Simulation of Full-scale Multi-stage Batchwise Chemical Plant

By P. V. Youle

A hypothetical multi-stage batchwise chemical plant has been simulated, using a Ferranti Mercury electronic computer. The plant has seventeen vessels in four stages. Results from the simulation program are given, to demonstrate their value to plant management in pointing to methods of increasing plant efficiency and output. The principles described can be applied to other chemical plants. This paper was presented at the Harrogate conference of The British Computer Society on 6 July 1960.

Introduction

Plant-study has been defined as the objective study of a piece of chemical plant in its totality (Youle, Tocher, Jessop, Musk, 1959). The simulation of the plant by means of a large electronic computer plays an important part in plant-study (Youle, 1960).

Where a full-scale plant has yet to be built, the simulation program can be used to guide all phases of the work:

Stage of work	*State of simulation program*
Initial laboratory studies.	The full simulation program is outlined roughly. The laboratory work having uncovered the reaction mechanism, that part of the program dealing with reactor kinetics can be written most fully.
Semi-technical design stage.	The simulation program is used to calculate the likely behaviour of various alternative semi-technical units, and from these calculations the most suitable form of unit is chosen. Gaps remaining in the program indicate the information required from the semi-technical work. These gaps refer principally to the scale-dependent factors in the system.
Semi-technical unit operational.	Information on scale-dependent factors is obtained and inserted in the program.
Full-scale plant design stage.	The program is completed by the addition of details of raw material handling and product storage. The complete program is run in various modified forms so as to check the designer's assumptions, and so as to show the points on which further work is most necessary.
Full-scale plant start-up.	Many difficulties have been anticipated by computer runs prior to the actual start-up. Plant performance is compared with that expected from the program, and start-up is made easier.
Full-scale plant operational.	Process development work is made easier by the existence of a computer program on which experimentation can be done without interference with the actual plant.

When the full-scale plant becomes operational, its output may best be planned on the basis of a simulation program of the activities of the whole of the parent concern. This leads to a serial arrangement of simulation programs, with the simulation of the actual chemical reactor forming part of the simulation of the full-scale plant, and this itself in turn forming part of a simulation of the whole firm's activities. The serial arrangement is illustrated in Fig. 1.

When a full-scale plant is already in existence, the objects of a simulation study come wholly under the last heading in the above tabulation. They can be defined more explicitly as follows.

1. To increase understanding of the process, the increased understanding leading to:
   - (*a*) Improved efficiency in running the plant.
   - (*b*) Increased output from the plant.
   - (*c*) Detection of bottlenecks.
   - (*d*) Assistance in planning expansion schemes.
   - (*e*) Rationalized maintenance schedules.
2. To facilitate calculations on experimental methods of plant operation without disturbance to the actual plant.

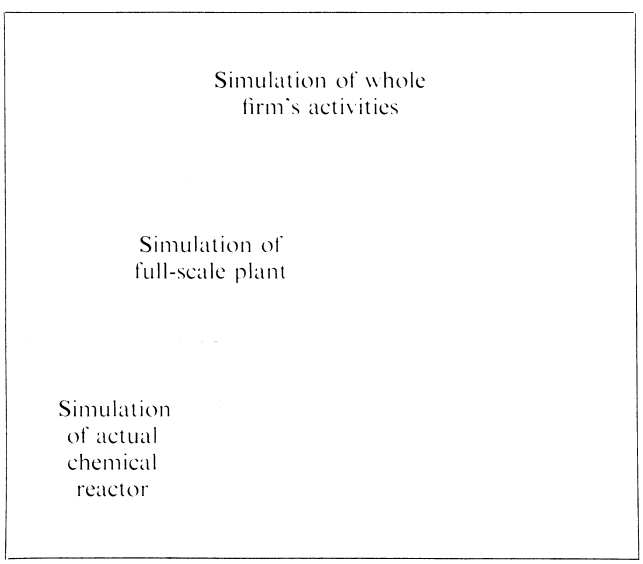

Fig. 1.—Serial nature of possible simulation programs

This paper describes a simulation study for a full-scale plant. The description relates to calculations that have been carried out for a typical, hypothetical, chemical plant. The underlying principles are emphasized because they are applicable to all similar plants.

Plant to be Simulated

The present paper first describes the hypothetical chemical plant, then gives details of the procedure adopted for simulating it, and finally gives examples of the results obtained from the simulation. Continuous processes may be less difficult to simulate than batchwise processes; for this reason, the example chosen is a typical batchwise multi-stage plant, as shown in Fig. 2. The procedure used to simulate this plant could be used for any similar plant in chemical industry. Practical use of such procedures has been made on a Ferranti Mercury computer, the program being written in Autocode.

For the present exercise, the stock of raw materials, and the storage capacity for plant product, were both assumed to be adequate, though, in a fuller exercise, both these assumptions could be modified. The process is pictured as involving seventeen vessels in four stages: stage A (three vessels), stage B (five vessels), stage C (four vessels) and stage D (five vessels). Fig. 2 depicts these stages in a typical chemical engineering flowsheet.

The essence of the simulation exercise is to make a model of this plant with the aid of an electronic computer. In making this model, the procedure is to cause the computer to create and maintain a continuous activity chart for the plant. All that follows is directed to describing how this simulation was accomplished, and the sort of information that accomplishing it then made available.

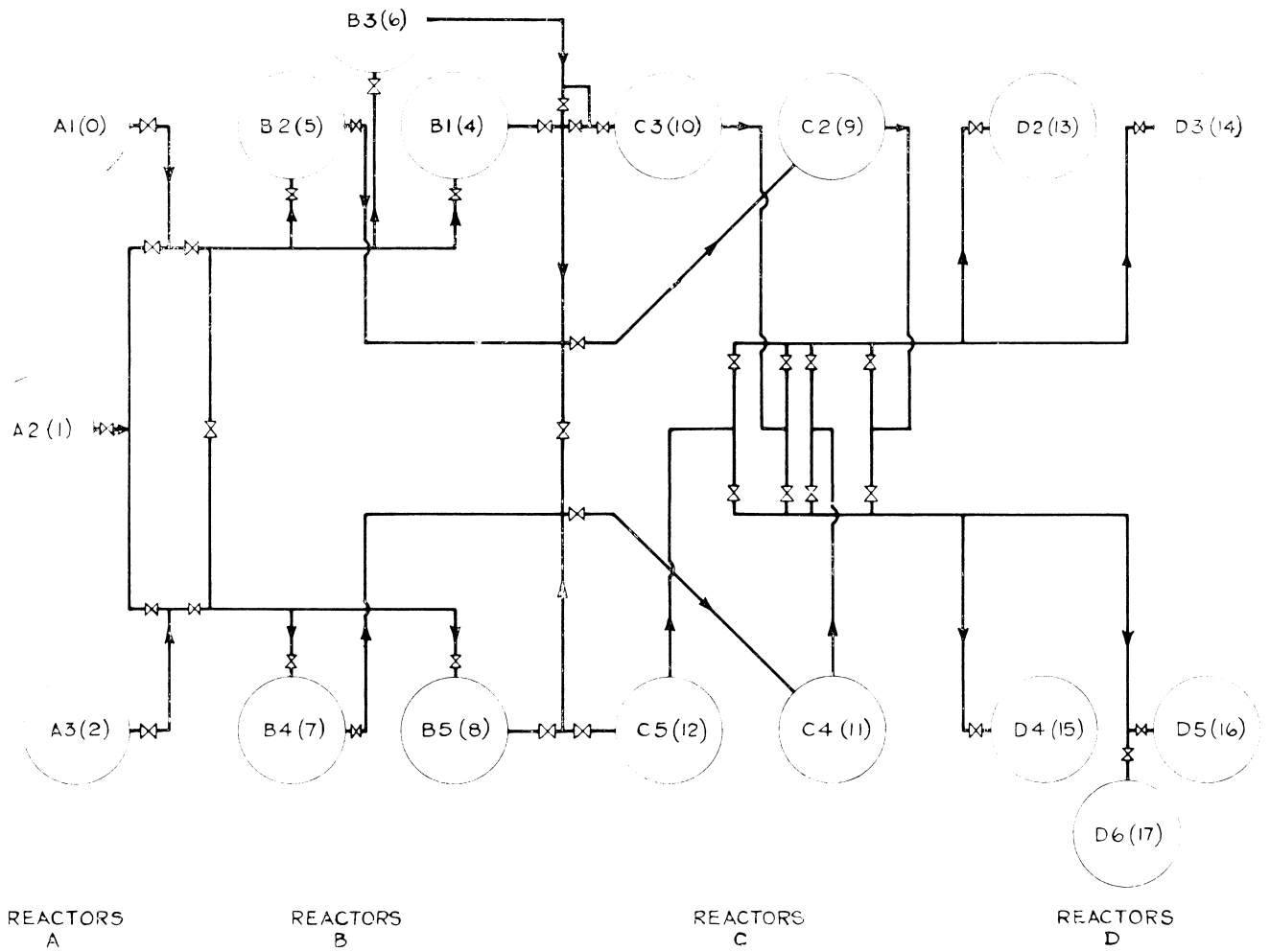

Fig. 2.—Line diagram of hypothetical multi-stage batchwise chemical plant

Programming Procedure

The procedure that was involved in setting up the computer simulation can be divided into the following eight stages, each set out in the form of an instruction applicable to an existing full-scale plant:

1. Get the co-operation of the plant staff.
2. Get a line diagram of the plant.
3. Supplement the line diagram by the fullest possible analysis of actual plant behaviour.
4. Do a complete logical analysis of the steps to be taken when each plant activity ends.
5. Add to this a series of subsections governing the transfer of batches from stage to stage on the plant.
6. Write the detailed computer program.
7. Collect relevant plant-record sheets.
8. Calculate mean cycle times and examine the distribution of cycle times.

The following discussion describes how these eight stages were applied to the hypothetical plant shown in Fig. 2. Special comments are made in places where the procedure for a real plant would have been different.

1. *Co-operation of Plant Staff*

Taking the stages in turn, it is necessary, throughout, to emphasize the importance of gaining the co-operation of the plant personnel. This, in the first place, ensures that the logical analysis of plant behaviour corresponds to reality as completely as possible. At a later stage, when the simulation shows up plant deficiencies, co-operation with plant personnel avoids rancour, and ensures that suggestions made to rectify deficiencies are soundly based, in practice as well as in theory.

2. *Line Diagram of Plant*

The vessels in Fig. 2 are numbered within each group and also (as shown below by the figures within brackets) consecutively throughout the whole plant:

A1(0), A2(1), A3(2), Dummy number (3),
B1(4), B2(5), B3(6), B4(7), B5(8),
C2(9), C3(10), C4(11), C5(12),
D2(13), D3(14), D4(15), D5(16), D6(17).

3. *Analysis of Plant Behaviour*

All special arrangements of valves must be noted, together with any restrictions due to plant layout.

The activities in any one unit can be reduced to a standard pattern. These activities will occupy a certain length of time on the plant. Since the main activity of a unit is "processing," the time taken for "processing" is crucially important and is often referred to as the *cycle time* for that unit.

If the unit in question has an adequate supply of raw materials, if there is adequate storage capacity for the product, and if pipework connections are adequate throughout, then there are only three possible activities for the unit:

(*a*) charging,
(*b*) processing,
(*c*) discharging.

In an actual plant, however, there may be no unit available from which to recharge raw materials, or there may be no empty unit into which to run the product, and these deficiencies lead to two further possible activities:

(*d*) waiting full, and
(*e*) waiting empty.

Furthermore, even though the necessary units may be available, there may be no free transfer lines, and such a deficiency leads to two further possible activities:

(*f*) temporarily waiting full, and
(*g*) temporarily waiting empty.

The computer is able to plot the progress of a unit through all the seven activities listed. To do this, the following routines are employed for the four types of delay times:

Delay time	*Computer action*
Waiting empty and waiting full.	Add a large constant number of minutes to the time at which waiting starts.
Temporarily waiting empty and temporarily waiting full.	The time at which the temporary waiting time will end is set to the time at which the interfering transfer will end.

The above analysis of possible unit activities is of general applicability and is not, by any means, confined to the plant sketched out in Fig. 2.

4. *Logical Analysis*

At this stage the main flow diagram for the computer program was drawn up. It is set out in Fig. 3.

5. *Routines for Stage-to-Stage Transfers of Batches*

For the plant in Fig. 2 six sets of transfer routines are required, and detailed flow diagrams must be drawn for these. An example of one of these is given in Fig. 4, which deals with the question, "Can a reactor waiting full in group A charge to a reactor waiting empty in group B?" The six transfer routines are set out in Table 1.

6. *Autocoding*

The main program was next written. Mercury Autocode was employed and Table 1 shows the arrangement of chapters in the program, Table 2 shows the symbols used in the program, and Table 3 the code numbers used to designate operations. This program contains the full analysis of possible unit activities, and a complete plan of the pathways by which material flows through the

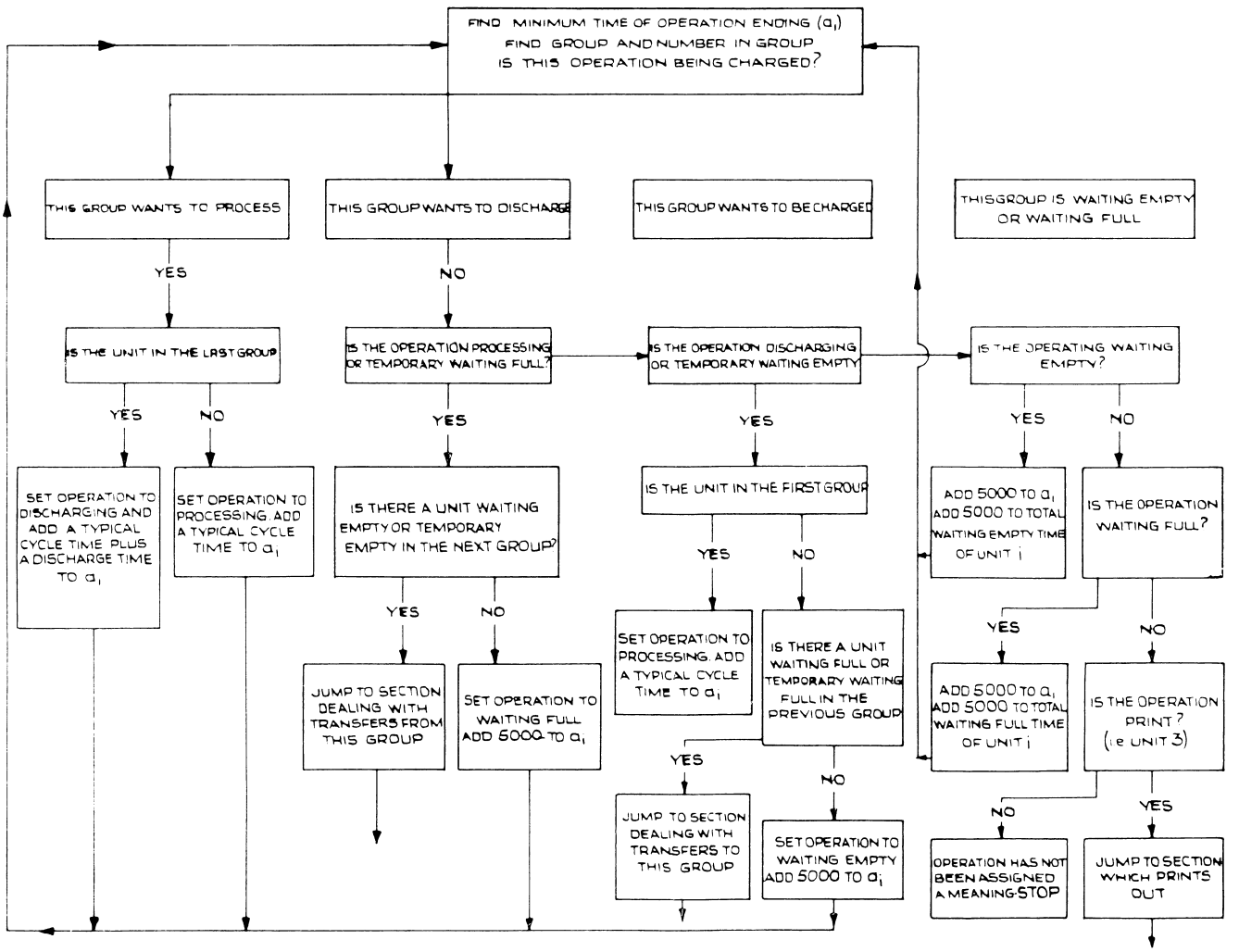

Fig. 3.—Flowsheet for main program

plant. It is ready to be run on the computer just as soon as representative time data can be supplied, and the aim of the next two stages is to get these time data.

7. *Collection of Data Sheets*

For an actual chemical plant, time data are obtained by analysing a large number of plant-record sheets. So many sheets may be available for inspection that the labour of examining them may call for subsidiary computer programs.

For the hypothetical plant sketched in Fig. 2, this problem does not arise: fictitious cycle times were invented.

8. *Cycle Times*

For this plant, hypothetical cycle times have been set up as in Table 4. The distribution of times has been assumed to be normal. The computer program is there-

Table 1

Simulation Program: Arrangement of Chapters

Chapter		
1	Main program (Fig. 3)	
2	Print	
TRANSFER ROUTINES:		
3	A discharging to B (Fig. 4)	Looking forward
4	B discharging to C	
5	C discharging to D	
6	B being charged by A	Looking backward
7	C being charged by B	
8	D being charged by C	
9	Read in	
0	Start	

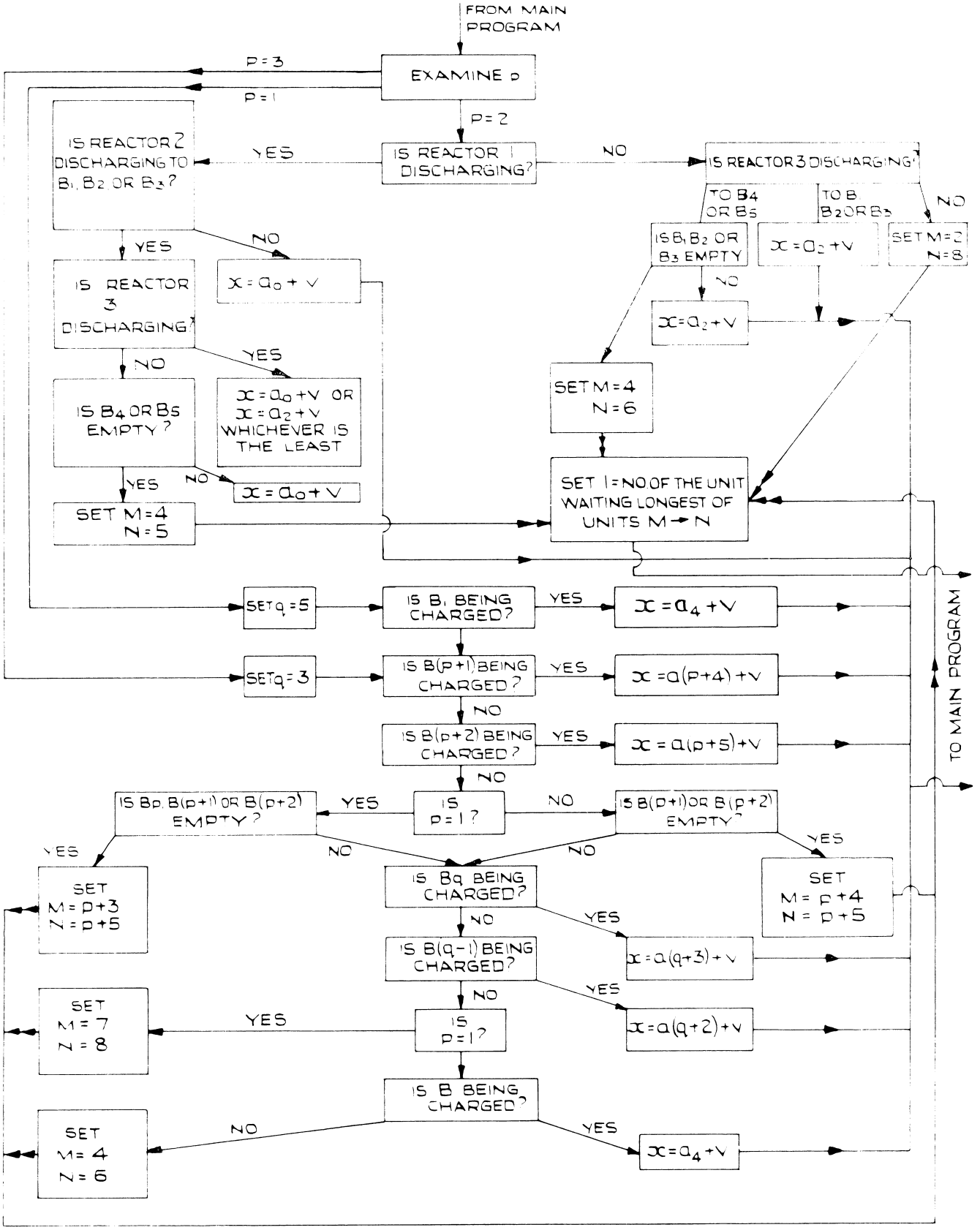

Fig. 4.—Flowsheet for Chapter 3

fore supplied with mean times and their standard deviation, so that it can generate an appropriate sequence of cycle times and so imitate plant operation.

For an actual plant, cycle times will usually be found to have a normal distribution. If any deviation from a normal distribution is detected, the cause should be sought by critically examining the plant performance. Skew distributions can be successfully generated by the computer, but it is unwise to arrange to do this until the cause of the skew distribution has been found out.

Operation of Computer Program

The computer simulation program was set up for the plant of Fig. 2 by following the eight stages described. The program was next run on the computer, with the objective of causing the computer to create and maintain a continuous activity chart for the plant. This activity chart can be printed out for any given instant.

Table 5 shows part of the print-out obtained at times of approximately 21,000 minutes from the start of the exercise.

The operation of the simulation program can be described in terms of Table 5. The computer scans through the list of times given in the last column of Table 5 and picks out the lowest. It then identifies the unit associated with that time. By consulting the logical analysis, embodied in its program, the computer progresses that unit forward, on to its next activity, and associates with it a new time. The table of times is then scanned again and the operation is repeated.

In Table 5 units A2 and B5 show identical times. This arises because unit A2 is emptying itself into unit B5. An exact identity of times would cause the calculation to stagnate and so, in practice, an extra 0·1 of a

Table 2

Symbols used in Program

i	The number of the unit (i.e. 0–17)
k	The number of the group to which the unit belongs
p	The number of the unit in the group
a_i	The time at which the operation ends in unit i
b_i	The code number for the operation proceeding in unit i
c_i	The total waiting full time of unit i
d_i	The total waiting empty time of unit i
e_i	The total number of batches processed in unit i
f_i	The mean cycle time of unit i
g_i	The standard deviation on cycle time of unit i
h_i	The discharge time of unit i
u_i	The total temporarily waiting full time of unit i
v_i	The total temporarily waiting empty time of unit i

Table 3

Code Numbers to Designate Operations

5	Being charged by unit 5 of the previous group
4	Being charged by unit 4 of the previous group
3	Being charged by unit 3 of the previous group
2	Being charged by unit 2 of the previous group
1	Being charged by unit 1 of the previous group
1	Processing
2	Temporarily waiting full
5	Print (applies only to unit no. i 3)
8	Waiting empty
9	Waiting full
10	Temporarily waiting empty
11	Discharging to unit 1 of the next group
12	Discharging to unit 2 of the next group
13	Discharging to unit 3 of the next group
14	Discharging to unit 4 of the next group
15	Discharging to unit 5 of the next group
16	Discharging to unit 6 of the next group

Table 4

Summary of Cycle Times Assumed

UNITS	DISCHARGE TIME MEAN (MIN.)	CYCLE TIME (MIN.)	
		MEAN	STANDARD DEVIATION
Reactors A	35	90*	18
Reactors B	30	160	35
Reactors C	40	121	30
Reactors D	35	166	40

* Includes charging time.

Table 5

Simulation of Hypothetical Chemical Plant: Part of Activity Chart

UNIT		ACTIVITY		TIME (MIN. FROM START)
GROUP	NO.	CODE NO.		
Reactors A	1	1	Processing	20,183
	2	15	Discharging	20,166
	3	11	Discharging	20,170
Reactors B	1	3	Being charged	20,170
	2	12	Discharging	20,180
	3	8	Waiting empty	25,012
	4	8	Waiting empty	25,012
	5	2	Being charged	20,166

minute is always added to the time associated, in such a pair of units, with that unit which is being filled.

The times for units B3 and B4 show the additional 5,000 minutes called for by their activity of waiting empty.

Results from Computer Program

Table 6 shows actual results for the second week of simulated plant operation. These results, typical of those obtained with a real plant, show an output of 190 batches. When a real plant is being simulated, considerable time should be spent comparing calculated performance with actual plant performance. It is wrong to use the simulation program for calculation on experimental methods of plant operation, until proof is available of the correctness of calculations for normal methods of operation. In the present exercise with a hypothetical plant, this proof is assumed to be available. The correctness of the simulation being assumed, a discussion of results is permissible. The two columns which list temporary waiting times show only small delays. This indicates that the pipework on this plant is adequate for the present production rate. The two columns listing waiting times show that reactors A and B wait full for a high proportion of the time. This betrays a lack of capacity in the second half of the plant. On a short-term basis, this can be dealt with by reducing mean cycle times in reactors A and B. On a longer-term basis, new units at stages C and D may be needed, and calculations should be carried out for one extra reactor in both of stages C and D. Reactors C wait full for about 6% of the time, and reactors D wait empty for about 8% of the time. This apparent inconsistency indicates that cycle time variability is restricting output.

Table 6

Results for Second Week of Plant Operation

UNIT		WAITING TIMES		TEMPORARY WAITING TIMES		OUTPUT	
GROUP	NO.	FULL (MIN.)	EMPTY (MIN.)	FULL (MIN.)	EMPTY (MIN.)	BATCHES MADE	
A	1	2,244	—	0	—	60	
	2	1,907	—	15	—	65	
	3	1,841	—	24	—	66	
B	1	1,521	123	11	21	38	
	2	1,250	93	11	10	38	
	3	1,143	166	4	69	40	
	4	1,659	64	21	5	38	
	5	1,347	63	5	23	37	
C	2	556	203	82	53	48	
	3	800	294	54	13	47	
	4	666	212	78	11	49	
	5	651	282	74	47	47	
D	2	—	1,047	—	24	38	Total 190
	3	—	845	—	51	37	
	4	—	833	—	139	38	
	5	—	626	—	61	38	
	6	—	812	—	71	39	

Successive weekly output figures are given in Table 7. Variability and carry-over from week to week are having a pronounced oscillating effect on the output. The mean is 189·25 batches/week and the standard deviation of the mean is 0·7.

In a real-life simulation exercise, the calculated plant output would be compared with the actual plant output week by week, and any discrepancy would be immediately investigated.

The effect of cycle time variability is important in the present example. Reducing the standard deviation of cycle time by a quarter would increase weekly output by 1·7%. Eliminating variability altogether would give an increase of 11·2%.

Unit occupation times have been calculated for the plant and are illustrated in Table 8. The first column gives results for the plant as sketched in Fig. 2. The second column in the Table shows the unit occupation times to be expected for a 25% cut in cycle time variability. The last column shows unit occupation times for a plant with additional units at stages C and D, as suggested by the earlier results in Table 6. Calculations are clearly possible for many such experimental methods of plant operation.

Conclusion

The above results justify the claim that computer simulation of a chemical plant will lead to valuable information on the following points:

1. *Calculations for the Plant as it is:*
   - (*a*) Plant output.
   - (*b*) Unit occupation times.
   - (*c*) Delays due to inadequate pipework and to cycle time variability.
2. *Calculations for experimental methods of operation:*
   - (*a*) Output at different cycle times.
   - (*b*) Output with reduced cycle time variability.
   - (*c*) Output with different arrangement of vessels and pipework.
   - (*d*) Effect of different maintenance schedules.
   - (*e*) Possible methods of on-line computer control.
3. *Leading to:*
   - (*a*) Ways of improving efficiency.
   - (*b*) Ways of improving output.
   - (*c*) Detection of bottlenecks.
   - (*d*) Assistance in planning expansion schemes.

Table 7

Calculated Weekly Output Figures

WEEK	OUTPUT (BATCHES WEEK)
1	184 (start-up)
2	190
3	187
4	190
5	187
6	191
7	190
8	187
9	192
Mean	189·3

Table 8

Calculated Unit Occupation Times

EQUIPMENT	UTILIZATION (%)		
	NORMAL OPERATION	VARIABILITY CUT BY 25%	EXTRA UNIT AT C AND D
Reactors A	79·8	79·5	85·6
B	84·8	87·2	94·0
C	89·8	90·7	80·2
D	91·0	91·6	85·6

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References

YOULE, P. V., TOCHER, K. D., JESSOP, W. N., and MUSK, F. I. (1959). "Simulation Studies of Industrial Operations," *J. Roy. Stat. Soc.*, Vol. 122, p. 484.

YOULE, P. V. (1960). Proceedings of the Second European Symposium on Chemical Reaction Engineering: "Simulation Techniques in Chemical Reaction Engineering." (To be published.)

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