held constant during the 8 ms reset period of the HSRO cycle and transferred to digital memory. The integrators in the HSRO portion of the simulation were speeded up by a factor of 100.

Table 2: Summary of Scaled Voltage Equations

REACTOR

$$\frac{d\,[100y]}{d\tau} = \left(\frac{1}{\beta}\right)[100]$$

$$\frac{-d\,[50A]}{d\tau} = \left(\frac{10k_1}{\beta}\right)[5AB] - \left(\frac{4k_3}{\beta}\right)\left[\frac{25}{2}CD\right]$$

$$\frac{-d\,[50E]}{d\tau} = \left(\frac{4k_4}{\beta}\right)\left[\frac{25}{2}ED\right] - \left(\frac{10k_2}{\beta}\right)[5BC]$$

$$[25D] = 2.5\left[\left(\frac{B_o}{10}\right)[100] - [10B]\right]$$

$$[10B] = \left(\frac{B_o}{10}\right)[100] - \left(\frac{1}{5}\right)\left[50\,(A_o - A)\right] - \left(\frac{1}{5}\right)[50E]$$

$$[50C] = \left[50\,C_o\right] + \left[50\,(A_o - A)\right] - [50E]$$

SEPARATOR

$$\frac{[50\,\Delta A_1]}{[5\,\Delta A_L]} = \frac{10}{\tau S+1}\,;\quad \frac{[50\,\Delta C_1]}{[5\,\Delta C_L]} = \frac{10}{\tau S+1}\,;$$

$$\frac{[50\,\epsilon]}{[5\,\Delta E_L]} = \frac{-10}{\tau S+1}$$

CONTROL LOOP†

$$\frac{[2\,\Delta 1]}{[100\,\epsilon]} = \frac{[10\,\epsilon_1]}{[100\,\epsilon]} \times \frac{[2\,\epsilon_2]}{[10\,\epsilon_1]} \times \frac{[2\,\Delta 1]}{[2\,\epsilon_2]}$$

$$\frac{[10\,\epsilon_1]}{[100\,\epsilon]} = \frac{S + 1/\tau_D}{(10\,\alpha)\,S + 10/\tau_D}$$

$$\frac{[2\,\epsilon_2]}{[10\,\epsilon_1]} = \left(\frac{K_c}{10}\right)$$

$$\frac{[2\,\Delta 1]}{[2\,\epsilon_2]} = \frac{S + 1/\tau_r}{S + 1/K_r\tau_r}$$

FEED EQUATIONS

$$[50A_o] = [50\,\Delta A_1] + \left(\frac{A_S}{2}\right)[100] + [50f]$$

$$[50C_o] = [50\,\Delta C_1] + \left(\frac{C_S}{2}\right)[100] + \left(\frac{C_m}{4}\right)[2\,\Delta 1]$$

DISTURBANCE EQUATIONS

Step Input

$$[50f] = \left(\frac{K}{2}\right)[100]$$

Sinusoidal Input

$$[50f] = \left(\frac{K}{2}\right)[100\,\sin\omega_i t]$$

Notes: ( ) = pot setting, [ ] = computer variable or reference voltage, and τ = machine time = βy in reactor equations.

† Since L_s is assumed to be 50%, $2\Delta 1$ is limited to ± 100 volts.

Track-store units 27 and 28 held A_o and C_o constant during the operate portion of a HSRO run. During this period their input was updated, but the updated values were not used in the present computation. They represented new feed flows for the next "slug" of fluid integrated down the reactor length.

All digital to analog conversion (DAC) was performed during the operate portion of the HSRO cycle, while analog to digital conversion (ADC) was performed during the reset period.

Integrators involved in the "real-time" simulation of the separator and control system have a unity R-C time constant.

Signals generated on the MLG patch panel used in the DOS program include the mode of computer operation (OP, HD, IC). A logical one appeared at the mode termination when the computer was in a particular mode. The HSRO, A, and $\bar{A}$ signals were required for conversion purposes. The A signal was "high" during the reset period and "low" during the operate period ($\bar{A}$ is the complement of A).

The pulse train which produces A and $\bar{A}$ operates continuously regardless of the computer mode; therefore, it must be synchronized with the DOS clock if it is to be used on the DOS to initiate conversion operations.

DOS Programming: The programming of the DOS is best discussed by considering the principle areas of the over-all program, which is shown in Appendix A. These areas are ADC, DAC, and conversion timing; the initialization abstracts of the over-all circuit diagram will be used in the discussion of the over-all DOS program.

ADC

The circuit shown in Figure 5 is designed to convert three analog voltages, appearing on trunks 100-102, after receiving a blip input signal. A blip completion signal is generated after the three conversions are completed.

The blip input resets the multiplexer, selects channel zero, and simultaneously calls for a conversion (CONV input to ADC). When the ADC is complete, a FIN signal is gated with a ready signal from the DCS 375 Computer (OC 12) to enable (TE_i) the transfer of information to the digital memory. When this occurs, the Input-Output Buffer Register (IOBR) between the DOS-350 and the DCS 375 is simultaneously cleared and loaded in a parallel manner (L_p, CLR inputs to IOBR). The ADC is reset (RST) as is OC 12 at this time.

When transfer into memory is complete a blip appears at TC_i which increments (INC) the multiplexer to channel one and initiates the conversion cycle. After the third conversion has been completed a blip appears at the output of AND gate 28B signifying completion of all three conversions.

DAC

Consider Figure 6, where a blip input sets a flip-flop (211) to signify conversion is required and simultaneously clears (CLR) the general purpose counter (GC 10) which is a channel selector for the DAC. A digital ready signal (OC 11) through an "AND" gate (240) enables transfer out of the digital computer into the IOBR. A blip from the TC_o termination loads the digital word into the assembly register (L_p), whose completion is signified by a LFIN-RST blip which initiates conversion (TRA) to channel zero. When conversion is complete a blip from TFIN-RST advances the BCD counter to channel one as well as initiating another DAC conversion by sending a reset signal to flip-flop 220.

After three conversions have been completed, the AND of the TFIN-RST signal with channel 2 signal (AND gate 28A) produces a blip finish signal, which resets flip-flop 211 inhibiting further conversion signals.

Conversion Timing

The OP, HD, IC, and $\bar{A}$ signals received from the MLG unit (as shown in Figure 7) are passed through AND gates as a safeguard against noise

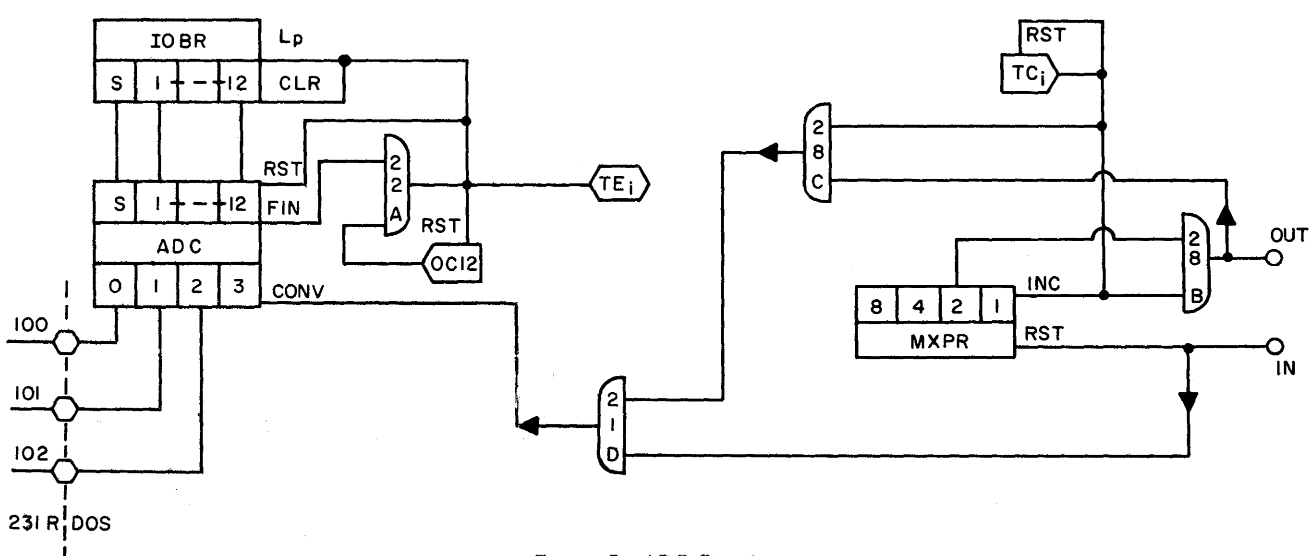

Figure 5: ADC Circuit

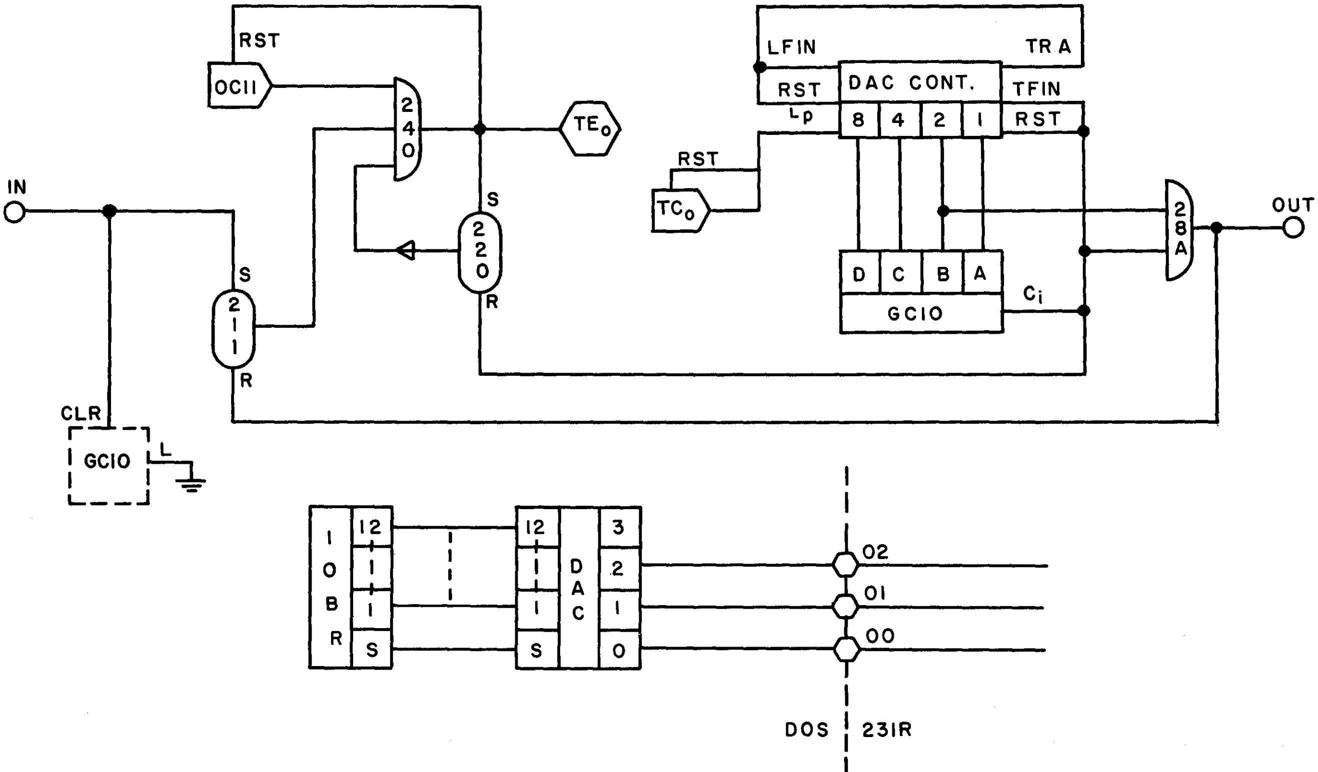

Figure 6: DAC Circuit

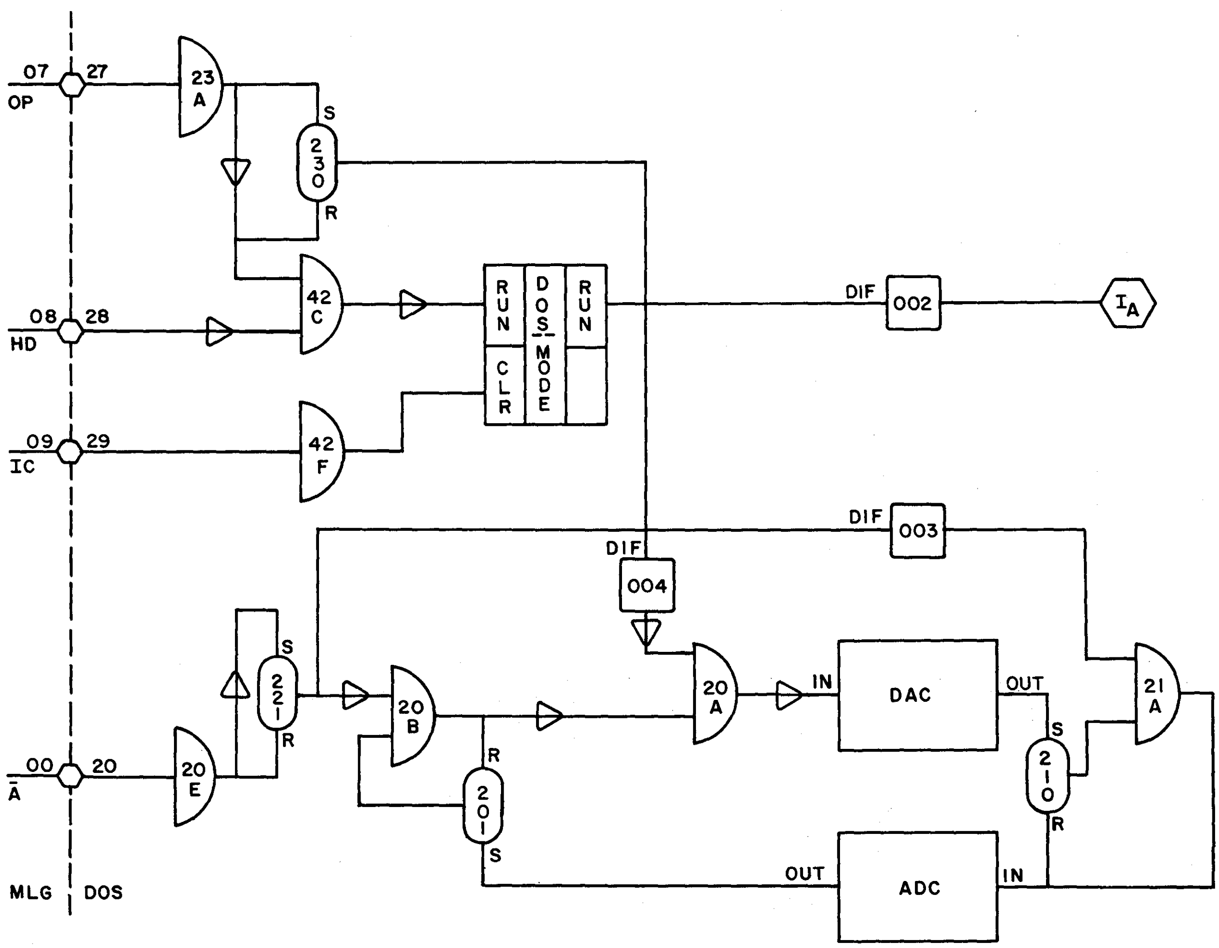

Figure 7: Conversion Timing and Initialization Circuit

or spikes. The OP and $\bar{A}$ signal are sent to flip-flops to insure that they are synchronized with the DOS clock.

Temporarily disregarding initialization, after an ADC is complete (flip-flops 201 is high) and the rep. op. cycle is in operate (flip-flop 221 is low), a blip is sent to the DAC program through the initializing circuit. After the DAC program is complete, flip-flop 210 is set and waits for the reset part of the rep. op. cycle. At this time a blip appears at the output of AND gate 21A to initiate the ADC routine. The ADC completion signal sets flip-flop 201 and the above procedure is repeated.

Initialization

To insure proper operation of the system, the correct initial values of reactor recycles must appear prior to the first ADC. If the reactor feed voltages are not correct, its effluent voltages will be incorrect. In setting up the problem it has been assumed that prior to an entering disturbance the reactor is operating at steady-state. Therefore, the digital memory cells used for the delay are filled with the steady-state effluent flow rate values. In lieu of the above, a DAC must take place prior to an ADC.

This is accomplished by DIF 004 (Figure 7), which is passed through the OR circuit feeding the DAC. After the first set of DAC is complete and the start of the next reset period is reached, an ADC is initiated. DIF 003 is used to prevent an ADC from taking place after the reset period has started in the event that the first DAC was completed during a reset period.

The digital program, which will be discussed later, replaces values removed by DAC with the next ADC values and then advances to the next set of memory locations.

Digital Computer Programming

The stored-program digital computer program provides storage and playback of the ΔA_L, ΔC_L, and ΔE_L reactor outlet flow rates. The total delay required is 3 seconds and each high-speed analog run requires 20 ms.; therefore, a total of 150 points must be stored per variable. Since the reactor is assumed to start from steady-state, the digital program also loads the table initially with the steady-state values (in this case zero).

The flow diagram for the digital program is shown in Figure 8 and the assembler program is listed in Appendix A.

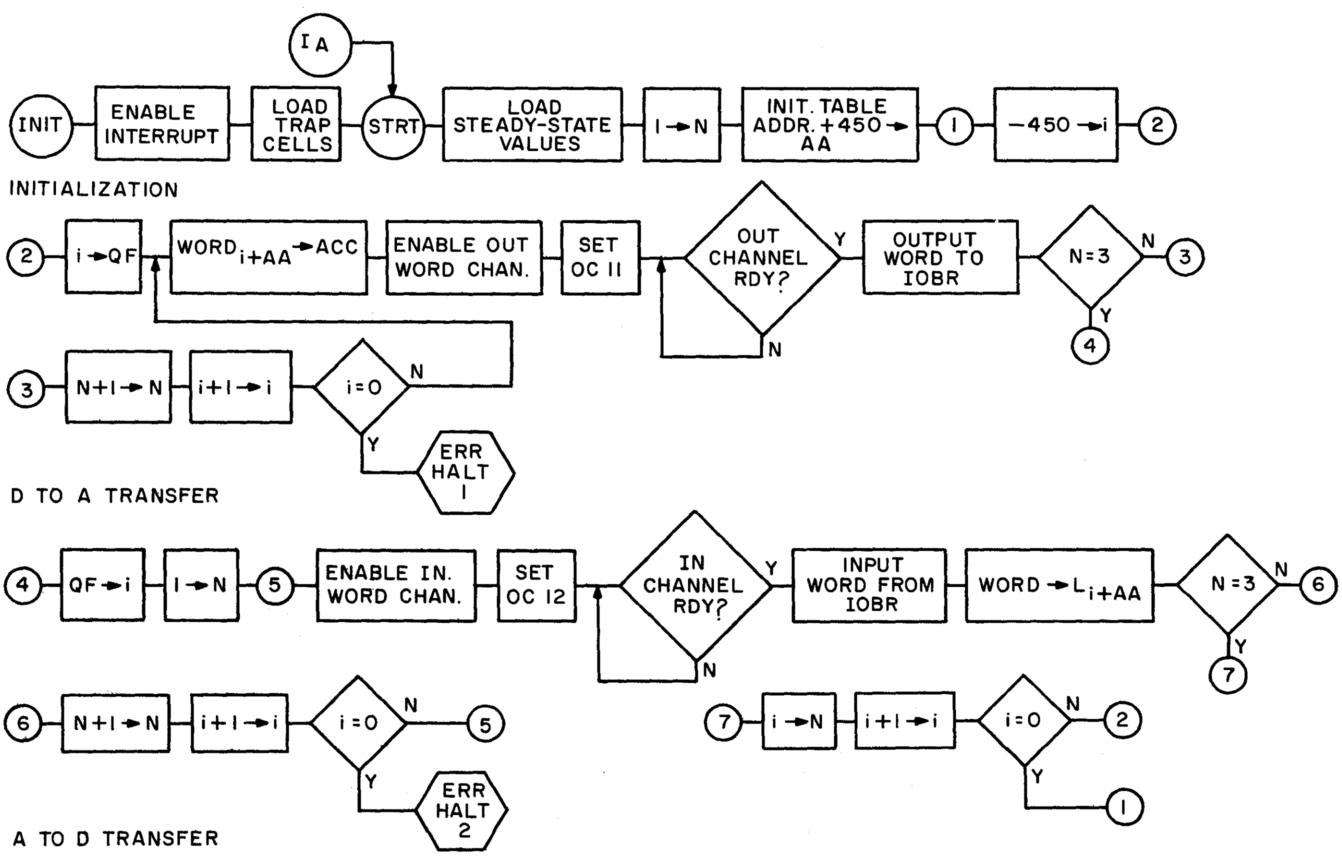

Figure 8: Flow Diagram of Digital Program

The computer is started from location INIT where interrupts are enabled and the interrupt trap cells are loaded with the appropriate jump instructions. The program then goes to STRT where the initial steady-state values are loaded into the table, and the initial address of the table is established in memory. Table indexing is then initialized after which the program proceeds to the D to A transfer routine. The index is then stored in memory for use in the A to D transfer routine.

The first data word then is loaded into the accumulator and the parallel output channel is enabled (OC 11 is set to indicate to the DOS that the DCS 375 is ready to output a word). The output channel is tested for the ready flip-flop set, which halts the digital program until the DOS commands the data to be transferred. When the channel becomes ready, the DCS 375 outputs the word to the IOBR of the appropriate DAC channel.

The index, N, is tested then for readout of the last DAC channel. If it is the last channel, the program proceeds to prepare for the A to D conversions. If not, N and i are indexed and a test is performed; i is tested for the end of the table. At the end, an error halt will occur since the routine should have exited at the N test. If the index is non-zero, the routine loads the accumulator with the next word and repeats the output cycle.

The A to D transfer program first establishes the proper index, i, from the memory location QF and reinitializes the variable count, N. The parallel input channel then is enabled and OC 12 is set to inform the DOS that the program is ready to input analog data. The program then enters a waiting loop until the input channel ready signal is brought high at the completion of an A to D conversion.

The program inputs the data word from the IOBR and stores it in the proper indexed location. The variable count, N, is tested for 3 and, if it is not the last channel, the routine increments N and i and tests i for the last table address. At the last table address, the program executes an error halt since an exit should have occurred at the N test. For a non-zero, the program returns to point 5 to prepare to input the next channel.

For a variable count N = 3, the routine reinitializes N, increments i, and tests for the last data point. If it is not the last point, the program returns to point 2 to prepare for the next D to A transfer. If the index is zero, i is reinitialized before reentering the D to A transfer routine.

Computer Control: When the analog computer is in the IC mode the DOS is in CLR; it can only be put into the RUN mode if the analog is in operate, OP, or hold, HD. If the DOS is put in RUN, an interrupt signal is fed to the digital computer, thru I_A, which causes the digital program to clear its memory and load delay cells with initial, steady-state values of A, C, and E. DIF 002 disables the interrupt signal until the analog computer again goes from the IC to the HD mode.

This computer control set-up uses the analog computer as the master computer. It permits parameters to be varied on the analog without clearing the DOS or reprogramming the digital computer. To obtain this flexibility of operation, the HD mode cannot be by-passed; to start a run, one must go through the HD mode.

Since both the ADC and DAC are completed in less than 1 ms, there is no need to remain in HD for any predetermined period of time.

COMPUTER RESULTS

The results of the simulation are shown in Figures 9 thru 15 and are summarized in Table 3.

Runs 1 through 3 (Figures 9 thru 11) are illustrative. They show typical steady-state reactor concentration profiles, the L/V transport delay in the reactor, and the insensitivity of the control variable to a 10-radian-per-second sinusoid. This proves that the separator will filter out high frequency disturbances.

Run 2 proves that the step input disturbance does not result in instability, but establishes a new set of steady-state operating conditions. The function of the control system, of course, is to maintain the design outflow of E in spite of this change.

Adding proportional control (run 4), indicates that a gain of 10 will yield a steady-state off-set whose magnitude is much less than that obtained without proportional control.

Increasing the gain to 20 (run 5), results in periodic response (period equal to 9 sec) indicating that the system is at or approaching its critical gain (-180° phase shift). Applying the Ziegler-Nichols‡ criteria for a proportional plus integral controller resulted in approximate controller settings of $K_c = 10$ and $\tau_r = 5$ seconds.

‡$K_c = 0.45$ (CRITICAL GAIN), $\tau_r = 0.8$ (PERIOD OF OSCILLATION AT CRITICAL GAIN) – *in this case,* $K_c = 10$, $\tau_r = 5$ *sec.*

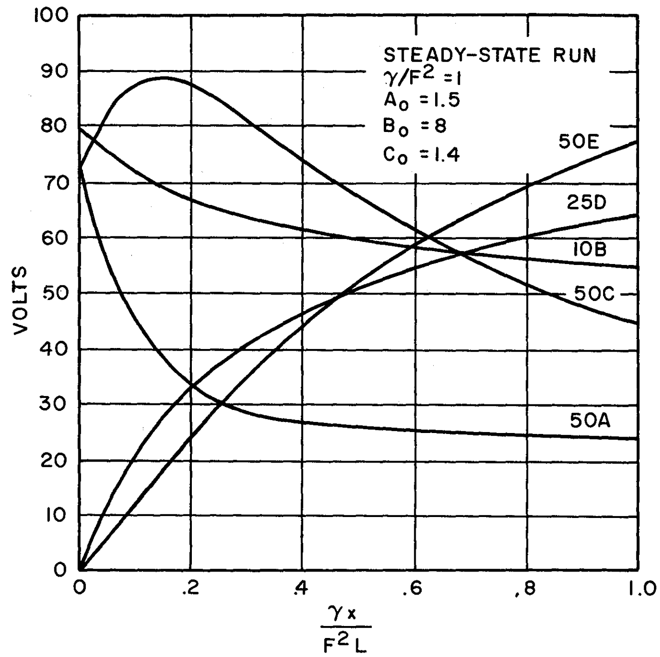

Figure 9: Steady-State Concentrations Versus Reactor Length Variable

System response to these settings, show in Figure 7, is reasonable, and the controlled variable returns to its set-point in about 20 sec. Further refinements could have been attempted but these results were adequate and satisfied the objectives of the study.

It should be noted that the response obtained in run 7 is typical of that expected for a load change imposed on a controlled system.

Run 6 justifies undertaking a study of this type since it proves that unstable control settings exist. Failure to maintain proper control can of course lead to:

1. Increased operating costs due to high recycle rates, low production of product, etc.

2. Potential danger to operating personnel due to toxic materials, fires, etc., which could result from a run-away or improperly controlled system,

which are typical motivations for applying computational techniques to chemical process problems.

The advantages of simulating this system on a hybrid computer are worthy of comment. A parallel simulation of the reactor equations would have required a complete 120-amplifier, 231-R computer to perform this simulation; the analog requirement for the hybrid simulation was less than 50 amplifiers. If the reactions were exothermic and thermal equations were required in the simulation, a conventional all-analog approach would have required two complete 231-R computers. Only one analog computer would be required in the hybrid simulation of the system if the thermal equations were added. Therefore, one advantage of the hybrid computer simulation of partial differential equations is a definite saving of analog components over the conventional parallel approach.

Table 3: Summary of Computer Results

Figure No.	Run No.	Description
9	1	Typical steady-state concentration profiles of components A thru E versus reactor length
10	2	System response to a step change (no control system)
11	3	System response to a sinusoidal disturbance (no control system)
12	4	System response to a step change with proportional control; $K_c=10$
13	5	System response to a step change with proportional control, $K_c=20$
14	6	Example of system instability with improper control settings
15	7	System response to a step change with proportional plus integral control; $K_c = 10$, $\tau_r = 5$

REFERENCES

(1) Rijnsdorp, J.E., Vichnevetsky, R., and van de Vusse, J.C. "Application of the Analogue Computer in the Study of the Esterification of Terephthalic Acid", "Analog Computation Applied to the Study of Chemical Processes", edited by Vichnevetsky, R.; Gordon and Breach, Science Publishers, Inc., New York, New York.

(2) Vichnevetsky, R., "Method of Characteristics in the Hybrid Solution of First Order Partial Differential Equations", ECC Report No. 60, Electronic Associates, Inc.

(3) "The Simulation of Transport Delay with the HYDAC Computing System", EAI Applications Reference Library, Application Study: 1.3.7h.

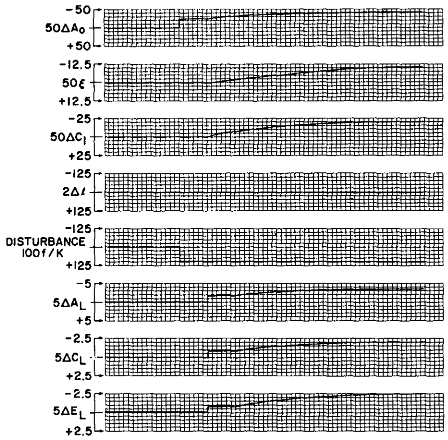

Figure 10: Run 1, System Response to Step Input (No Control System)

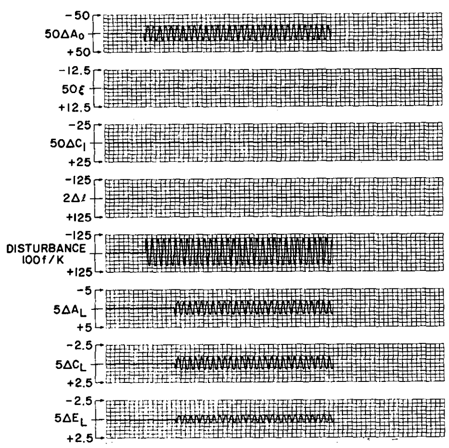

Figure 11: Run 3, System Response to Sinusoidal Input (No Control System)

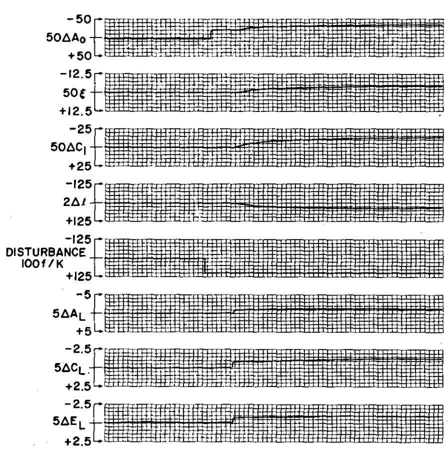

Figure 12: Run 4, System Response to Step Input (K_c = 10)

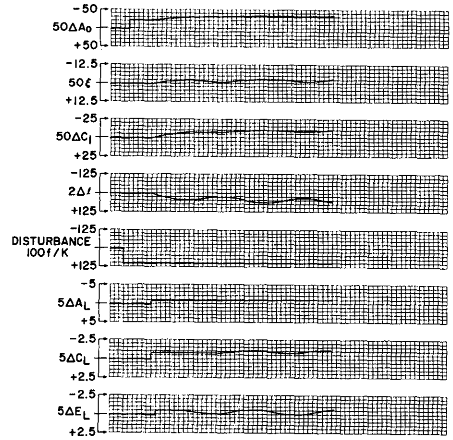

Figure 13: Run 5, System Response to Step Input (K_c = 20)

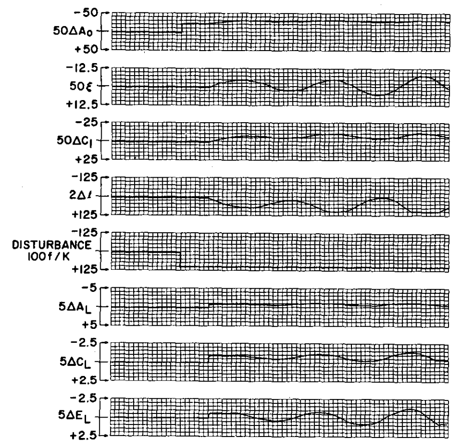

Figure 14: Run 6, System Behavior with Improper Control Settings

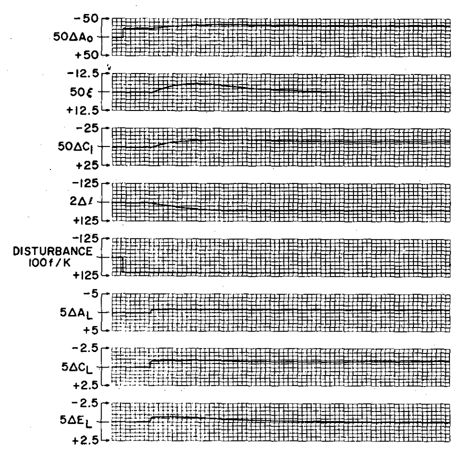

Figure 15: Run 7, System Response to Step Input (K_c = 10, Tr = 5)

APPENDIX A

COMPUTER DIAGRAMS AND PROGRAMS

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POTENTIOMETER ASSIGNMENT SHEET — SHEET 1 OF 2

POT. NO.	STATIC SETTING CHECK RUN NO.	SETTING RUN NO.	SETTING RUN NO.	SETTING RUN NO.	NOTES	PARAMETER DESCRIPTION $\beta = 10$	POT. NO.
P00							P00
Q00	0.1000					$1/\beta$	Q00
P01							P01
Q01	0.7400					$10k_1/\beta$	Q01
P02							P02
Q02						CONSTANT	Q02
P03	0.5000						P03
Q03							Q03
P04							P04
Q04							Q04
5							P05
Q05							Q05
P06	0.5000					$E_0/2$	P06
Q06	0.1000	0.0296				$4k_4/\beta$	Q06
P07							P07
Q07							Q07
P08							P08
Q08							Q08
P09	0.4000	0.3200				$4k_3/\beta$	P09
Q09							Q09
P10							P10
Q10	0.8000					$B_0/10$	Q10
P11							P11
Q11							Q11
P12							P12
Q12							Q12
P13							P13
3	0.1992	0.2383				$A_{LS}/2$	Q13
P14							P14
Q14	0.5000	0.2000				$10k_2/\beta$	Q14

POT. NO.	STATIC SETTING CHECK RUN NO.	SETTING RUN NO.	SETTING RUN NO.	SETTING RUN NO.	NOTES	PARAMETER DESCRIPTION	POT. NO.
P15	0.2500					CONSTANT	P15
Q15							Q15
P16							P16
Q16							Q16
P17							P17
Q17							Q17
P18							P18
Q18	0.3991	0.4434				$C_{LS}/2$	Q18
P19	0.1000					CONSTANT	P19
Q19							Q19
P20							P20
Q20							Q20
P21							P21
Q21							Q21
P22							P22
Q22							Q22
P23							P23
Q23							Q23
P24							P24
Q24							Q24
P25							P25
Q25							Q25
P26							P26
Q26							Q26
P27							P27
Q27							Q27
P28							P28
Q28	0.6700	0.7061				$E_{LS}/2$	Q28
P29	0.3750					$E^\circ/2$	P29
Q29							Q29

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POTENTIOMETER ASSIGNMENT SHEET — SHEET 2 OF 3

POT. NO.	STATIC SETTING CHECK RUN NO.	SETTING RUN NO.	SETTING RUN NO.	SETTING RUN NO.	NOTES	PARAMETER DESCRIPTION	POT. NO.
P30	0.1000					$\Delta H_1^\circ/2$	P30
Q30	0.5000					$1/\tau$	Q30
P31	0.7500					$\Delta C_1^\circ/2$	P31
Q31	0.5000					$1/\tau$	Q31
P32	0.5000					$1/\tau$	P32
Q32	0.7000					$C_{0s}/2$	Q32
P33							P33
Q33	0.5000					$1/\tau$	Q33
P34							P34
Q34							Q34
P35							P35
Q35	0.5000					$1/\tau$	Q35
P36	0.3000					$\alpha \mathcal{E}_1^\circ - \mathcal{E}$	P36
Q36	0.5000					$1/\tau$	Q36
P37							P37
Q37							Q37
P38							P38
Q38							Q38
P39	0.9000	0.5000				$C_m/4$	P39
Q39							Q39
P40	0.2000					$(\mathcal{E}_2^\circ - \Delta E^\circ)/50$	P40
Q40							Q40
P41							P41
Q41							Q41
P42							P42
Q42							Q42
P43							P43
Q43							Q43
P44							P44
Q44	1.0000	0.1000				$10/K_r$	Q44

POT. NO.	STATIC SETTING CHECK RUN NO.	SETTING RUN NO.	SETTING RUN NO.	SETTING RUN NO.	NOTES	PARAMETER DESCRIPTION	POT. NO.
P45							P45
Q45	0.1000	0.2500				$\|K\|/2$	Q45
P46							P46
Q46							Q46
P47							P47
Q47							Q47
P48							P48
Q48	0.7500					$A_{0s}/2$	Q48
P49							P49
Q49							Q50
Q50							Q50
Q51							Q51
Q52							Q52
Q53							Q53
Q54							Q54
Q55							Q55
~~Q56~~	0.1000				P57 } HAND-SET	$1/T_D$	~~Q56~~
~~Q57~~	0.2500				P58 } POTS	$1/K_c$	~~Q57~~
~~Q58~~	0.5000				P59 }	$1/T_r$	~~Q58~~
Q59							Q59
Q60	0.1000					$\omega/10$	Q60
Q61	0.1000					$\omega/10$	Q61
Q62							Q62
Q63							Q63
Q64							Q64
Q65							Q65
Q66							Q66
Q67							Q67
Q68							Q68
Q69							Q69

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231-R AMPLIFIER ASSIGNMENT SHEET

BOARD ____________

Amplifier Number	Feedback / Connection	OUTPUT: Function, and, or, variable	Check Point	Static Test
00	I	100(1-y)	-10	100
01	I	50A	-36.85	75
02	S	-50A		-75
03	HG	$10(B_0-B)$		10
04	HG	5AB		52.5
05	S	25D		25
06	I	50E	5.76	50
07	S	-50E		-50
08	HG	12.5 ED		12.5
09	HG	- 12.5 CD		-5
10	S	10B		70
11	S	-10B		-70
12	T/S	$-50A_L$		-75
13	T/S	$50\Delta A_L^*$		55.08
14	HG	-5BC		-14
15	S	-25D		-25
16	S	-50C		-20
17	T/S	$-50C_L$		-20
18	T/S	$50\Delta C_L^*$		-19.91
19	S	50C		20
20				
21				
22	T/S	$-50E_L$		-50
23	T/S	$50\Delta E_L^*$		-17
24	S	$50\Delta H_0$		20
25				
26				
27	T/S	$-50A_0$ ①		-95
28	T/S	$-50C_0$ ①		-44.6
29				

Amplifier Number	Feedback / Connection	OUTPUT: Function, and, or, variable	Check Point	Static Test
30	I	$-50\Delta A_1$	-45	-10
31	I	$-50\Delta C_1$	-12.5	-75
32	S	$50(\Delta C_1 + C_M \Delta \ell/100)$		24.6
33	S	$-50C_{0s}$		-70
34	HG	$10(\varepsilon_1-\varepsilon)$		-37.5
35	I	50ε or $-50\Delta E_1$	-31.25	-37.5
36	I	$100(\alpha\varepsilon_1-\varepsilon)$	37.5	30
37	HG	CONSTANT, 10 ST		10
38	S	$-50A_{0s}$		-75
39	S	$-2\Delta\ell$		56
40	I	$2(\Delta\ell-\varepsilon_2)$	-15.2	-20
41				
42	S	$-10\varepsilon_1$		45
43	HG	$2\varepsilon_2$		-36
44	HG	$2(\Delta\ell/K_r-\varepsilon_2)$		30.4
45				
46				
47				
48	S	$50(\Delta H_1+f)$		20
49				
50				
51				
52				
53				
54				
55	XY0 INV			
56	INV			
57	XY5 INV			
58	INV			
59				

Amplifier Number	Feedback / Connection	OUTPUT: Function, and, or, variable	Check Point	Static Test
60	I	100 Sin ωt	100	-100
61	I	100 Cos ωt	100	100
62	S	-100 Cos ωt		-100
63				
64				
65	XY1 INV			
66	INV			
67				
68				
69				
70				
71				
72				
73				
74				
75	XY2 INV			
76	INV			
77				
78				
79				
80				
81				
82				
83				
84				
85	XY3 INV			
86	INV			
87				
88				
89				

Amplifier Number	Feedback / Connection	OUTPUT: Function, and, or, variable	Check Point	Static Test
90				
91				
92				
93				
94				
95	XY4 INV			
96	INV			
97				
98				
99				

NOTES

① CHANGE STATE OF ELECTRONIC COMPARATOR #00 TO READ CORRECT OUTPUT

M353

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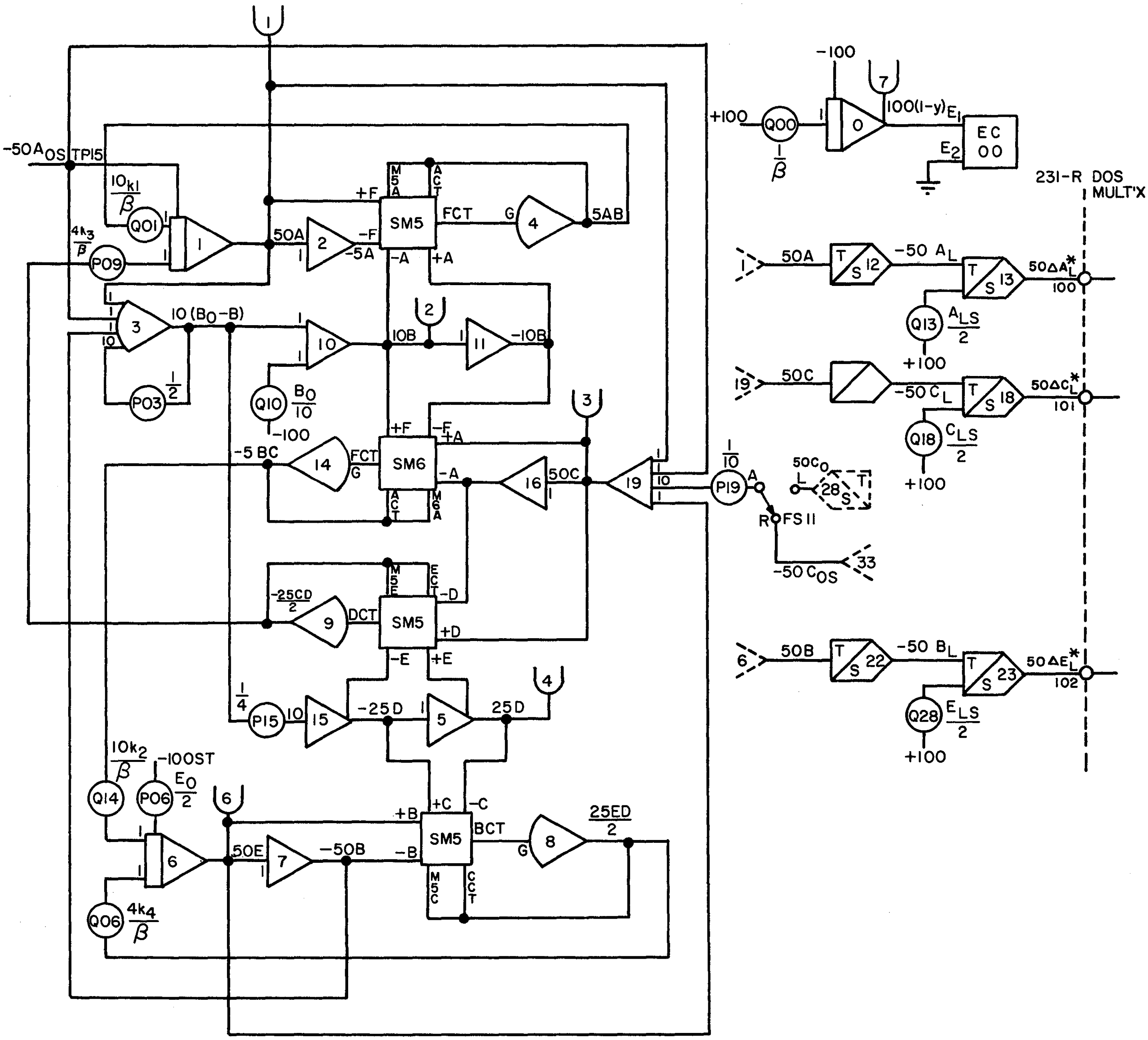
BY ______ SUBJECT TUBULAR REACTOR DOS DIAGRAM SHEET NO. 1 OF 1
DATE ______ PROJ. NO. ______



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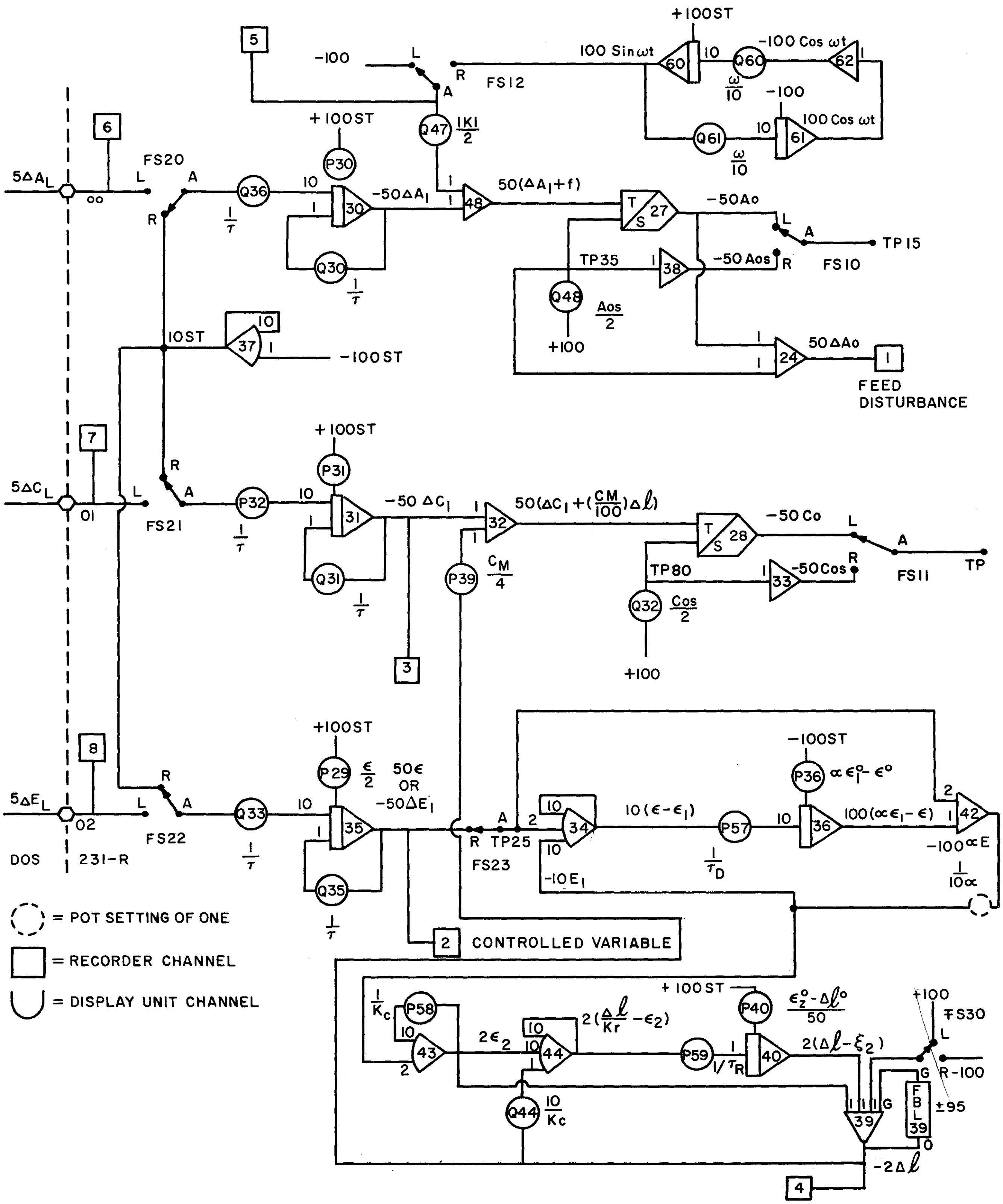
BY ________ SUBJECT TUBULAR REACTOR ANALOG COMPUTER DIAGRAM SHEET NO. 1 OF 2
DATE ________ PROJ. NO. ________



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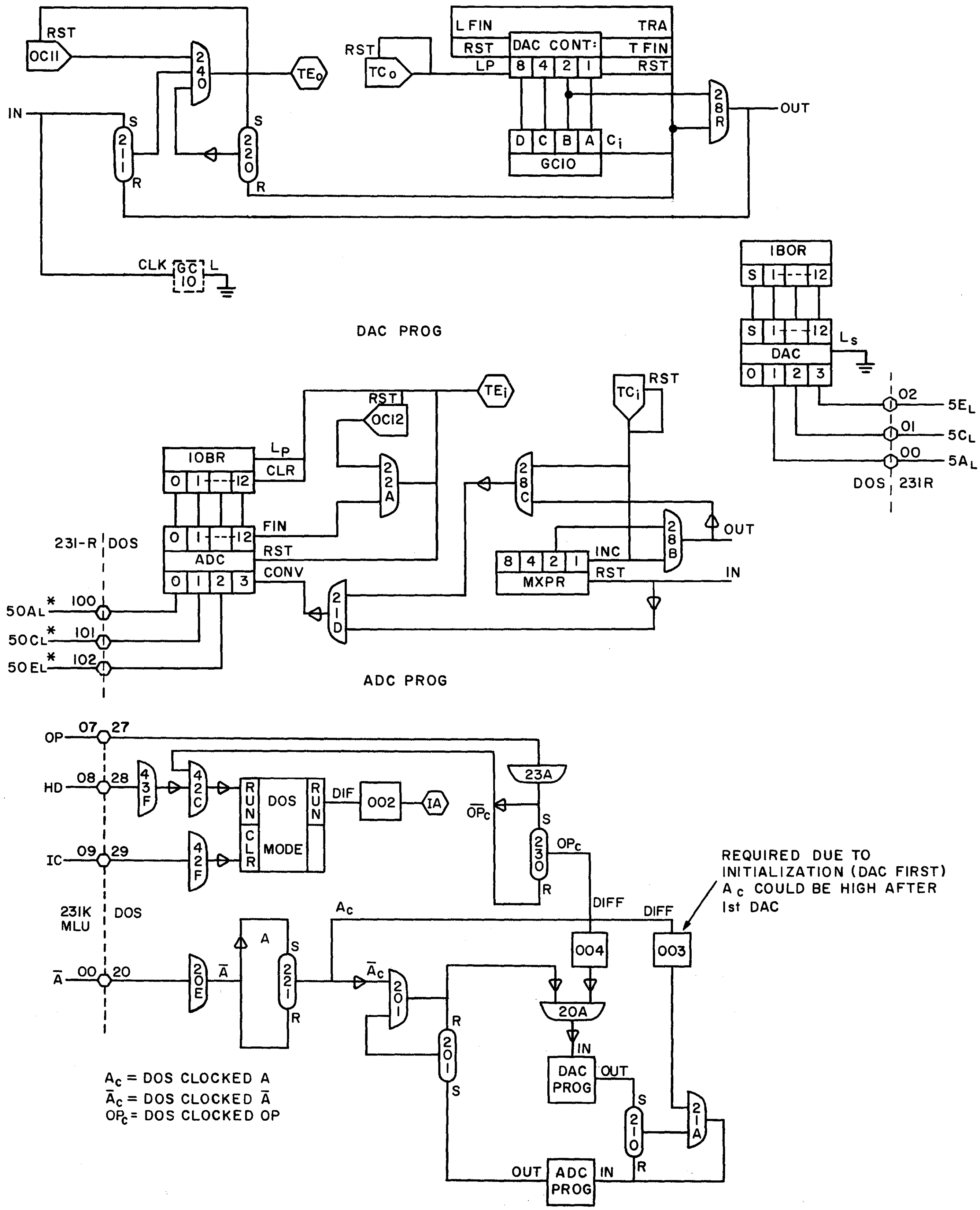
RESEARCH AND COMPUTATION DIV.
BOX 582, PRINCETON, N. J.

BY ______ DATE ______

SUBJECT TUBULAR REACTOR ANALOG COMPUTER DIAGRAM

SHEET NO. 2 OF 2 PROJ. NO. ______



RUN #	FUNCTION SWITCH POS. SWITCH NO 11	12	13	20	21	22	23	30
1. STATIC CHECK	R	R	R	R	R	R	R	L/R (1)
2. STEADY STATE CONCENTRATION PROFILES	R	C	R	C	C	C	C	C
		L - STEP CHANGE						
		R - SINUSOIDAL INPUT						
3. SYSTEM RESPONSE	R	C	R	L	L	L	C	C
TO STEP----------		L						
AND SINUSOID----------		R						
(NO CONTROL SYSTEM)								
4. SYSTEM RESPONSE PROPORTIONAL CONTROL	R	L	R	L	L	L	R	C
ONLY----------		K_C = 10		P58 = 0.1000				
STEP INPUT----------		K_C = 20		P58 = 0.0500				
5. SYSTEM RESPONSE	R	L	R	L	L	L	R	C
P&I CONTROL----------		K_C = 10		P58 = 0.1000				
STEP INPUT----------		τ_r = 5		P59 = 0.2000				

(1) SET FBL #39 IN IC MODE TO ±95 VOLTS USING FS 30 - RETURN TO "C" POSITION

MLG SET-UP

INTEGRATOR PATCHING & PUSH BUTTON SETTINGS

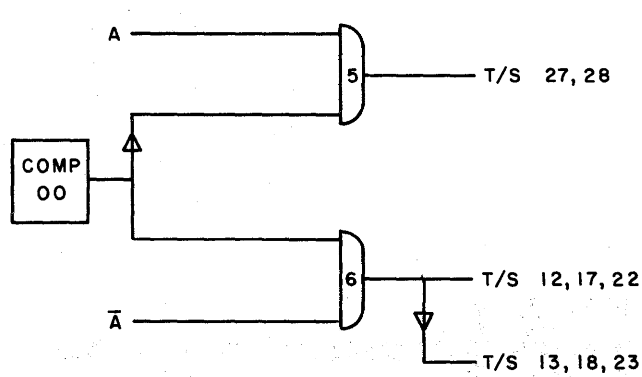
PATCHING MS ⟶ ES
.01 ⟶ F
N ⟶ 1
A/Ā SIGNALS TO INTEGRATORS
0, 1, & 6

PUSH-BUTTONS

	REAL TIME	HSRO
MASTER	N-SEC	N-MS
30-59	N-SEC	N-SEC
60-99	N-SEC	N-SEC

TIMING - OPR TIME - 12 MS; RST TIME - 8 MS

MLG PATCHING



```
          REL
A         BSS     1ØØØ          RESERVE MEMORY BLOCK
VW        OCT     77777777
NK        OCT     3             # OF POINTS PER TRASFER
V         DEC     45Ø
FW        OCT     1
INIT      ITC     '4ØØØØ        ENABLE INTERRUPTS
          LDA     TRCA          LOAD IA TRAP CELL
          STA     IATC
          LDA     TRCA&1        LOAD IA TRANSFER
          STA     IATC&1
STRT      LDX     -15Ø,1
          LDX     -45Ø,2
          LDA     SS1
          STA     A&45Ø,2
          LDA     SS2
          STA     A&451,2
          LDA     SS3
          STA     A&452,2
          ADX     3,2
          JXI     STRT&2,1
          LDA     FW
          STA     N
          LDA     CC
          ADD     V
          STA     AA            INITIAL LO & # OF POINTS
KC        LDA     V
          ERA     VW
          SUB     FW
          TAX     ,1            # OF POINTS COMPLEMENTED
          STX     QF,1          STORE INDEX REGISTER 1 IN QF
KK        STX     VF,1          STORE INDEX REGISTER 1 IN VF
          LDA     AA
          ADD     VF
          STA     AAA           LOCATION OF POINT
          LDA*    AAA           INDIRECT ADDRESSING
          OCP     2             ENABLE OUTPUT WORD CHANNEL
          OCP     '1Ø11         SET OCP LINE 11
          SKS     '11ØØØ        OUTPUT WORD CHANNEL READY
          JMP     *&2           YES
          JMP     *-2           NO
          OTA                   TRANSFER D TO A
          LDA     N
          SUB     NK            # OF POINTS PER TRANSFER
          JZE     GG            N-NK=Ø  YES
          LDA     N             NO
          ADD     FW            INCREMENT COUNTER BY 1
          STA     N
          JXI     KK,1          INCREMENT INDEX REGISTER 1
          HLT     '3415         ERROR
GG        LDA     QF
          TAX     ,1            TRANSFER CONTENTS OF QF INTO INDEX REGISTER 1
          LDA     FW
          STA     N
QP        STX     VF,1          STORE INDEX REGISTER 1 IN VF
          LDA     AA            SET UP FOR A TO D
          ADD     VF
          STA     AAA
          OCP     1             ENABLE INPUT WORD CHANNEL
          OCP     '1Ø12         SET OCP LINE 12
          SKS     '12ØØØ        INPUT WORD CHANNEL READY
          JMP     *&2           YES
          JMP     *-2           NO
          INA                   TRANSFER A TO D
          STA*    AAA
          LDA     N
          SUB     NK            # OF POINTS PER TRANSFER
          JZE     QV            N-NK=Ø YES
          LDA     N             NO
          ADD     FW            INCREMENT COUNTER BY 1
          STA     N
          JXI     QP,1          TEST AND INCREMENT INDEX REGISTFR 1
          HLT     '1266         ERROR
QV        LDA     FW
          STA     N             RESTORE COUNTER TO 1
          JXI     KK-1,1
          JMP     KC
CC        PZE     A
AA        OCT     Ø
AAA       OCT     Ø
VF        OCT     Ø
N         OCT     1
QF        OCT     Ø
SS1       DEC     Ø
SS2       DEC     Ø
SS3       DEC     Ø
TRCA      JRT     IATC&1
          PZE     STRT
IATC      EQU     3
          END
```