EAI®

HYBRID COMPUTATION

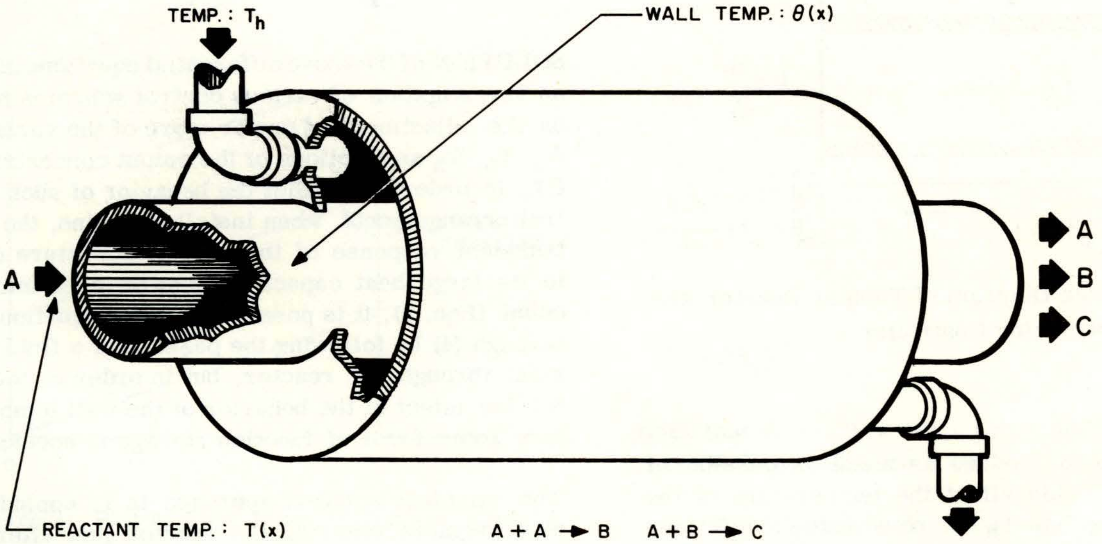
Chemical/Petro-Chemical

Application Study: 6.4.1h

DEVELOPMENT OF A PROGRAM FOR THE HYBRID SIMULATION OF A TUBULAR REACTOR

ABSTRACT: The conceptual details of the hybrid solution of the equations necessary for the study of the transient behavior of a chemical tubular reactor are discussed in the following material. This behavior is considered under various conditions when an optimizing controller is installed. The analog and digital operations available in the EAI HYDAC* system are utilized to advantage to solve the partial differential equations which describe the flow of reacting material down the length of the reactor.

The solutions to these equations are based on a function iteration scheme utilizing digital function storage to reduce the amount of analog non-linear equipment required through the time-sharing of analog operations. The advantages of analog simulation over purely numerical solutions are retained in evaluating the stability of the control scheme in this way.



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STATEMENT OF THE PROBLEM

The problem used as a basis for discussion is concerned with the investigation of the control characteristics of a chemical reactor under various operating conditions for purposes of evaluating a particular optimizing control scheme. Major components of the physical system are shown in the block diagram of Figure 1.

A stream of reacting material flows through the reactor at a fixed velocity V. At the reactor input a feed of reactant A, with molar concentration A_o is introduced. A_o is, in general, a function of time t. Material A is assumed to undergo an intermediate reaction.

$$A + A \rightarrow B$$

at a temperature dependent rate, $R = f(T)$, while the intermediate B reacts with A at a rate K, to produce a product C such that

$$A + B \rightarrow C$$

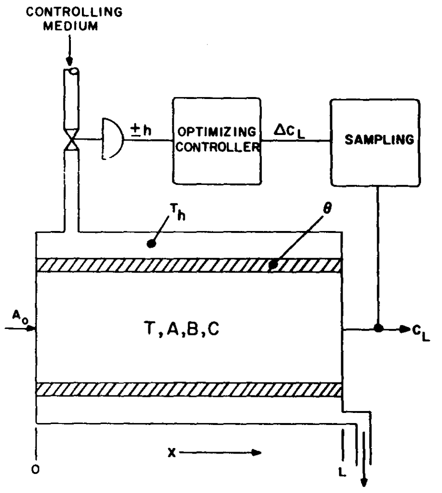

Figure 1. Block Diagram of Tubular Reactor with Optimizing Controller

It is desired to produce as much as possible of product C. To this effect the temperature of the controlling medium T_h can be adjusted to influence the reactor wall temperature θ which, in turn, influences the temperature T of the reacting material and thus the reaction rate.

EQUATIONS based on material and heat balances can be written taking into consideration the following simplifying assumptions:

1. Temperature T_h is constant over the length of the reactor.
2. Temperature θ has no axial diffusion.
3. Only convection and no diffusion take place in the reacting material.

Appropriate equations are:

$$\frac{\partial A}{\partial t} + V\frac{\partial A}{\partial x} = -2RA^2 - K\,AB \qquad (1)$$

$$\frac{\partial B}{\partial t} + V\frac{\partial B}{\partial x} = RA^2 - K\,AB \qquad (2)$$

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} = K\,AB \qquad (3)$$

$$a_1\left(\frac{\partial T}{\partial t} + V\frac{\partial T}{\partial x}\right) = -b_1RA^2 + b_2(\theta - T) \qquad (4)$$

$$a_2\frac{\partial \theta}{\partial t} = b_2(T - \theta) + b_3(T_h - \theta) \qquad (5)$$

$$R = f(T) \qquad (6)$$

$$x = 0 \rightarrow A = A_o;\ B = C = 0;\ T = T_o \qquad (7)$$

$$x = L \rightarrow C = C_L \qquad (8)$$

SOLUTION of the above differential equations allows an investigation of various control schemes based on the adjustment of one or more of the variables A_o, T_o, T_h as functions of the output concentration C_L. In order to predict the behavior of such control arrangements, when installed on line, the slow transient response of the wall temperature θ due to its large heat capacity has to be taken into account (Eqn. 5). It is possible to solve equations (1) through (4) by following the passage of a fluid segment through the reactor, but in order to account for the effect of the behavior of the wall temperature some form of function storage is necessary.

The simplest solution approach is to consider a new segment entering the reactor just after the previously considered segment has left it, so that only one segment is considered at a time. Alternately, it is possible to consider more closely spaced segments (at distance L/n) and to carry out the analog solution n times faster.* However, for clarity in explanation, the first, and simplest, approach will be used.

Referring to the diagram of Figure 2 the solution scheme chosen would be equivalent to solutions performed along the flow lines (concentration lines) which amounts to a change of independent variable. This new variable is defined as

$$t' = t - \frac{x}{V}$$

such that the flow lines now become lines of constant t. Performing the change in variable results in

$$\frac{\partial}{\partial t} + V\frac{\partial}{\partial x} \text{ being changed to } V\frac{\partial}{\partial x}$$

and

$$\frac{\partial}{\partial t} \text{ being changed to } \frac{\partial}{\partial t'}$$

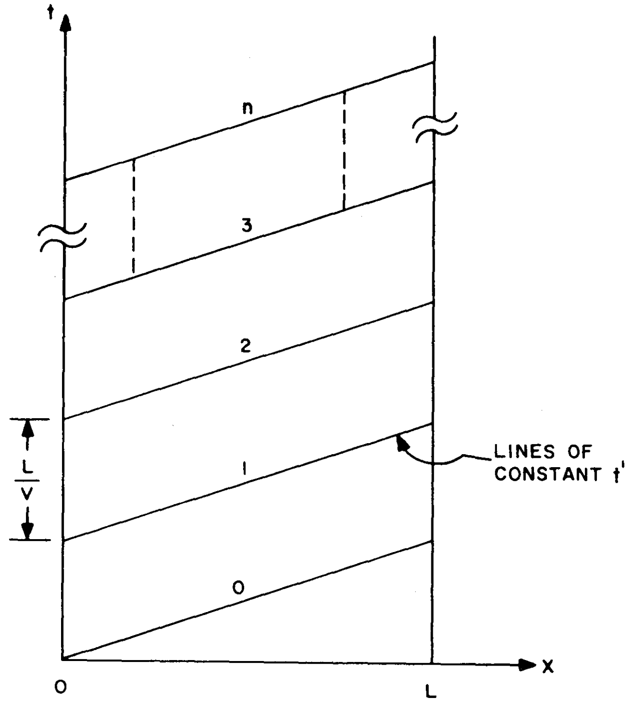

Figure 2. Plot of Flow Lines in Tubular Reactor

Thus, equations (1) through (4) are integrated at constant t' with x changing from O to L in one analog run. On the nth run, $t' = t'_n = nL/V$. Equation (5) is approximated by the finite-difference expression

$$a_2 \frac{\theta_n(x) - \theta_{n-1}(x)}{\frac{L}{V}} = b_2(T_n - \theta_n) + b_3(T_{h_n} - \theta_n) \quad (9)$$

Both $\theta_n(x)$ and $T_{h_n}(x)$ are defined on a flow line

$$x = x$$
$$t = \frac{nL + x}{V} \qquad 0 \leq x \leq L \qquad (10)$$

For θ_n this implies that the initial wall temperature distribution, $\theta_0(x)$, be given on the n = 0 flow line. For T_{h_n} it can be assumed, thanks to the sluggish response of the wall temperature, that T_h is constant in x for constant t', or

$$T_{h_n} = T_h(t'_n) = T_h(t_n) \qquad (11)$$

THE ANALOG PROGRAM, whose structure is shown in Figure 3, would then be required to solve the following equations (with run time proportional to x):

$$V\frac{dA_n}{dx} = -2RA_n^2 - KA_nB_n \qquad (12)$$

$$V\frac{dB_n}{dx} = RA_n^2 - KA_nB_n \qquad (13)$$

$$V\frac{dC_n}{dx} = KA_nB_n \qquad (14)$$

$$a_1V\frac{dT_n}{dx} = -b_1RA_n^2 + b_2(\theta_n - T_n) \qquad (15)$$

$$\frac{a_2V}{L}(\theta_n - \theta_{n-1}) = b_2(T_n - \theta_n) + b_3(T_{h_n} - \theta_n) \qquad (16)$$

$$R = f(T_n) \qquad (17)$$

Note that A + 2B + 3C = Constant, which makes it possible to calculate B by

$$B_n = 1/2\,(A_{o_n} - A_n - 3C_n) \qquad (18)$$

where $A_{o_n} = A_n(0)$, the input concentration of material A ($x = 0$) at time $t = t_n$. At the end of an analog run the output ($x = L$) concentration C_{n_L} is

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*A time delay of n samples must then be placed on C_L to obtain it in compatible time with the input.

obtained at time $t = t_n + \frac{L}{V} \cdot C_{n_L}$ is obtained simultaneously in real time with $A_{o,\ n+1}$, $T_{h,\ n+1}$ and and $T_{o,\ n+1}$ (the initial condition for T_n on the n+1 run).

The function $\theta_{n-1}(x)$ obtained on the previous run is stored in the HYDAC memory. While it is being read out $\theta_n(x)$ is stored in its place for use in the following run. A function iteration is thus performed, an operation for which a standard "cookbook" program has been formulated. The structure of such a program is shown in Figure 4.

In this program the "iteration control" calls for successive analog runs and insures the timing for function storage. The converters communicate with the serial memory via a buffer. "Conversion timing" calls for a complete cycle of sampling, A/D conversion, transfer to buffer, writing into the memory, reading out the memory, loading the D/A conversion, and interpolating.

THE OPTIMIZING CONTROLLER attempts to maximize production of component C by acting on variable T_h. It operates on successive samples of the output concentration C_{L_n} taken at time intervals

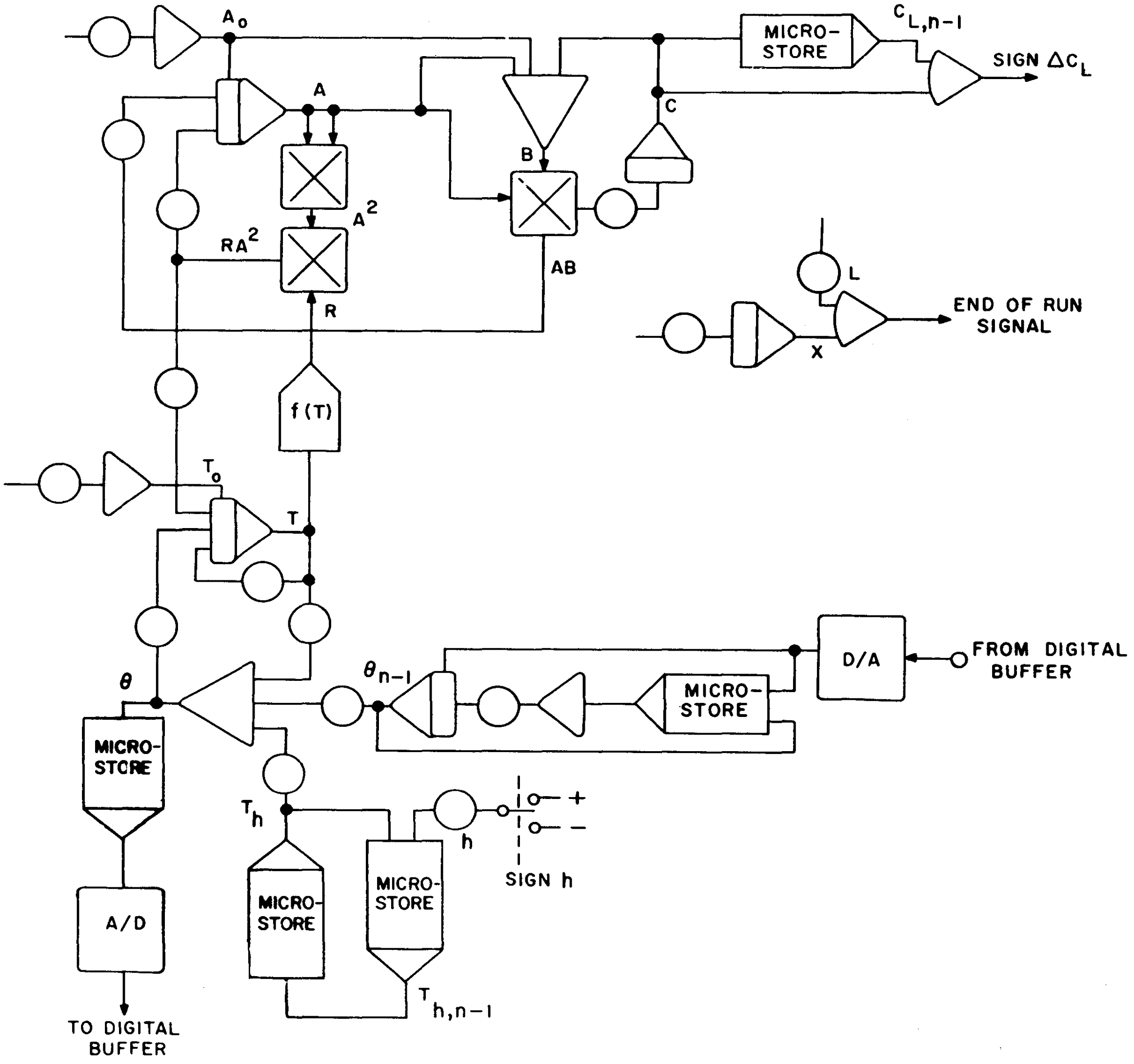


Figure 3. General Structure of Analog Program Simulating Reactor and Controller

L/V. The new sample is compared with the previous one, and if an increase in C_L is detected, T_h is changed up or down by an amount h. When a decrease in concentration is sensed a counter is advanced. When this counter carries out, indicating that T_h is moved in the wrong direction, the direction is reversed and the counter is cleared. Due to the system time lags between T_h and C_L this arrangement is extremely critical from the point of view of stability. This is what makes the analog simulation mandatory. Due to the non-linearity of the equations the transient behavior and stability of the system will depend on the values of the input concentration A_0 and temperature T_0 which vary in time. The "stable" situation corresponds to a steady "hunting" oscillation across the maximum production point. In general, any optimizing controller must have such an oscillation since under entirely steady conditions it is impossible to know whether a higher yield can be obtained or not.

A small number of digital logic building blocks are assembled to provide the logic for the controller. Their function is to switch Microstore components at every run and determine the sign of the correction made to T_h, i.e., h.

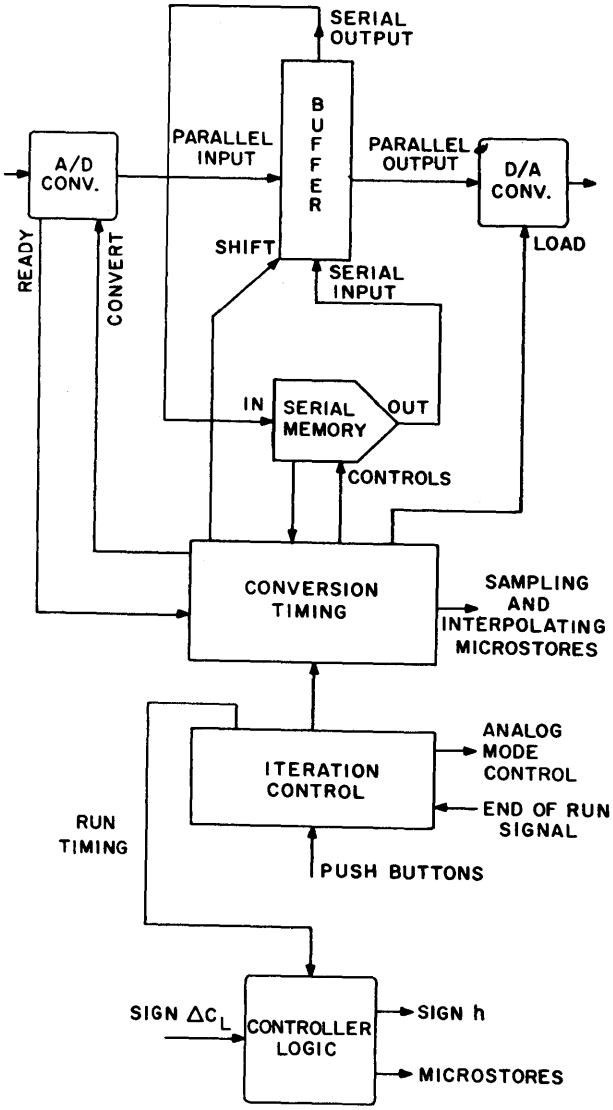


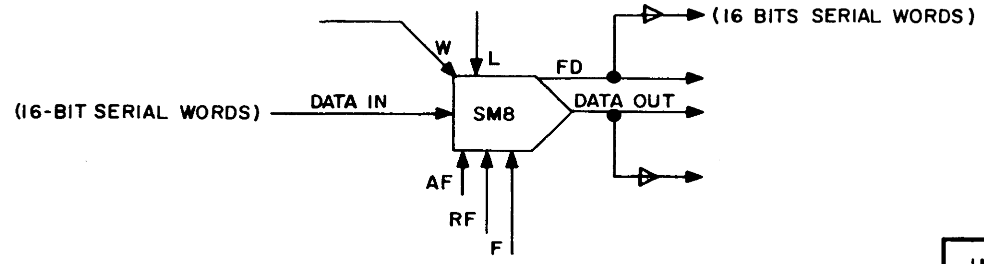
Figure 4. Structure of General Function Iteration Program for HYDAC

APPENDIX

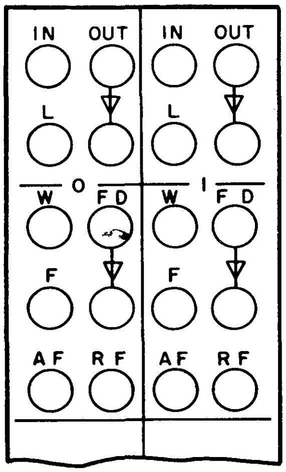
The Serial Memory Units

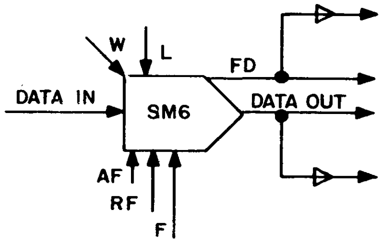
The Serial Memory Unit used to store $\theta_n(x)$ in the function iteration program may be described as a device for storing a table of numbers, or digital "words", that represent a sequence of sampled values of an analog signal. All numbers are stored as serial binary words of 16 bits each. Each unit has its own control circuitry for writing, addressing, and reading the tabular values in the proper sequence. Each size of memory unit (SM-8, SM-6, SM-4) has a different Read/Write Cycle Rate. This rate is the maximum number of data words per second that, in the normal mode of operation, can be written into and read from memory in sequence. Any lower rate may be used, as may be required by the analog-to-digital conversion rate or the analog sampling rate. The entire table of numbers can be read rapidly from memory in a single Read/Write cycle, but, in normal use a single word is selected from the table and a new word written into the same position in one cycle, and the selected position is moved to the next in the sequence.

Figures 5 and 6 illustrate the characteristics of the Serial Memory units. The tables of data

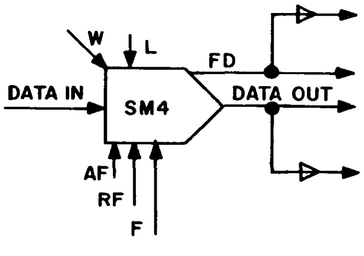


(A) SERIAL MEMORY, SM8 (2^8 OR 256 WORDS OF STORAGE)

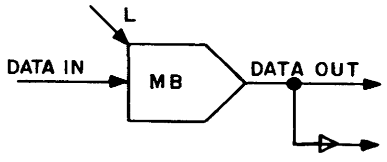




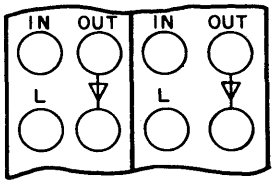
(B) SERIAL MEMORY, SM6 (2^6 OR 64 WORDS OF STORAGE)



(C) SERIAL MEMORY, SM4 (2^4 OR 16 WORDS OF STORAGE)



(D) MEMORY BUFFER (I WORD OF STORAGE)



PATCH PANEL LAYOUT

Figure 5. Digital Memory Unit for the Analog Computer

words are addressed by a moving index "flag". The flag is moved forward (left-to-right in Figure 6) one step each Read/Write Cycle during which the AF (advance flag) control line is energized. The flag may be moved in the reverse direction, one step per cycle, by the RF (reverse flag) control line. If the AF line is energized all the time, the entire table will be addressed at the maximum Read/Write cycle rate (512 cps, 2048 cps, or 8192 cps) and thus the flag will sweep the entire function table in the minimum sweep time (0.5 sec., 31 millisec., or 2 millisec.). If the flag is moved beyond the #256 position it steps to position #1, in the SM-8.

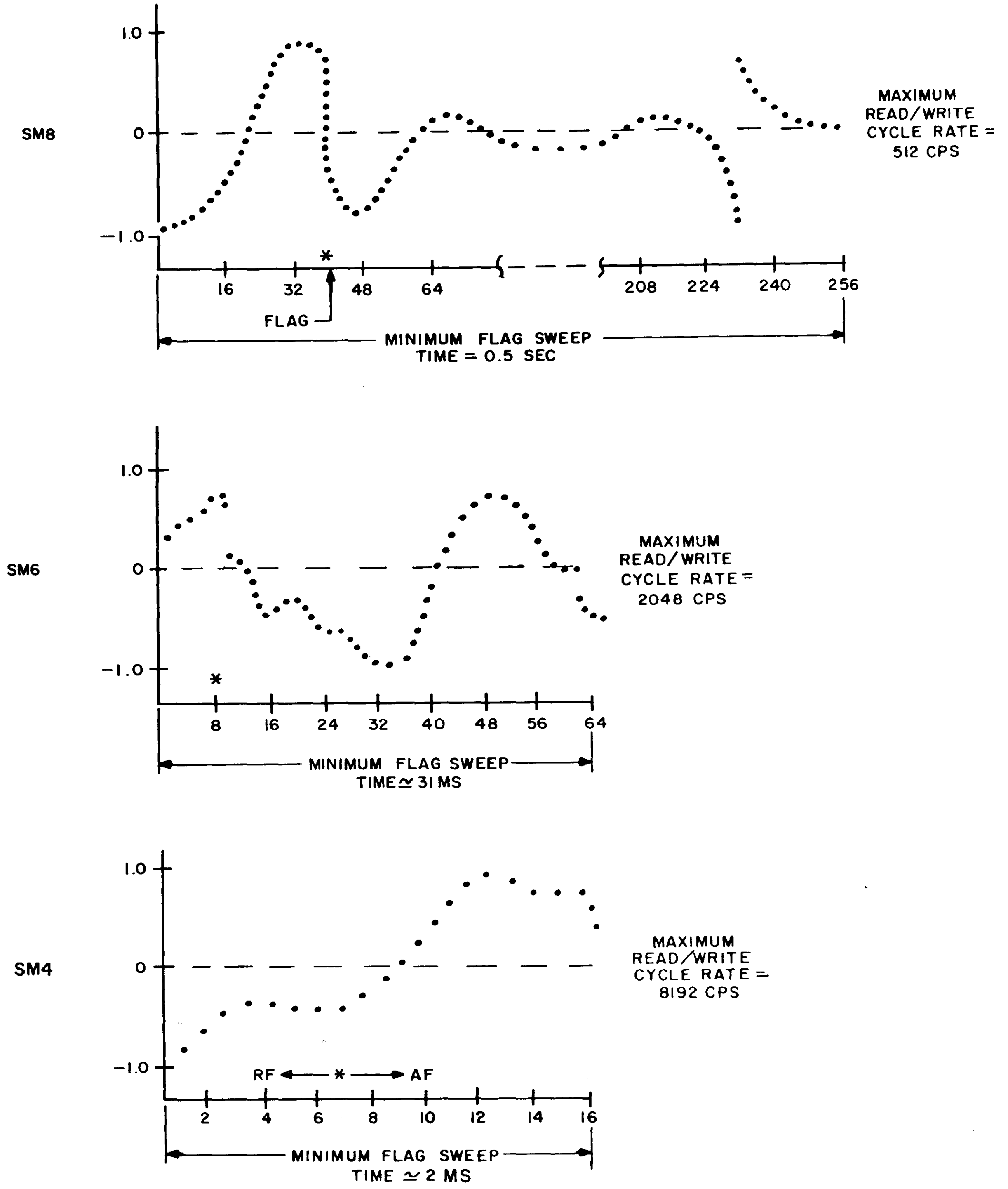


Figure 6. Characteristics of Serial Memory Units

The tabular data words selected by the moving flag are "read out" by forming the logical product (with an AND gate) of the data output and the FD control line. The FD (flagged-data) line provides an enabling signal long enough to pass the serial bits of the indexed or flagged word, once each Read/Write cycle. Thus reading from the memory is possible without employing any specific "read" control signal.

New data is written into the memory at the flagged position whenever the W control line is energized and the new serial data is available at the input.

The F (flags) control line permits the simultaneous use of as many as three independent flags in a Serial Memory Unit. Thus in special programs it is possible to move these flags back and forth independently to select the desired position for reading or writing. The L (load) control line is similar in function to the W line but is used to prestore or initialize the memory unit with special data, such as initial flag locations.

The range of memory sizes and maximum Read/Write cycle rates satisfies a wide range of problem requirements. For transport delay programs the required minimum sampling rate and the delay time may determine the choice of memory unit. For function storage and generation the SM-8 unit will handle a 256-point function in as short a period as 0.5 second. Thus, for real time programs the SM-8 is very satisfactory; however, for high speed repetitive programs the SM-6 is better since it can be used with a time base as short as 31 milliseconds. The SM-4 is useful mostly for very short delays, and with other units. It must be noted that function tables of any size can be programmed simply by cascading Serial Memory Units. If different size units are employed the lowest maximum Read/Write cycle rate applies to the combination. Many additional useful operations may be performed with these memory units together with logic building blocks and the analog computer. These are presented in other reports on the Serial Memory Units for the analog computer.

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