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ABSTRACT

A computer program for the simulation of complex continuous process in real-time in an interactive mode is described. The program is user oriented, flexible, and provides both numerical and graphic output. The program has been used in classroom teaching and computer aided design. Typical input and output are illustrated for a sample problem to demonstrate its features. (Author/EMH)

DYNAMIC PROCESS SIMULATION FOR ANALYSIS AND DESIGN

EP-23/11/28/73

by

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SUMMARY

A computer program for the simulation of complex continuous processes in real-time in an interactive mode is described. The program is user oriented, flexible, and provides both numerical and graphical output. Applications of the program have been in classroom teaching and computer aided design. Typical input and output are illustrated for a sample problem to demonstrate its main features.

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INTRODUCTION

Users of digital or hybrid computers can now choose from a wide variety of software simulation packages suitable for process analysis, design, and simulation in contrast with the situation of just a few years ago. A number of steady-state simulation routines such as, Pacer (1), CSMP (2), FLOWTRAN (3), Chess (4), and many others, have evolved to model large and often complex chemical processes. In general, these routines are operated in the batchmode, and the user has to select and write the necessary software to model his process.

More recently, computer codes such as DYNSYS (5), DYFLO (6), PROPYC (7), REMUS (8), and LEANS (9), have been prepared to simulate the dynamic behavior of continuous processes. However, most of these routines are still designed to operate in the batchmode and lack interactive graphic capabilities. With the advent of the wide-spread use of time share computing and the development of auxiliary hardware of reasonable cost, the possibility now exists to provide a simulation program for multiple combinations of individual dynamic processes that operates in an interactive mode and provides both printed and graphical output. Although the program

to be described below has been developed at The University of Texas at Austin under Project C-BE (funded by the National Science Foundation) for the purpose of supplementing classroom teaching, it can be of particular value to designers in industry who need to evaluate the performance of various configurations of equipment.

The Combined Model Simulation (CMS) program makes use of the most recent hardware and techniques to provide a flexible program that can model in real time almost any process configuration incorporating almost any type of time dependent model for each process element. No additional user-written software is required unless additional process models are wanted. Special attention has been paid to make the program inexpensive to operate and user-oriented so that users do not need to have programming experience in order to employ effectively the CMS Program. About 70,000 words of storage are required to load the program, although a version with overlays requires only one-third the storage at the expense of 50% increased computing time.

We believe that one of the major areas of application for such programs is in engineering design and education where the designer or student needs to rapidly explore and evaluate different equipment configurations to develop a process. A second application is in studying the dynamic behavior of various types of individual pieces of equipment. For the student, the program provides a powerful tool with which to learn applications of engineering principles without the often inefficient and time consuming task of writing

and debugging his own simulation code. Since no programming knowledge is required, both the practicing engineer and student find the CMS routine both convenient and cost effective. Because of the added feature of graphical output, the CMS program represents a significant contribution to computer aided design.

THE CMS PROGRAM CAPABILITIES

As explained above, the CMS program simulates the dynamic behavior of an arbitrary arrangement, or configuration, of chemical processing equipment. The program is arranged to meet four basic demands of the user. First, it offers the user his choice of the simulated equipment to be included in the configuration, and then gives him the freedom to arrange the selected equipment to represent a process. Second, it is interactive -- the user has complete on-line control of the program's operation. Third, in addition to numerical output, it provides an on-line graphical display of the process behavior in real time. Finally, the graphical capabilities of the program can be used to plot experimental data on the same coordinates as the process response for visual comparison of predicted performance with actual performance.

In its current state the equipment simulated in the program includes three different dynamic models of chemical reactors, a continuous stirred tank reactor (CSTR), a plug flow reactor (PFR), and a tubular reactor with axial dispersion (PFRD). Each reactor includes a user-specified

volume and, in addition, the dispersion reactor calls for a user-specified dispersion coefficient. All the reactors are isothermal to simplify the computations for students, but the program can easily be modified to include nonisothermal equipment.

The user may specify the reaction mechanism with choices of no reaction or reactions of various kinetic orders (first, second, etc.). The reactors are combined into arbitrary networks with the aid of splitters (subroutine SPLT divides one stream into two streams of arbitrary flow rates) and mixers (subroutine MIX combines two streams into one).

Any piece of equipment can be arbitrarily arranged by the user to form a process that is represented by a network. Reactors may appear in parallel, in series, or in any combination with the aid of splitters and mixers. Each piece of equipment in the network is assigned a unique number by the user. Figure 1 illustrates a sample process. Suppose that the user wanted to simulate the process. The CMS program forms the network from the information supplied by the user after he introduces the type and corresponding number of each piece of equipment, as well as the number corresponding to the next subsequent piece of equipment. The input for the network in Figure 1 is illustrated in Figure 2. The information provided by the user enables the computer to form adjacency and incidence matrices that represent the process configuration, and the matrices in turn are used to schedule the sequence of computations for the dynamic simulation. The theory associated with converting from a process flow sheet to an adjacency

and incidence matrix is discussed by Himmelblau and Bischoff (10). They also illustrate how the adjacency matrix can be treated to determine a precedence order for the equipment in a network so that the inputs and outputs of the specified equipment are arranged in a suitable sequence for solution of the entire process model. The respective matrices and the schematic outline of the network are printed by the CMS program, as illustrated in Figure 3. Note that the equipment configuration is printed out serially in a vertical descending order. Plotting of the network configuration is also possible.

The CMS software permits input/output at user-specified times during the simulation. Once the user has entered a process configuration into the computer, he has under his control an interactive dynamic simulation routine that models the specified network. He is at liberty to enter data to test the network's behavior and to choose various types of inputs such as a step, sinusoidal, pulse, or random noise input. At any time he may also redirect the operation of the program, as for example by re-start, stop, suppress printing or plotting, or change the time interval at which he enters information or receives output. In general, the user's control over the operating program is virtually unlimited. Almost any control options can be incorporated into the program so that flexibility is a key element in making the interactive computing a serviceable tool. Each mathematical model describing a specific type of equipment is established as a subroutine. Inlet and outlet values are transmitted to the subroutine along with a set of parameters associated

with the particular equipment being represented. Thus, initial user information defines each piece of equipment, its unique number, the equipment number to which it is connected, and the associated parameter set. In developing the program software, where possible we used R. Franks' (6) DYFLO subroutines and general structure. By taking advantage of this extensive collection of well documented software we hoped to improve the program transferability and ease of modification by potential users.

To assure that information generated by the program is rapidly interpreted by the user and to avoid long pauses during program execution, the output consists of both numerical information and a series of graphs. Only inlet and outlet stream properties are recorded because (a) these are of primary importance in studying process behavior and (b) only a limited, condensed amount of information can be immediately absorbed by the user.

Two important questions that have to be answered by any designer of a simulation code are: when during the simulation should program output information be printed and plotted; and what information should be included. Our approach was to transmit output information at user-specified intervals during the simulation. Since the user can control the time interval during the actual simulation, process output information can be viewed as frequently as desired. As to the type of information provided, our choice was to print all the numerical data on the inlet and outlet streams at the times specified by the user. The data for the plots are accumulated during one time interval and then released to the plotter at the end of that interval. Figure 4 illus-

trates typical numerical results from the simulation of the process represented by the network in Figure 1. After each ENTER DATA line is printed by the teletype or teleprinter, the user can enter new information. Otherwise, he types GO, and the results for the next incremental time(s) are printed out. Figure 5 illustrates the corresponding graphical output (the axes and their labels have been plotted by the program, as well as the curves), namely the inlet and exit reactant concentrations versus time.

One important additional feature of the CMS program is its ability to plot experimental data on the same coordinate axes as the process response, thus greatly facilitating model development and verification. For example, in studying the mixing characteristics of a network, as discussed by Himmelblau and Bischoff (10), the dimensionless external age distribution proves to be a convenient tool for analysis. When the user introduces a pulse input to the network, the program automatically asks for experimental data and, if supplied, the program plots this data using special symbols. Figure 6 shows the user supplied information for one example. Experimental data are entered into the program as shown at the bottom of the Figure. The lower figure in Figure 7 illustrates how both the experimental data and the simulated CST responses are plotted. By comparing the behavior of the model to the experimental data (plus computing the variance associated with the least squares fit), the user can readily evaluate the adequacy of his mathematical model and immediately modify the model and repeat the simulation until a suitable model is synthesized.

In summary, the Combined Model Simulation program performs the following functions:

1. Accepts user input suitable for specification of a network of process equipment
2. Translates user input into adjacency and incidence matrices (labeling and numbering all streams)
3. Uses the adjacency matrix to arrange the specified equipment in the proper precedence order for solution
4. Determines and assigns flow rates to all streams in the network
5. Solves the network model interactively
6. Provides interactive input and output for the simulation model
7. Generates (interactive) graphical output
8. Allows the user to enter experimental data that can be plotted
9. Provides for immediately restarting of the simulation with or without network modifications.

PROGRAM SUBROUTINES

The following are the subroutines comprising the CMS Program and their respective roles in the CMS Program:

Name	Description
(1) Subprograms from R. Franks text	
PRL	Provides numerical output
INTI	Increments the independent variable time
INT	Integrates the dynamic material and energy balances
(2) Supplementary subprograms	
ZERO	Initializes arrays and parameters
DAT	Sets initial boundary conditions, default values, and initializes program variables
REACT	Contains reaction kinetics
READ	The input-interactions of the program are created through Subroutine READ.
NDS	Completes user input for the network and performs the following tasks: (1) Develops the adjacency matrix (2) Develops the incidence matrix (3) Numbers the streams (4) Assigns numbers to the equipment. These numbers correspond to the order in which the equipment is called in Subroutine EQUIP (5) Outputs the adjacency matrix, the incidence matrix, and the network.
EQUIP	Calls the subroutines containing the equipment models.
FLOW	Sets the flow rates within the defined network
CSTR	Continuous-Stirred-Tank Reactor model
PFR	Plug Flow Reactor model
PFRD	Tubular Reactor model with axial dispersion
SPLIT	Divides one stream into two. The flow ratio is set by the user.
SUM	Combines two streams

(3) Special subroutines

IOSUB	Free field reader
RECORD	Internal accounting routine

(4) Graphics subroutines

GRAPH	Links graphics routines to main program
SUMM1	Collects numerical data for plotting
CURVE	Graphs numerical data
AXIS4	Draws axes

The complete program and documentation is available from Project C-BE, College of Engineering, at The University of Texas at Austin upon request.

CLASSROOM EXPERIENCE

Program CMS with its time share operation and interactive graphics has been evaluated in the Chemical Engineering Department at The University of Texas at Austin both by instructors and students. It has been successful in simulating the dynamic behavior of chemical processes, and also in conveying much the same feeling and improved understanding associated with laboratory experience and previously used analog computer simulations. In teaching, the CMS program has changed the student's role of passively learning abstract concepts by the traditional lecture method to one in which the student interacts with the computer in real time. Course concepts and ideas are implemented and the results viewed immediately.

Plotted output from the CMS program can be viewed simultaneously by the entire class with the aid of an inexpensive overhead projection system,

thus providing the instructor with a new tool for classroom teaching; refer to Muller, Nuttall, and Himmelblau (11). Figure 8 illustrates the computer terminal equipment used both in the classroom and by students while executing the CMS program. If for some reason the time sharing system cannot be connected to or contacted by the remote teletype, in emergencies the tape recorder can be turned on to emulate the entire operation of the CMS program (without user input, of course).

DESIGN EXPERIENCE

The CMS program has been used to assess the dynamic effects of a recycle stream in the design of a catalytic packed bed tubular reactor for converting producer gas to synthetic natural gas. The methanation reaction is quite exothermic and temperature excursions in the tubular reactor must be prevented. The CMS program was used to simulate the recycle fraction of the methane that served as a diluent so as to minimize transie t temperature excursions that would damage the catalyst and decompose the product.

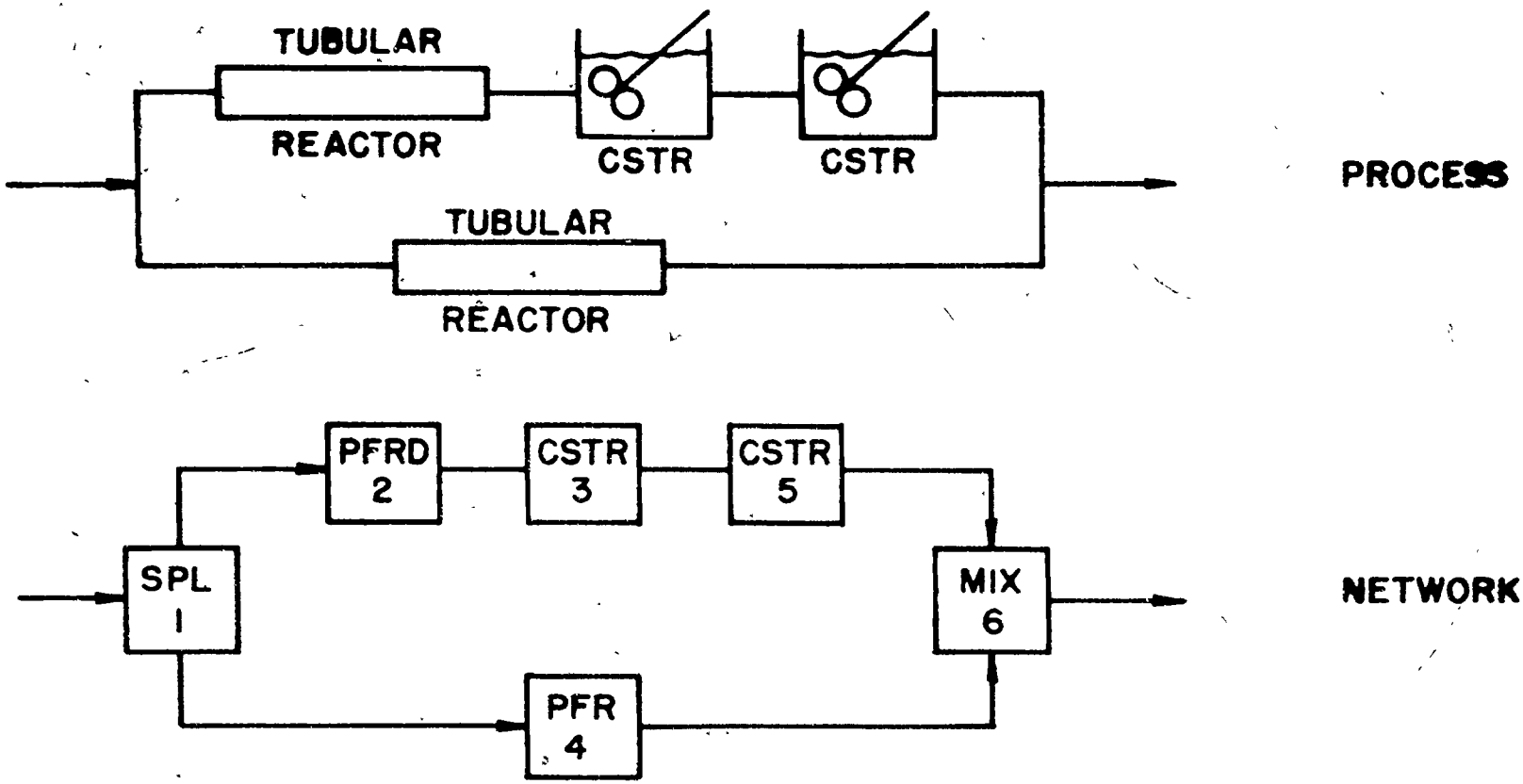
CONCLUSIONS

We have described a generalized process simulation program (CMS) and some of its applications in chemical engineering. The CMS program has evolved in part because of recent advances in the use of computers (time-share computing) and the improved terminal equipment (time-share graphics).

Recently, improved hardware, together with software, has provided a new and powerful tool for teaching and interactive design at less cost than the traditional batchmode of computing. Furthermore, the techniques and concepts presented here can be readily implemented in fields other than chemical engineering.

ACKNOWLEDGEMENT

This research was supported in part by Project C-BE under Grant GY-9340 "The Use of Computer-Based Teaching Techniques in Undergraduate Science and Engineering Education" from the National Science Foundation to The University of Texas at Austin, Drs. John J. Allan and J. J. Lagowski, Co-Directors.



Definition of Equipment

SPL - Splitter
MIX - Mixer
PFR - Plug Flow Reactor
PFRD - Tubular Reactor with axial dispersion
CSTR - Continuous Stirred Tank Reactor

Figure 1. Schematic Diagram of a Simple Process and Its Representation by the Corresponding Network.

```
        COMBINED MODEL

    DO YOU WANT TO BEGIN A NEW NETWORK?
YES
    HOW MANY PIECES OF EQUIPMENT ARE IN THE NETWORK?
6
    ENTER EQUIPMENT SPECIFICATIONS

SPLT(1,2,4,0.25)
PFRD(2,3)
VOLUME = 10
    PECLET NUMBER
20
CSTR(3,5)
VOLUME = 20
CSTR(5,6)
VOLUME = 20
PFR(4,6)
VOLUME = 50
MIX(6,7)
GO
```

NOTE: Underlined information was supplied by the user; other statements by the CMS Program.

Figure 2. User Input and CMS Program Interactive Statements Used to Specify the Network Illustrated in Figure 1

ADJACENCY MATRIX

	1	2	3	4	5	6
1	0.000	.250	0.000	.750	0.000	0.000
2	0.000	0.000	1.000	0.000	0.000	0.000
3	0.000	0.000	0.000	0.000	1.000	0.000
4	0.000	0.000	0.000	0.000	0.000	1.000
5	0.000	0.000	0.000	0.000	0.000	1.000
6	0.000	0.000	0.000	0.000	0.000	0.000

INCIDENCE MATRIX

	1	2	3	4	5	6	7	8
1	1	-1	-1	0	0	0	0	0
2	0	1	0	-1	0	0	0	0
3	0	0	0	1	-1	0	0	0
4	0	0	1	0	0	-1	0	0
5	0	0	0	0	1	-	-1	0
6	0	0	0	0	0	1	1	-1

REACTOR NETWORK

```
     SPLT
PFR       PFRD
          CSTR
          CSTR
     MIX
```

IS EVERYTHING OK?

<u>YES</u>

NOTE: Underlined information was supplied by the user; other statements by the CMS Program.

Figure 3. Information Provided by the Program to Aid the User in Verifying His Network

```
                    ENTER DATA

GO


 TIME = 0
STRM NO              1              8
   FLOW        1.800E+01      1.800E+01
   TEMP        1.900E+02      1.900E+02
   COMP B      2.480E+00      3.480E+00
   COMP A      1.000E+00      0.



 TIME = 2.0000E+00
STRM NO              1              8
   FLOW        1.800E+01      1.800E+01
   TEMP        1.900E+02      1.900E+02
   COMP B      2.480E+00      3.244E+00
   COMP A      1.000E+00      2.580E-01

                    ENTER DATA

GO


 TIME = 4.0000E+00
STRM NO              1              8
   FLOW        1.800E+01      1.800E+01
   TEMP        1.900E+02      1.900E+02
   COMP B      2.480E+00      2.936E+00
   COMP A      1.000E+00      5.454E-01

                    ENTER DATA
GO
```

NOTE: Underlined information was supplied by the user; other statements by the CMS Program.

Parameter changes may be entered after each ENTER DATA statement and prior to typing GO.

Figure 4. User/Program Record During the Simulation of the Network Shown in Figure 1

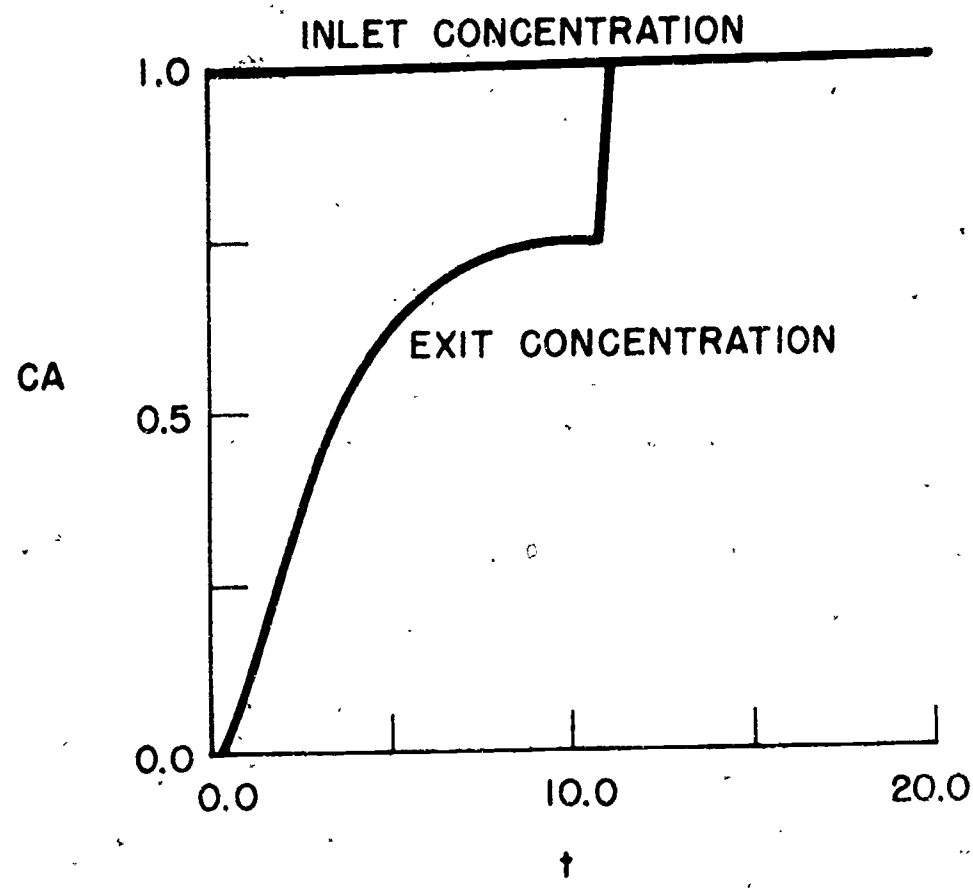


Figure 5. Graph of Inlet and Exit Concentration of Species A Versus Time

```
        DO YOU WANT TO BEGIN A NEW NETWORK?
YES
        HOW MANY PIECES OF EQUIPMENT ARE IN THE NETWORK?


        ENTER EQUIPMENT SPECIFICATIONS
CSTR (1, 2)
VOLUME = 100
GO
        ADJACENCY MATIRX
              1
        1   0.000

        INCIDENCE MATRIX
              1     2
      1       1    -1
        REACTOR NETWORK
        CSTR
        IS EVERYTHING OK?
YES
        ENTER DATA
PX = 1.0
PC = 1.0
GO
        DO YOU WANT TO ENTER RTD EXPERIMENTAL DATA?
YES
        HOW MANY DATA POINTS ARE YOU GOING TO ENTER?
10
        ENTER DATA IN A THETA, E(THETA) FORM
.11   .92
.33   .75
.47   .62
1.1   .348
1.8   .221
2.4   .086
2.99  .044
3.6   .024
4.7   .0073
8.6   .0013
```

Figure 6. Using Program CMS to Compare the Mixing Characteristics of a Continuously Stirred Tank to Experimental Residence Time Distribution Data

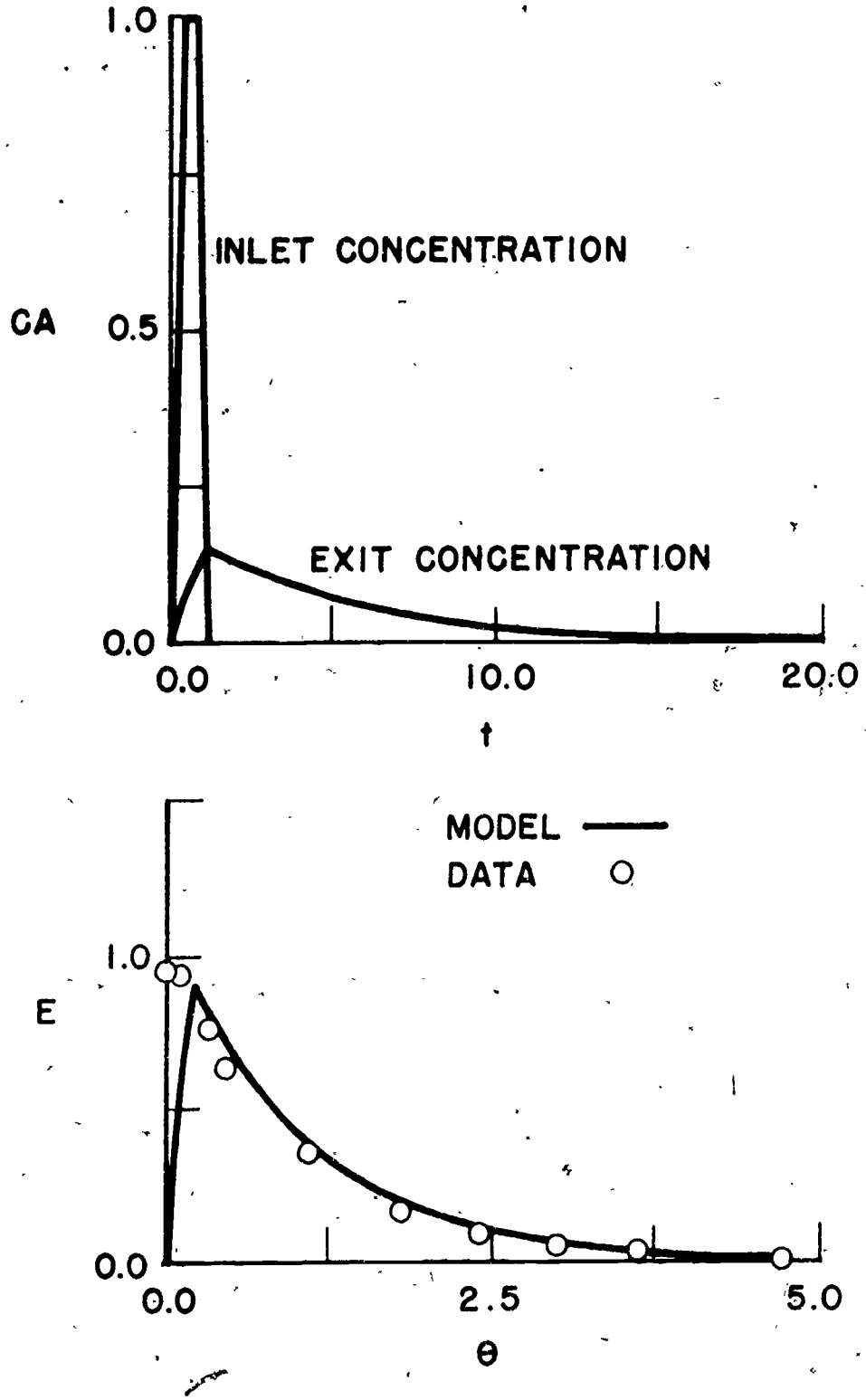


Figure 7. Graphical Information Provided by Program CMS during a Study of the Mixing Characteristics of a Continuously Stirred Tank

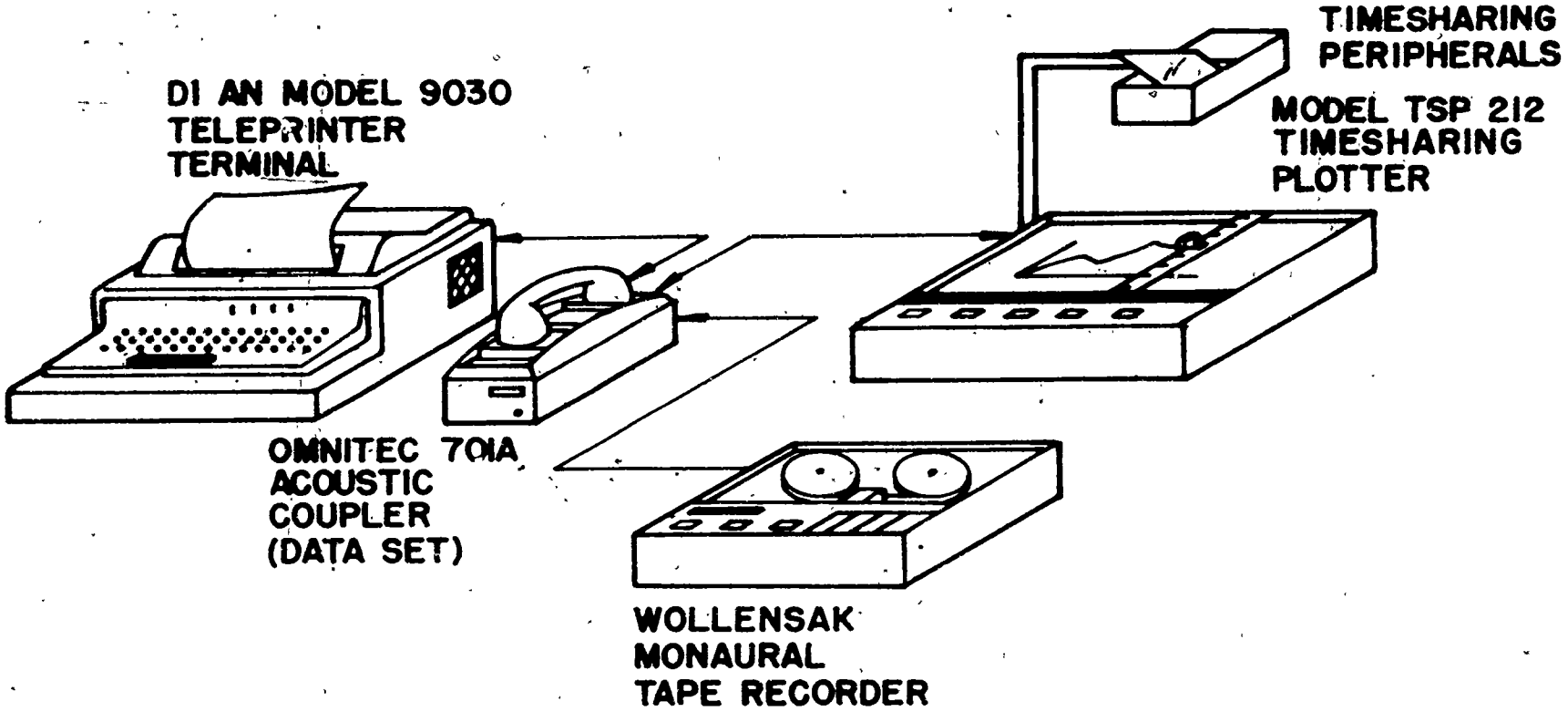


Figure 8. Computer Terminal Equipment Used with the CMS Program

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