

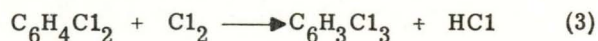
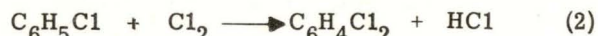
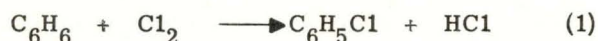
ANALOG COMPUTER STUDY
OF A SEMI-BATCH REACTOR

INTRODUCTION: This paper considers a reactor design application of the PACE® TR-48 General Purpose Analog Computer, viz: the chlorination of benzene in a semi-batch reactor. The major objective of the study will be to relate the maximum production of intermediate chlorobenzenes to the chlorine feed rate and the time of reaction. Another objective consists of illustrating how experimental kinetic data can be fitted on such a computer to obtain reaction rate constants.

Since the majority of both inorganic and organic chemical products of the chemical industry are formed by one or more chemical reactions, the chemical engineer is continually faced with the problem of designing flow, batch, or semi-batch reactors. In recent years, the cost of designing and optimizing a reactor has been sharply reduced through the use of the general purpose analog computer. The computer is used to simulate the behavior of the process in question. Proposed changes in the process and its eventual optimization can then be accomplished quickly, and without expensive equipment modifications.

THE PHYSICAL SYSTEM

The chlorination of benzene (C_6H_6) produces monochlorobenzene (C_6H_5Cl), dichlorobenzene ($C_6H_4Cl_2$), and trichlorobenzene ($C_6H_3Cl_3$) through successive, competing chemical reactions:



These reactions are carried out in a lead-lined or iron vessel, which is shown in Figure 1, with ferric chloride ($FeCl_3$) as a catalyst. The vessel is fitted with cooling coils, since the chlorination reactions are exothermic, and a reflux condenser. The purpose of the reflux condenser is to return vaporized chlorobenzenes to the system, while allowing the hydrogen chloride and excess chlorine vapor to leave the system. In order to maintain the reacting mixture at a uniform temperature and to minimize mass-transfer effects, the reacting mixture is well agitated.

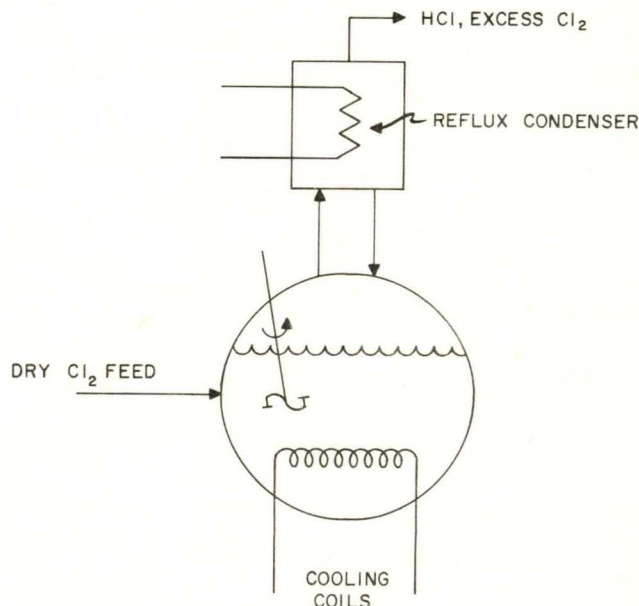


Figure 1. Semi-Batch Reactor Diagram

No chlorobenzenes can be formed until some of the chlorine gas, which is being bubbled through the liquid benzene, has gone into solution. The amount of chlorine which is capable of going into solution

is limited by the solubility of chlorine in the reacting mixture, which depends on the operating conditions of the reactor. Since the chlorobenzenes are formed successively, the concentrations of mono- and dichlorobenzene will each pass through a definite maximum at some time during the process. Eventually, all of the benzene will have reacted to pure trichlorobenzene (and other chloro-hydrocarbons, which have been neglected).

The following restrictions can be made on the system:

- (1) No liquid or vapor hold-up occurs in the reflux condenser.
- (2) The system operates under isothermic and isobaric conditions.
- (3) Changes in the volume of the reacting mixture are negligible.
- (4) Hydrogen chloride gas vaporizes and leaves the system.
- (5) Negligible mass transfer resistance occurs between the gaseous chlorine and the chlorine in solution (up to solubility limit of chlorine).

THE MATHEMATICAL MODEL

The equations defining the reaction kinetics of the system, given in several references (2,5), are

$$V \frac{dN_B(t)}{dt} = -k_1 N_B(t) N_C(t) \quad (4)$$

$$V \frac{dN_M(t)}{dt} = k_1 N_B(t) N_C(t) - k_2 N_M(t) N_C(t) \quad (5)$$

$$V \frac{dN_D(t)}{dt} = k_2 N_M(t) N_C(t) - k_3 N_D(t) N_C(t) \quad (6)$$

and

$$V \frac{dN_T(t)}{dt} = k_3 N_D(t) N_C(t) \quad (7)$$

where

V = Volume of reacting mixture

t = Time

N(t) = Moles per unit volume

k = Rate constant in volume per unit mole per unit time.

and the subscripts represent the following:

C = Chlorine

M = Monochlorobenzene

D = Dichlorobenzene

T = Trichlorobenzene

B = Benzene

1 = Reaction producing monochlorobenzene

2 = Reaction producing dichlorobenzene

3 = Reaction producing trichlorobenzene

These equations have the initial conditions:

$$N_B(0) = N_O \quad (8A)$$

$$N_C(0) = 0 \quad (8B)$$

$$N_M(0) = 0 \quad (8C)$$

$$N_D(0) = 0 \quad (8D)$$

$$N_T(0) = 0 \quad (8E)$$

Equations 4-7 can be added and integrated to obtain the benzene material balance equation

$$N_O = N_B(t) + N_M(t) + N_D(t) + N_T(t) \quad (9)$$

If the mass transfer effect of chlorine being transferred from the vapor to the liquid phase is neglected, the chlorine concentration in the system is described by the material balance equation

$$\underbrace{N_C(t)}_{\text{moles of chlorine in solution}} = \underbrace{\int_0^t r dt}_{\text{moles of chlorine supplied}} - \underbrace{x(t)}_{\text{moles of chlorine reacted}} \quad (10)$$

where x(t) represents the moles of chlorine reacted and r denotes a constant chlorine feed rate in moles per unit time. The chlorine reacted can be obtained

(in terms of the chlorobenzene concentrations) from the stoichiometry of the system, namely

$$x(t) = N_M(t) + 2 N_D(t) + 3N_T(t) \quad (11)$$

The solubility of chlorine in the reacting mixture was obtained by considering the total pressure above the liquid, π , which is equal to the sum of the partial pressures, p , of the individual components in the vapor phase. Thus

$$\pi = p_C(t) + p_B(t) + p_M(t) + p_D(t) + p_T(t) \quad (12)$$

Since its tenure in the system is only momentary, the partial pressure of hydrogen chloride was neglected.* By applying Raoult's Law, which states that the partial pressure is equal to the product of the mole fraction, $\frac{N(t)}{N_O + N_C(t)}$, and the vapor pressure, p° , equation 12 becomes

$$\begin{aligned} \pi = & \frac{N_C(t)}{N_O + N_C(t)} p_C^\circ + \frac{N_B(t)}{N_O + N_C(t)} p_B^\circ + \frac{N_M(t)}{N_O + N_C(t)} p_M^\circ + \\ & \frac{N_D(t)}{N_O + N_C(t)} p_D^\circ + \frac{N_T(t)}{N_O + N_C(t)} p_T^\circ \end{aligned} \quad (13)$$

This equation can be solved for the maximum chlorine concentration, $N_C(t)$, to obtain

$$\begin{aligned} \bar{N}_C(t) = & \frac{N_O}{p_C^\circ - \pi} \left[\pi - \frac{N_B(t)}{N_O} p_B^\circ - \frac{N_D(t)}{N_O} p_D^\circ \right. \\ & \left. - \frac{N_T(t)}{N_D} p_T^\circ \right] \end{aligned} \quad (14)$$

Since the vapor pressures are functions of temperature only and the system is isothermal and isobaric, the maximum chlorine concentration depends only on the chlorobenzene concentrations. Any excess chlorine supplied to the system leaves it through the reflux condenser.

A more convenient form** of the system equations may be obtained by defining

$$h = \frac{k N_O}{V} \quad (15)$$

$$\theta = h t \quad (16)$$

*System operated above critical temperature of HCl.

**The equations were written in terms of θ , $\frac{k_2}{k_1}$, and $\frac{k_3}{k_1}$ because experimental data was available on the ratios of the rate constants; and k_1 was unknown.

$$C(\theta) = N_C(\theta) / N_O \quad (17)$$

$$B(\theta) = N_B(\theta) / N_O \quad (18)$$

$$M(\theta) = N_M(\theta) / N_O \quad (19)$$

$$D(\theta) = N_D(\theta) / N_O \quad (20)$$

$$T(\theta) = N_T(\theta) / N_O \quad (21)$$

$$X(\theta) = x(\theta) / N_O \quad (22)$$

$$G = \frac{r}{N_O h_1} \quad (23)$$

Using these definitions, equations 4 - 7, 9 and 11 become

$$\frac{dB(\theta)}{d\theta} = -B(\theta)C(\theta) \quad (24)$$

$$\frac{dM(\theta)}{d\theta} = B(\theta)C(\theta) - \left[\frac{k_2}{k_1} \right] M(\theta)C(\theta) \quad (25)$$

$$\frac{dD(\theta)}{d\theta} = \left[\frac{k_2}{k_1} \right] M(\theta)C(\theta) - \left[\frac{k_3}{k_1} \right] D(\theta)C(\theta) \quad (26)$$

$$\frac{dT(\theta)}{d\theta} = \left[\frac{k_3}{k_1} \right] D(\theta)C(\theta) \quad (27)$$

$$1 = B(\theta) + M(\theta) + D(\theta) + T(\theta) \quad (28)$$

$$X(\theta) = M(\theta) + 2D(\theta) + 3T(\theta) \quad (29)$$

Equation 10 can now be represented as

$$C(\theta) = \int_0^\theta G d\theta - X(\theta) \quad (30)$$

which can be differentiated to obtain

$$\frac{dC(\theta)}{d\theta} = G - \frac{dX(\theta)}{d\theta} \quad (31)$$

or, by substituting

$$\begin{aligned} \frac{dC(\theta)}{d\theta} = & G - \left[B(\theta)C(\theta) + \left(\frac{k_2}{k_1} \right) M(\theta)C(\theta) + \left(\frac{k_3}{k_1} \right) \right. \\ & \left. D(\theta)C(\theta) \right] \end{aligned} \quad (32)$$

Equation 32 is the best form of the chlorine concentration equation for computational purposes.

The operating temperature and pressure used in this investigation are 55 deg. C--which is typical of the operating temperature used in industry for

this system (4)--and 2 absolute atmospheres-- which was assumed. Based on these operating conditions, the saturation concentration of chlorine, $C(\theta)$, can be assumed constant and equal to 0.120. The proof of this fact is shown in Appendix A. This means that the constraint on equation 32 is

$$C(\theta) \leq \bar{C} = 0.120 \quad (33)$$

PROGRAMMING THE COMPUTER***

This problem, which was solved on a ± 10 volt PACE[®], TR-10 General Purpose Analog Computer, presents no magnitude scaling problems. From the stoichiometry of the system it is obvious that $B(\theta)$, $M(\theta)$, $D(\theta)$, and $T(\theta)$ cannot exceed unity and that $X(\theta)$ cannot exceed three. The chlorine concentration, $C(\theta)$, is limited to 0.120; therefore its maximum value is obvious. These maximum values and their associated scale factors and computer voltages are tabulated in Table I. Table II lists the systems parametric data.

TABLE I. MAGNITUDE SCALING

Physical Variable (Dimensionless)	Estimated Maximum Value (Dimensionless)	Scale Factor Volts Per Dim. Unit	Computer Variable (Volts)
B	1.0	10	[10 B]
M	1.0	10	[10 M]
D	1.0	10	[10 D]
T	1.0	10	[10 T]
X	3.0 < 4.0	2.5	[2.5 X]
C	0.12 < 0.2	50	[50 C]

TABLE II. PARAMETER DATA

$$\frac{k_2}{k_1} = 0.125^{(2)} \quad \text{Dimensionless}$$

$$\frac{k_3}{k_1} = 0.00417^{(2)} \quad \text{Dimensionless}$$

$$0 \leq G \leq 0.008 \quad (\text{ASSUMED}) \quad \text{Dimensionless}$$

The scaled voltage equations, which are based on the information contained in Tables I and II, are

$$\frac{d}{d\tau} [10 B] = -10 \left(\frac{1}{50\beta} \right) \frac{[10B] [50C]}{10} \quad (34)$$

$$\frac{d}{d\tau} [10M] = 10 \left(\frac{1}{50\beta} \right) \frac{[10B][50C]}{10} - \left(\frac{k_2}{5k_1} \right) \frac{[10M][50C]}{10} \quad (35)$$

$$\frac{d}{d\tau} [10T] = \left(\frac{k_2}{5k_1\beta} \right) \frac{[10M][50C]}{10} - \left(\frac{k_3}{5k_1\beta} \right) \frac{[10D][50C]}{10} \quad (36)$$

$$\frac{d}{d\tau} [10T] = \left(\frac{k_3}{5k_1\beta} \right) \frac{[10D][50C]}{10} \quad (37)$$

$$[2.5X] = 0.250 [10M] + 0.500 [10D] + 0.750 [10T] \quad (38)$$

$$\frac{d}{d\tau} [50C] = \left(\frac{5G}{\beta} \right) [10] - \left[\left(\frac{1}{\beta} \right) \frac{[10B][50B]}{10} + \left(\frac{k_2}{k_1\beta} \right) \frac{[10M][50C]}{10} + \left(\frac{k_3}{k_1\beta} \right) \frac{[10D][50C]}{10} \right] \quad (39)$$

4

$$[50 C] \leq [50 \bar{C}] = 6.00 \text{ volts} \quad (40)$$

where machine time, τ , is defined in terms of the time scale factor β , and θ as

$$\tau = \beta \theta \quad (41)$$

The computer diagram implementing these equations is shown in Figure 2 and the components used are summarized in Appendix C. Potentiometer and amplifier assignments are tabulated in Tables III and IV. The time scale factor chosen for this problem was 0.05 (seconds of machine time per dimensionless unit). This choice was based on the fact that the feedback to the integrators had to be attenuated by responsible potentiometer settings in order to run the problem in a reasonable length of computer time ($20 \leq \tau \leq 100$ seconds).

When fitting experimental data to determine rate constants, it is advantageous to plot the results in time, t , rather than in the dimensionless variable, θ , since the kinetic data will be in terms of time. Time, which is related to θ by equation 16, can be obtained from the equation

$$\frac{dt}{d\theta} = \frac{1}{h_1} = \frac{V}{k_1 N_0} \quad (42)$$

***It is assumed that the reader is familiar with fundamentals of analog computer programming.

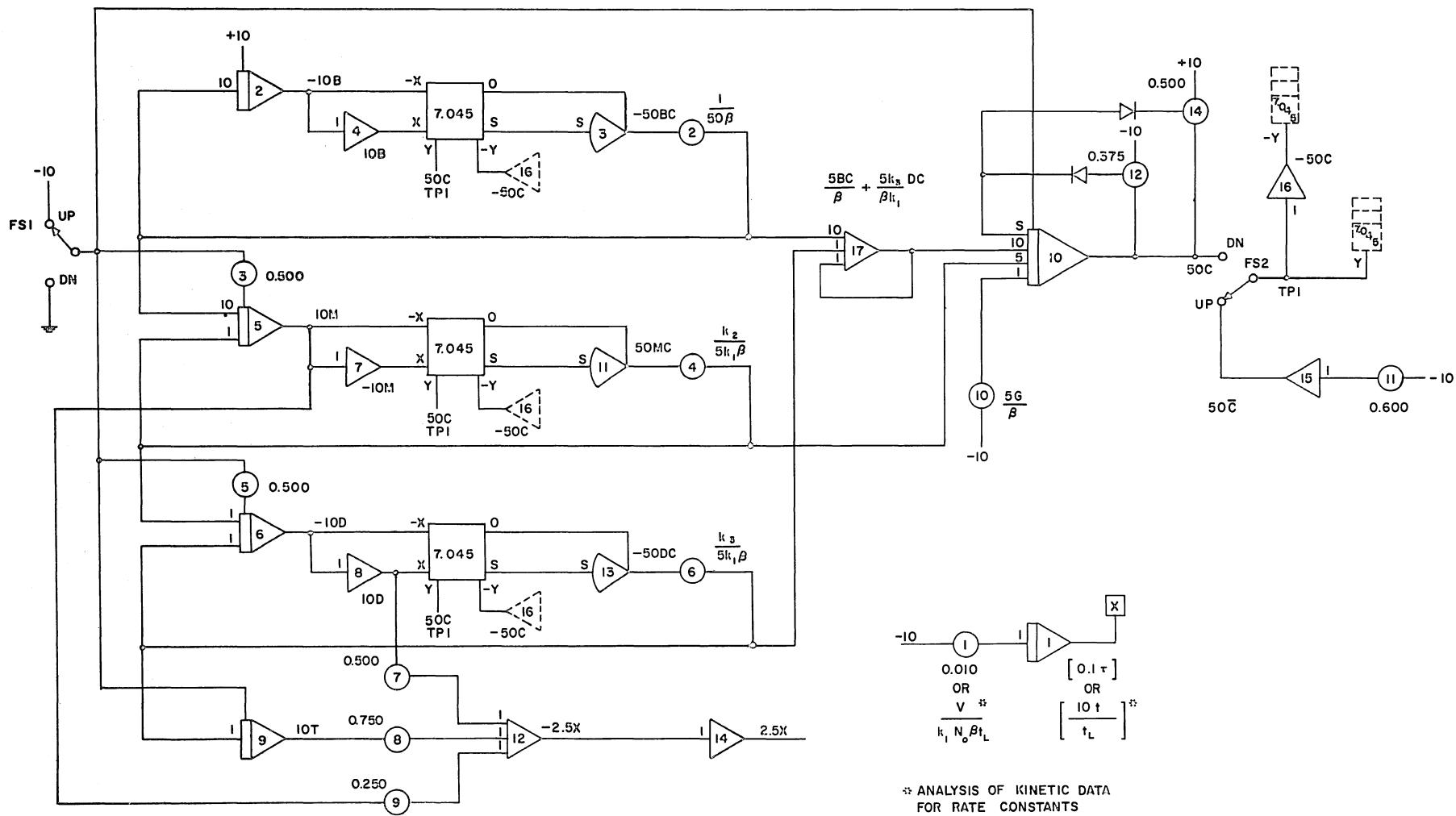


Figure 2. Computer Diagram

TABLE III

ELECTRONIC ASSOCIATES INC.
EDUCATION & TRAINING GROUP

TR-10 POTENTIOMETER ASSIGNMENT SHEET

PROBLEM Semi-Batch Reactor

DATE _____

POT NO.	PARAMETER DESCRIPTION	SETTING STATIC CHECK	STATIC CHECK OUTPUT VOLTAGE	SETTING RUN NUMBER I	NOTES	POT NO.
1	CONSTANT $\alpha V/k, N_0 t_L \beta$	0.010			→	1
2	$1/50\beta$	0.100	0.400		→	2
3	CONSTANT	0.500			→	3
4	$k_2/5k, \beta$	0.500			→	4
5	CONSTANT	0.500			→	5
6	$k_3/5k, \beta$	0.500	0.017		→	6
7	CONSTANT	0.500			→	7
8	CONSTANT	0.750			→	8
9	CONSTANT	0.250			→	9
10	$5G/\beta$	0.100	0.000		→	10
11	CONSTANT	0.600			→	11
12	LIMIT	0.375			→ APPROXIMATE	12
13						13
14	LIMIT	0.500			→ APPROXIMATE	14
15						15
16						16
17						17
18						18
19						19
20						20
21						21
22						22
23	FS1	UP	DN		→	23
24	FS2	UP	UP	DN	→	24

TABLE IV

ELECTRONIC ASSOCIATES INC
EDUCATION & TRAINING GROUP

TR-10 AMPLIFIER ASSIGNMENT SHEET

PROBLEM Semi-Patch Reactor

DATE _____

AMP NO.	FB	OUTPUT VARIABLE	STATIC CHECK				NOTES
			CALCULATED		MEASURED		
			INTEGRATOR INPUT SUM	OUTPUT	INTEGRATOR INPUT SUM	OUTPUT	
1	I	$v_{10} \text{ or } 10t/t_L^*$	0.10 [†]	10.00			
2	I	-10B	6.00 [†]	-10.00			
3	HG	-50BC		-6.00			
4	S	10B		10.00			
5	I	10M	4.50 [†]	5.00			
6	I	-10D	-3.00 [†]	5.00			
7	S	-10M		-5.00			
8	S	10D		-5.00			
9	I	10T	-1.50 [†]	10.00			
10	I	50C	-3.00 ^{**}	10.00			LIMIT TO 6.00volts
11	HG	50MC		3.00			
12	S	-2.5X		-6.25			
13	HG	-50DC		3.00			
14	S	2.5X		6.25			
15	S	50C		6.00			
16	S	-50C		6.00			
17	S	$5BC/\beta + 5R_3 DC/R_2\beta$		2.38			
18		* ANALYSIS OF KINETIC DATA FOR RATE CONSTANTS					
19		† 100K FEEDBACK IN CHECK AMPLIFIER					
20		** 10K FEEDBACK IN CHECK AMPLIFIER					

TABLE V. TIME OF MAXIMUM PRODUCTION
VERSUS CHLORINE FLOWRATE
DATA

θ Max Dimensionless		G Dimensionless	1/G Dimensionless
M	D		
22	264		0
160	430	0.008	125
210	520	0.006	167
305	680	0.004	250
585	1230	0.002	500

whose scaled voltage representation is

$$\frac{d [IO t / t_L]}{d \tau} = \left(\frac{V}{\beta k_1 N_{O^+} t_L} \right) [IO] \quad (43)$$

The symbol t_L is the maximum time required for the data analysis, and depends on the data being fitted.

A dynamic check of the computer circuit was made after completion of successful static check. The dynamic check consisted of checking the maximum concentration of monochlorobenzene and the time at which the maximum occurred, against the computer results for a special case of reactor operation. The special case (FSI - DN, FS2-UP) assumes that the chlorine flow rate is infinite and that the reaction mixture is always saturated with chlorine. Calculations made on this basis indicate the maximum value of $M(\theta)$ will be 0.74 when θ is 22 (Refer to Appendix B).

RESULTS

In addition to the dynamic check run, as shown in Figure 3, four additional runs were made at values of G ranging from 0.002 to 0.008. These results, which are plots of $B(\theta)$, $M(\theta)$, $D(\theta)$, $T(\theta)$, $X(\theta)$ and $C(\theta)$ versus θ , are shown in Figures 4-7. From this information, it was possible to obtain the values of θ , θ_{max} at which the maximum amount of

the intermediate products was present in the system. This data and the corresponding values of the flow rate variable, G , are tabulated in Table V. A plot of $\log \theta_{max}$ versus $1/G$ is shown in Figure 8 for each of the intermediate products.

Figure 9, which is a plot of $B(t)$, $M(t)$, $D(t)$, and $T(t)$ versus time for three values of k_3/k_1 , serves to illustrate how experimental data can be fitted using the analog computer. By varying the reaction rate constants, which are unknown, the computer solution can be made to coincide with the experimental results to obtain these constants.

When this trial and error process is performed in real time, using an X-Y plotter, it is quite time-consuming. However, when high speed repetitive operation, which yields up to 60 solutions per second, is used in conjunction with an oscilloscope, a transparent overlay of the experimental data can be fitted in a matter of minutes, due to the fact that the effect of parameter variations on computer results can be observed instantly on the high persistence scope.

CONCLUSIONS

From Figure 3-7 it is obvious that the maximum reduced concentration of the intermediates is independent of the chlorine flow rate. These maximums, which occur at 0.74 and 0.88, can only be altered by changes in the reaction rate constants. This can be verified by consulting Figure 9. The chlorine feed rate, which controls the amount of chlorine available for reaction, affects the time at which the maximum concentrations occur. As shown in Figure 8, when the chlorine flow rate is infinite ($1/G = 0$) and the reaction mixture is always saturated with chlorine, θ_{max} has its minimum values of 22 and 264. When the chlorine feed rate is reduced, θ_{max} increases. Obviously, if the feed rate of chlorine is zero ($1/G \rightarrow \infty$), θ_{max} must be infinite.

The curve fitting technique mentioned in the results section, which is for the most part qualitative, serves only as an illustration of what can and has been done on the general purpose analog computer in regard to the analysis of kinetics data.

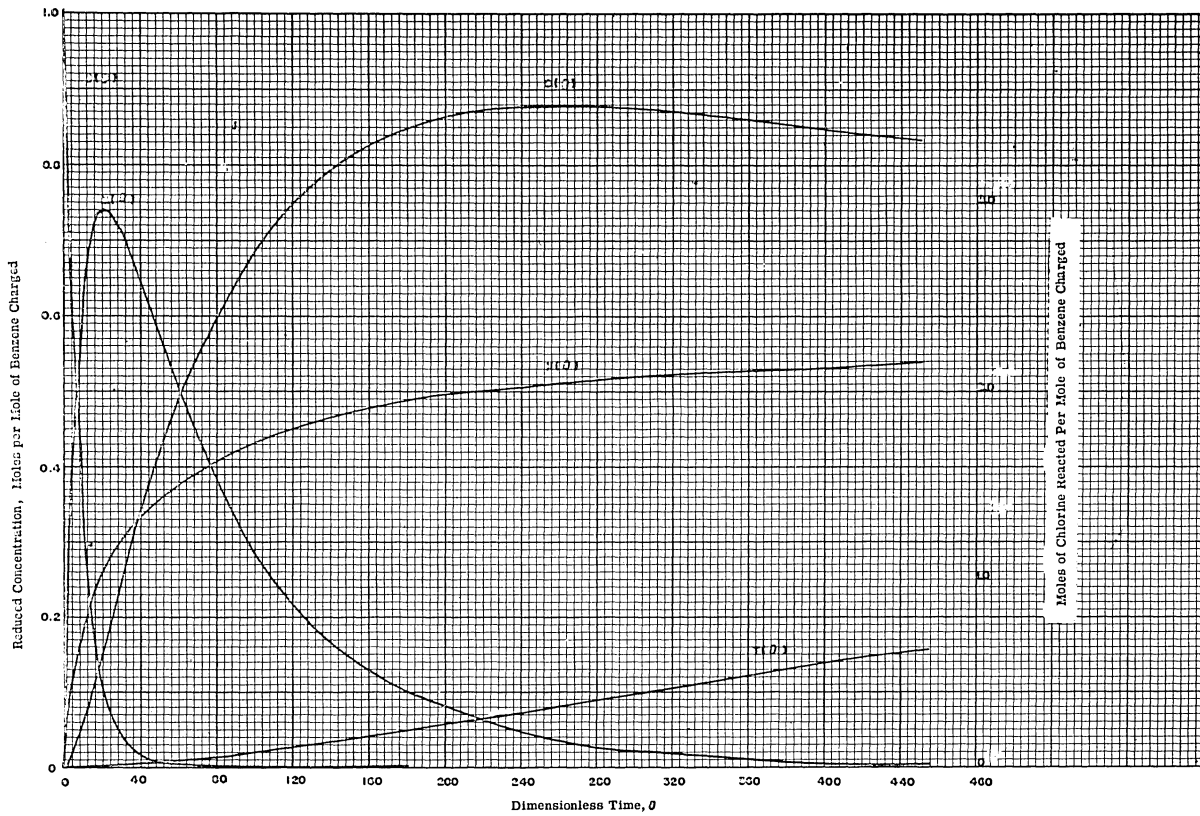


Figure 3. Reduced Concentrations Versus Dimensionless Time For Infinite Chlorine Feed Rate

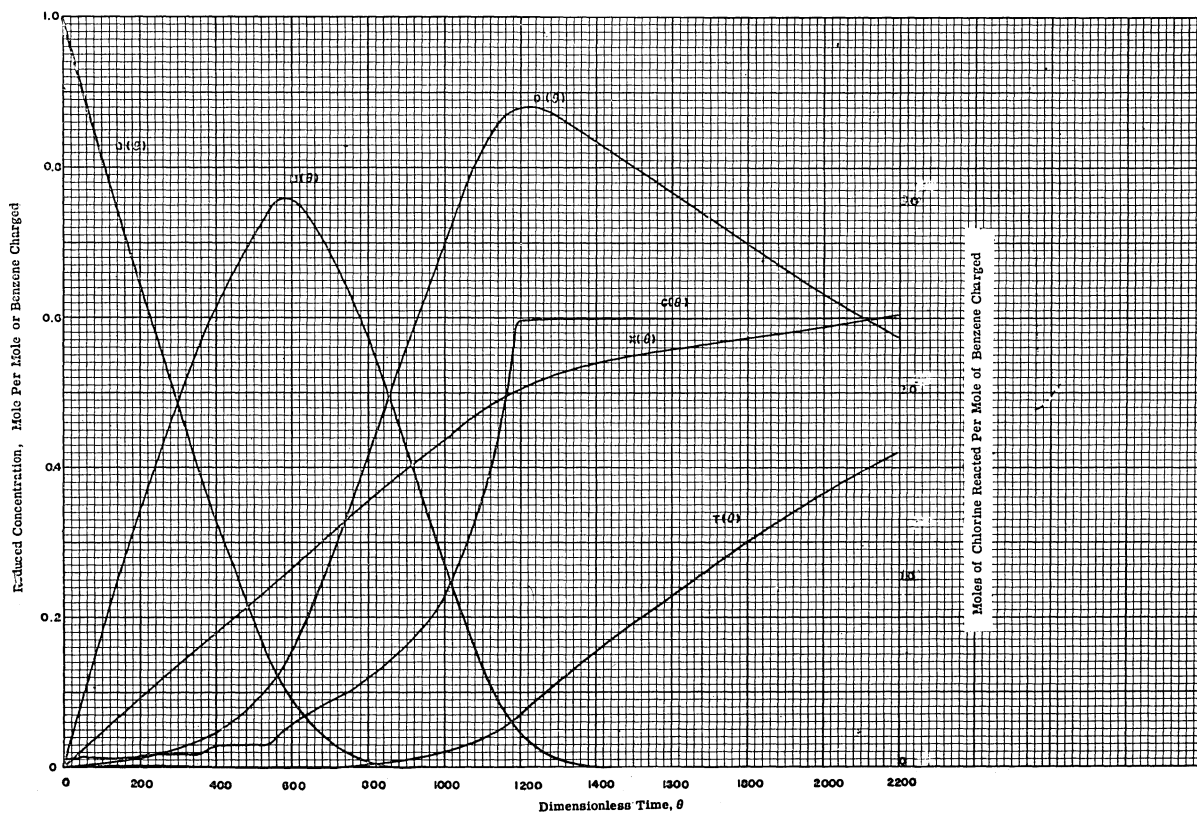


Figure 4. Reduced Concentrations Versus Dimensionless Time ($G = 2.0 \times 10^{-3}$)

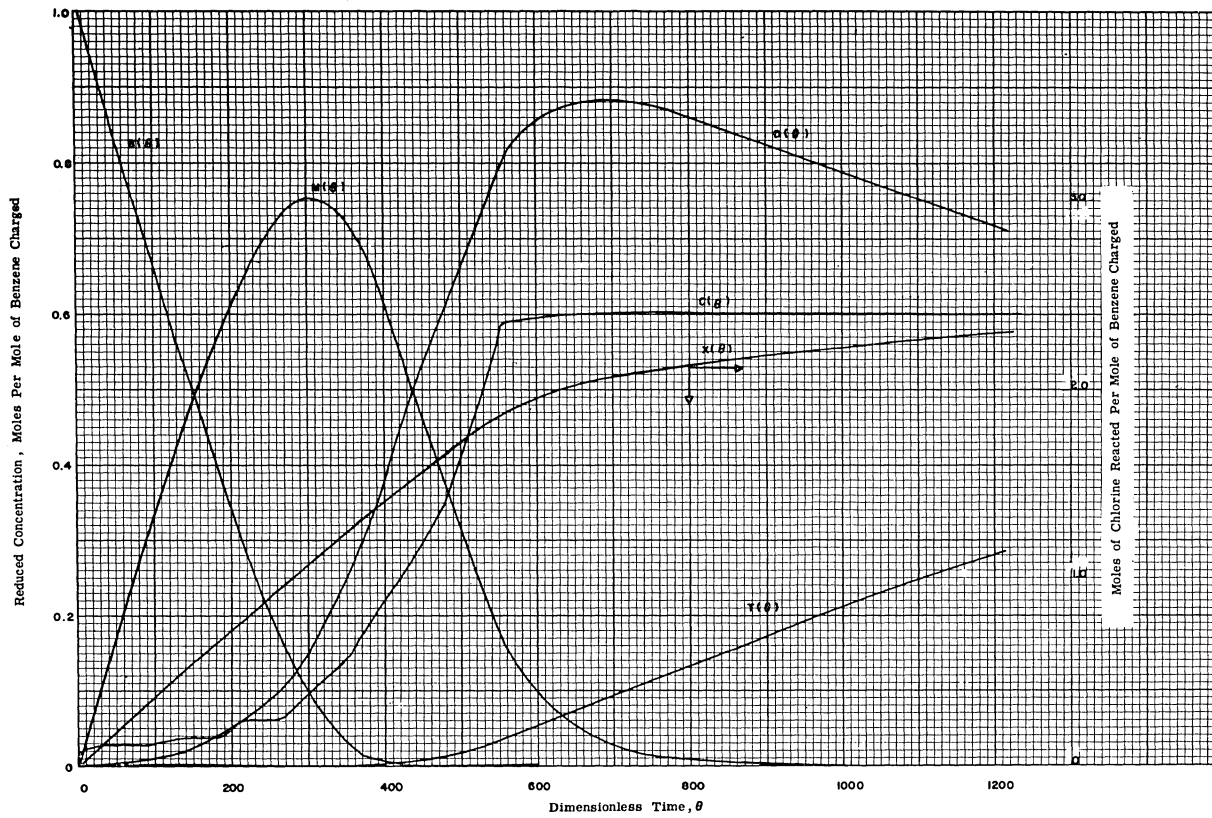


Figure 5. Reduced Concentrations Versus Dimensionless Time ($G = 4.0 \times 10^{-3}$)

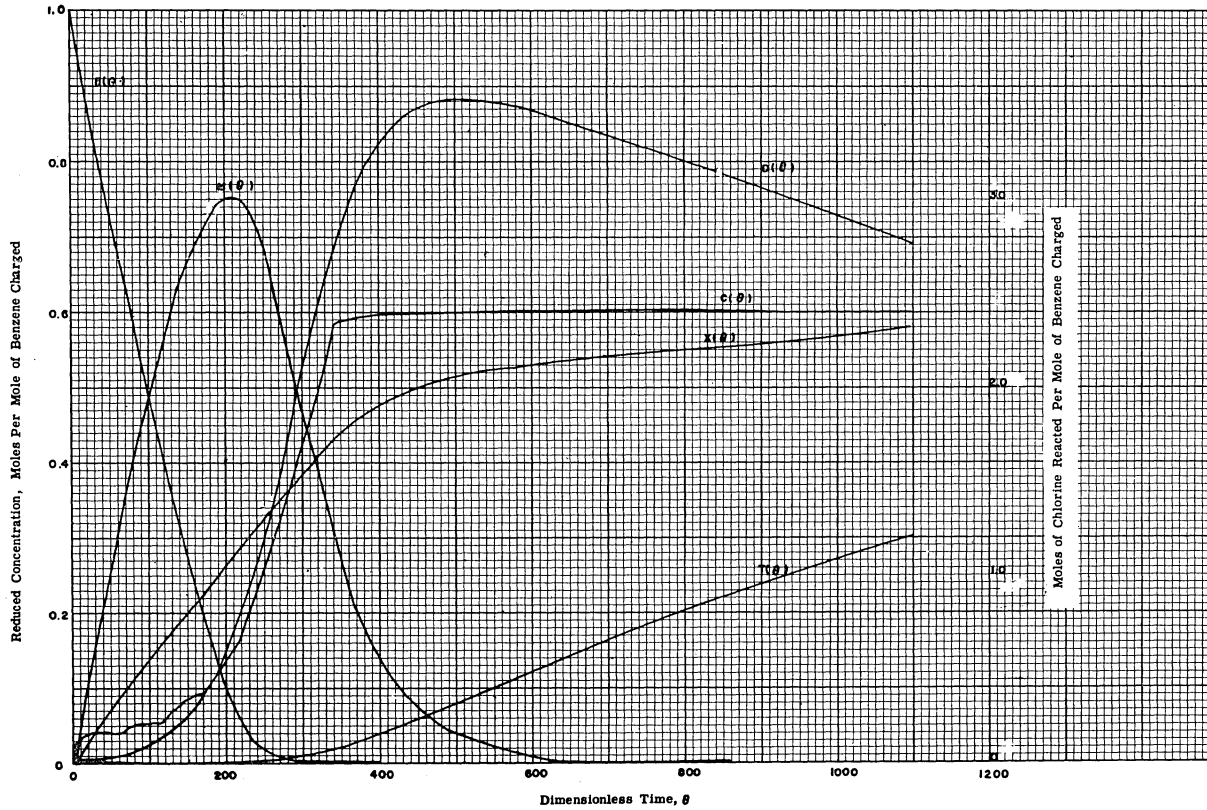


Figure 6. Reduced Concentrations Versus Dimensionless Time ($G = 6.0 \times 10^{-3}$)

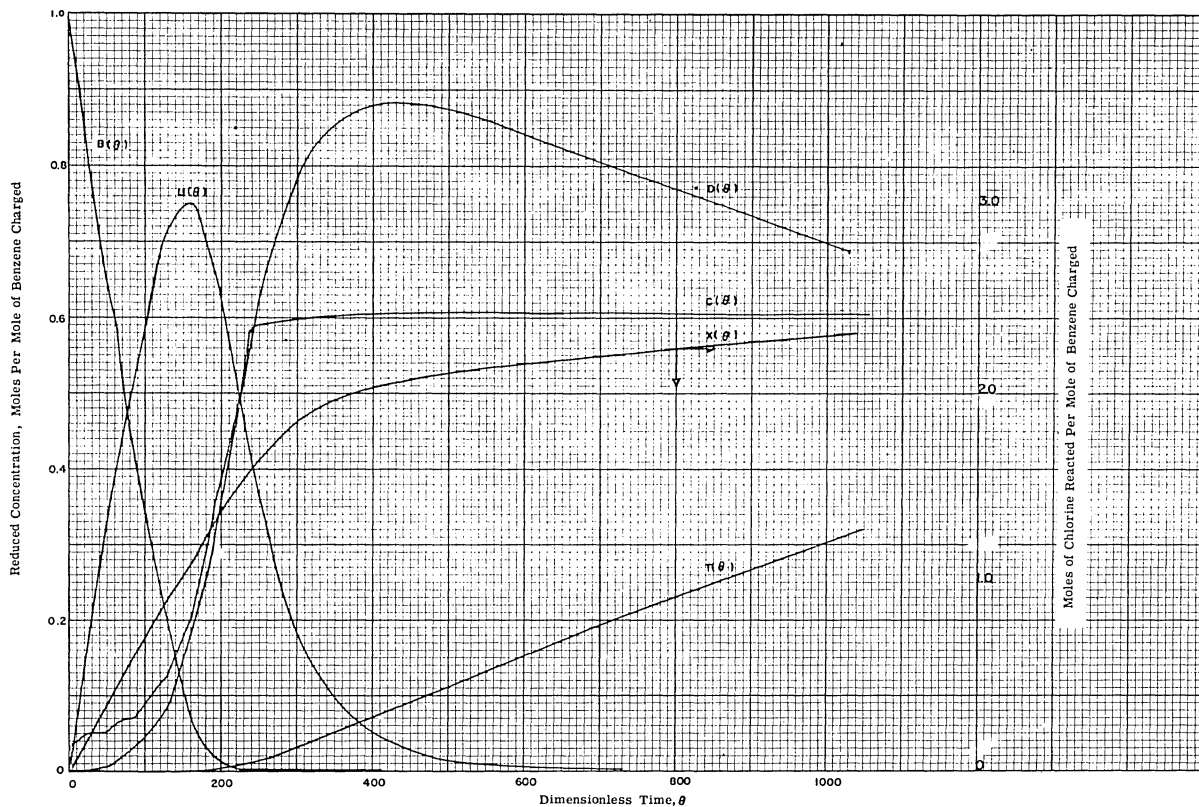


Figure 7. Reduced Concentration Versus Dimensionless Time ($G = 8.0 \times 10^{-3}$)

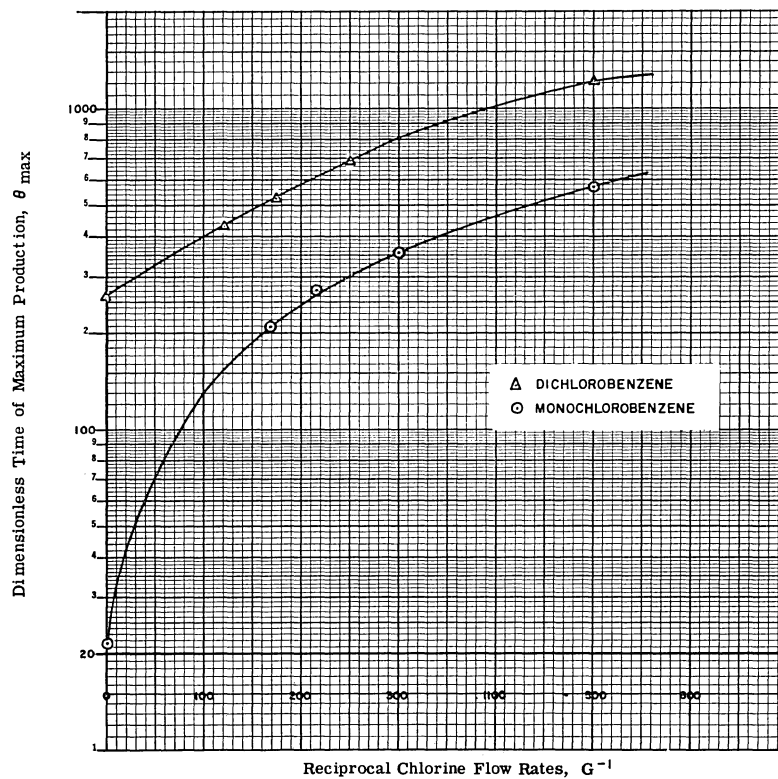


Figure 8. Dimensionless Time of Maximum Mono- and Dichlorobenzene Production Versus Reciprocal Chlorine Flow Rate

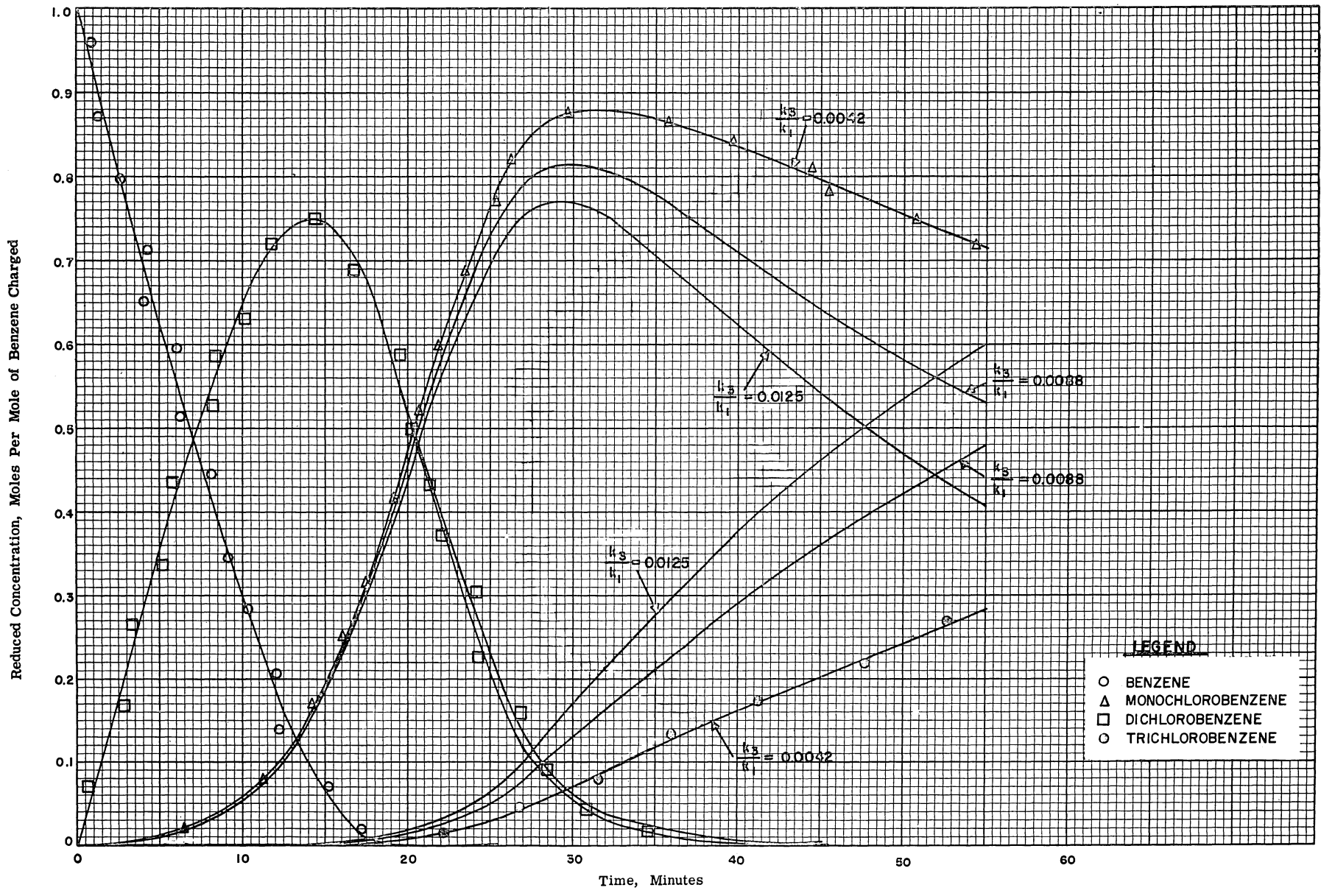


Figure 9. Reduced Concentrations Versus Time, Comparison of Experimental and Computer Results

APPENDIX A
SOLUBILITY CONSTRAINT CALCULATIONS

The vapor pressure data at the 55 deg. C operating temperature, necessary to solve the equation

$$\bar{C}(t) = \frac{1}{p_C^\circ - \pi} \left[\pi - B(t)p_B^\circ - M(t)p_M^\circ - D(t)p_D^\circ - T(t)p_T^\circ \right] \quad (A-1)$$

is tabulated in Table VI.

TABLE VI. VAPOR PRESSURE DATA AT 55 C

<u>Component</u>	<u>Vapor Pressure</u>	<u>Data Source</u>
Benzene	327 mm of HG	3
Monochlorobenzene	48,8 mm of HG	3
Dichorobenzene	11,5 mm of HG	3
Trichlorobenzene	<5 mm of HG	3
Chlorine	16,9 ATM	1

If this data is substituted into equation A-1, it can be seen that for all practical purposes since the total pressure is two atmospheres (see Table II), and the concentration variables cannot exceed unity. Based on equation A-2 the range of C(t) is

$$\bar{C}(t) = \frac{1}{p_C^\circ - \pi} \left(\pi - B(t)p_B^\circ \right) \quad (A-2)$$

$$0.105 < \bar{C}(t) < 0.134 \quad (A-3)$$

which is very narrow; therefore, variations in C(t) will have little effect on the results of the problem. The average value of C(t), 0.120, was considered sufficiently accurate for this study.

APPENDIX B

DYNAMIC CHECK CALCULATIONS

If the reacting mixture is always saturated with chlorine, the equations describing the behavior of monochlorobenzene and benzene are

$$\frac{dB}{d\xi}(\xi) = -B(\xi) \quad (B-1)$$

and

$$\frac{dM}{d\xi}(\xi) = B(\xi) - \frac{k_2}{k_1} M(\xi) \quad (B-2)$$

where

$$\xi = \bar{C}\theta \quad (B-3)$$

These equations have the initial conditions

$$B(0) = 1 \quad (B-4)$$

$$\text{and } M(0) = 0 \quad (B-5)$$

The solution to equation B-1 is

$$B(\xi) = e^{-\xi} \quad (B-6)$$

which can be substituted into equation B-2 to obtain

$$\frac{dM(\xi)}{d\xi} + \frac{k_2}{k_1} M(\xi) = e^{-\xi} \quad (B-7)$$

whose solution is

$$M(\xi) = \frac{1}{1 - \frac{k_2}{k_1}} \left[e^{-\frac{k_2}{k_1}\xi} - e^{-\xi} \right] \quad (B-8)$$

The maximum concentration of $M(\xi)$ occurs when

$$\frac{dM(\xi)}{d\xi} = 0 = e^{\xi'} - \frac{k_2}{k_1} e^{-\frac{k_2}{k_1}\xi'} \quad (B-9)$$

where ξ' is the value of the argument at which the maximum occurs . . .

$$\xi' = \frac{1}{1 - \frac{k_2}{k_1}} \ln \frac{k_1}{k_2} \quad (B-10)$$

This may be substituted back into equation B-8 to obtain the maximum value of $M(\xi)$

$$M(\xi') = \left(\frac{k_2}{k_1} \right)^{\frac{k_2/k_1}{1 - k_2/k_1}} \quad (B-11)$$

Since $\frac{k_2}{k_1}$ is one-eighth (see Table II) and C is 0.12 (see Appendix A)

$$M(\xi) = 0.74 \quad (B-12)$$

$$\text{and } \theta' = \frac{\xi'}{C} = 22 \quad (B-13)$$

APPENDIX C

EQUIPMENT REQUIRED TO PERFORM SIMULATION

The equipment required to perform this simulation was:

1 - X-Y Plotter

3 - Quarter Square Multipliers

17 - Operational Amplifiers

6 - Integrator Networks

13 - Potentiometers

and

2 - Function Switches

NOMENCLATURE

B = Reduced Benzene concentration, dimensionless
C = Reduced Chlorine concentration, dimensionless
C = Reduced Maximum Chlorine concentration, dimensionless
D = Reduced Dichlorobenzene concentration, dimensionless
G = Modified chlorine flowrate, dimensionless
M = Reduced Monochlorobenzene concentration, dimensionless
N = Concentration variable, moles
 N_C = Maximum chlorine concentration, moles
T = Reduced trichlorobenzene concentration, dimensionless
V = Volume of reacting mixture, cubic feet
X = Reduced reacted chlorine variable, dimensionless
h = Modified rate constant, seconds⁻¹
k = Reaction rate constant, cubic feet/mole second

p = Partial pressure, atmospheres
 p^0 = Vapor pressure, atmospheres
r = Chlorine feed rate, moles/second
t = Time, seconds
 t_L = Maximum time, seconds
x = Moles of chlorine reacted
 π = Absolute pressure, atmospheres
 θ = Dimensionless time variable, dimensionless
T = Machine time, seconds
 β = Time scale factor, seconds/dimensionless unit
 ξ = Dimensionless time variable, dimensionless

SUBSCRIPTS

B = Benzene
C = Chlorine
D = Dichlorobenzene
M = Monochlorobenzene
O = Initial Value
T = Trichlorobenzene
1 = Reaction producing Monochlorobenzene
2 = Reaction producing Dichlorobenzene
3 = Reaction producing Trichlorobenzene

REFERENCES

1. Perry, J.H., Chemical Engineers Handbook; pg. 150; 3rd Ed.; McGraw-Hill Book Co., Inc., New York, N.Y. (1950)
2. MacMullin, R.B., Distribution Reaction Products in Benzene Chlorinations; Chem. Eng. Prog: 44; 183 (1948)
3. Lange, N.A., Handbook of Chemistry; pg. 962; Handbook Publishers, Inc., Sandusky, Ohio (1934)
4. Shreve, R.N., The Chemical Process Industries; 1st Ed.; pg. 851; McGraw-Hill Book Co., Inc., New York, N.Y. (1945)
5. Smith, J.M., Chemical Engineering Kinetics; pg. 62; McGraw-Hill Co., Inc., New York, N.Y. (1956)



ELECTRONIC ASSOCIATES, INC. Long Branch, New Jersey

ADVANCED SYSTEMS ANALYSIS AND COMPUTATION SERVICES/ANALOG COMPUTERS/HYBRID ANALOG-DIGITAL COMPUTATION EQUIPMENT/SIMULATION SYSTEMS/SCIENTIFIC AND LABORATORY INSTRUMENTS/INDUSTRIAL PROCESS CONTROL SYSTEMS/PHOTOGRAMMETRIC EQUIPMENT/RANGE INSTRUMENTATION SYSTEMS/TEST AND CHECK-OUT SYSTEMS/MILITARY AND INDUSTRIAL RESEARCH AND DEVELOPMENT SERVICES/FIELD ENGINEERING AND EQUIPMENT MAINTENANCE SERVICES.