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DESIGN OF AN UNDERGRADUATE CHEMICAL ENGINEERING EXPERIMENT

(Chlorination of Benzene)

by

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I. INTRODUCTION

In 1972, T. Kurucsev [14] investigated the analytical approach to the design of laboratory experiments. He explained that a student, when assigned to do a laboratory exercise, might have either explicitly or implicitly three basic questions in mind:

What is to be learned?

What is to be done?

Is it going to be interesting?

And in broad terms, laboratory exercises serve the dual purposes of teaching or illustrating theoretical principles and teaching technical skills. Students are then instructed what to do and how to do it in order to achieve the above aims. Thus the concepts implied by the two basic questions may be referred to as:

Aims or Theory/Skill

Instructions or Do What/How?

The formalism suggested here is equivalent to arranging the above units in the form of a flowchart shown in Figure (1).

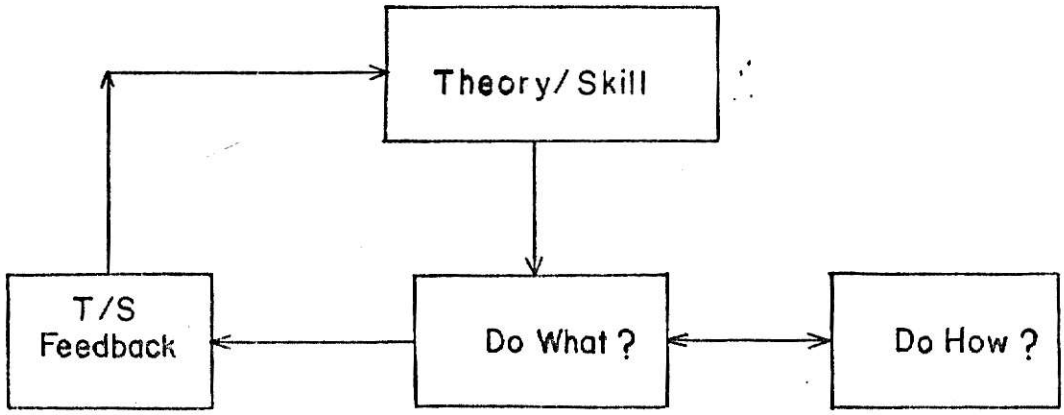

Figure 1. Block Diagram for Design and Analysis of Laboratory Exercises [14]

According to the flowchart, the design of an exercise may begin by defining a set of theoretical principles and practical skills that the students are expected to acquire. A set of experimental manipulations are then selected that serve as vehicles towards achieving the THEORY/SKILL aims. At this point the feedback from the DO WHAT/HOW? is examined to see what modifications of the original THEORY/SKILL set they may imply. The process of the design thus develops into a succession of iterations until the exercise is self-consistent. One might add that the possibility of taking DO WHAT? rather than THEORY/SKILL as the initial point of departure for the iterative process is not excluded.

The Marathon Oil Company [32]presented an industrial view of the undergraduate laboratories in which they concluded that the qualities which are most desirable for young engineers are: creativity, productivity, technical judgement, versatility, leadership, and communicability. In order to manifest these qualities, the young engineer needs to know:

1) What has to be done (problem analysis)
2) How to get it done (problem solving)
3) How to explain what has been done (communications)

Therefore an undergraduate laboratory must recognize these qualities and probably has to be designed to encourage their development.

Different universities have almost the same objectives and purposes for their chemical engineering laboratory courses. Generally in the laboratory, the basic laws and principles of chemical engineering are illustrated by actual measurements based on experimental work. The student also becomes familiar with the various instruments and apparatus used in

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the chemical industries. From his observations, he gains experience in the planning and execution of experimental work to attain specific objectives. Original thought, exercise of judgement, and resourcefulness broaden the scope of his training and install confidence in his own abilities. Therefore he develops valuable qualities of leadership through his direction of fellow students in these experiments. Also his ability to write effective reports, which adequately describe his findings and recommendations, are developed and improved [17]. In conclusion, it is possible to learn experimentation- an undergraduate engineering laboratory course can, and should, facilitate this kind of learning [6].

Presently, there is a lack of experiments containing more than one major chemical engineering operation. Most experiments are designed for a single experimental investigation, and there is little flexibility in their use. Therefore a new experiment with at least two different parts is needed to be able to investigate different chemical engineering aspects together or separately. Thus, the undergraduate would have the opportunity to see a whole chemical process presented as an experiment they can study and operate. Such an experiment must be relatively complex, but, at the same time, it must be simple enough for easy operation and understanding.

The proposed chlorination of benzene experiment (described in detail in the remainder of this thesis) seems to fulfill these requirements. It is an exothermic, heterogeneous, and catalytic reaction. A straightforward operation (distillation) may be used to separate the unreacted benzene and the chlorinated compounds. Hydrogen chloride and chlorine gases may be stripped off and absorbed by water in a packed column. The process is not difficult to control;

each stream may be controlled manually and some streams can be analyzed easily by using a gas chromatograph or approximate compositions obtained with a refractometer. Safety aspects must be considered in the design for safe operation and accident prevention. This experiment can be run as two separate units - the reactor and the distillation column as described in the flowsheet (section 3). Pressure, flow rate, concentration, and temperature may be measured to obtain data that can be used to study the process. The complete experiment involves the study of kinetics, separation techniques, and process control which can be investigated separately or as a unit. Classical control techniques or direct-digital control can be used in the study of the process.

In the following sections, a literature review, the design of the proposed experiment, the computer results, and the cost estimation will be presented. The different experimental investigations that can be made with this equipment will also be discussed in detail.

II. LITERATURE REVIEW

A) Chemical Engineering Undergraduate Laboratories

Kinetics, separation, and process control are the major parts of the proposed Chlorination of Benzene Experiment. A general review of experiments, in these areas will be given as well as a brief description of the experiments presently done in the laboratories at Kansas State.

Generally, the first experiments in kinetics are to demonstrate the difference in the behavior of batch, continuous tank, and tubular reactors with the hydrolysis of acetic anhydride as the most commonly used reaction. Often the batch experiment consists of determining the order of reaction, the rate constant, and the activation energy. Some of the objectives of CST experiments are to demonstrate both transient and steady state behavior of single stage or two-stage reactors, and to compare the results with theoretical predictions. For the tubular reactor, the extent of conversion is measured at varying flow rates in the Reynolds number range of 400 to 3500 so that the effects of transition between laminar and turbulent flow may be investigated. A typical heterogeneous catalysis experiment - isopropanol dehydrogenation and dehydration - gives the students experience with several of the important principles of heterogeneous catalysis and tubular flow reactors. The students examine the behavior of the system, at a certain temperature range, for different contact times, with emphasis on determining the effects of major variables on the conversion and selectivity of reaction. At some institutions, there are experiments such as Thermofor Catalytic cracking for the

study of the process of combustion of carbonaceous matter in the pores of a Silica-Alumina cracking catalyst and for observations of the effects of operation under diffusion-controlled, intermediate, and reaction-controlled conditions. Usually the final kinetics experiment is the modeling and simulation of one or two stirred reactors which is done by using analog and/or digital computer [1 and 17].

In distillation, the operation of the different distillation columns (such as bubble cap, packed, and sieve tray) are studied, and their behavior at equilibrium is observed. The students have to determine the overall column efficiency by using Ponchon-Savarit or McCabe-Thiele methods, the Murphree plate efficiencies for each plate, the relationship between the composition of the liquid on each plate and the plate number, and the effect of the feed location. They may also examine the mechanism of steam distillation. The analysis of transient response and feed plate location for the bubble cap distillation column is a classical experiment. Its objective is to determine the effect of feed plate location on operation of the column for various reflux ratios, to analyze the system's response to sudden changes in reflux ratio, and to model the system in accordance with this response. Few experiments deal with multicomponent distillation in the undergraduate laboratories.

In the typical undergraduate process control laboratory, the student first becomes familiar with the instrumentation. In the first experiments, he examines the response and calibration of measuring instruments. He then may investigate the characteristics of different controllers, for example the operation of a pneumatic controller with changeable control modes. Next the dynamic

parameters, which characterize the different systems, are predicted and determined by using a first or second order processes (two hydraulic tanks in series is common). Also the operating characteristics for different equipment such as distillation columns, steam jet ejectors, or centrifugal pumps are determined and their transient behavior studied. Analog and digital simulations are usually a vital part of the process control laboratory. The study and simulation of the response of the liquid level in a tank to a step changes in flow rate or of the tank temperature to a step changes in inlet water temperature, are widely used for computer simulation. By simulating the control system on an analog computer, the students have the opportunity to investigate the performance of different types of control without losing sight of the more fundamental systems relationships. Often a process can be fully analyzed without requiring access to the system components [17].

One of the recent successful approaches to large-scale computer controlled experiments has been at the University of Alberta in Canada, where a pilot-plant sized double-effect evaporater has been controlled and studied by a digital computer. Most of the control applications have been based on classical, single-variable, feedback control techniques and have not taken maximum advantage of new approaches based on modern control theory. Some of the reasons why these new methods have not been adopted include: lack of experience with experimental applications, a shortage of people trained in both the theoretical and procatical aspects of the design of such systems, and the lack of a suitable process model.

In this experiment, a generalized approach to the modeling of multi-effect evaporators is presented which separates the development of dynamic equations from the specification of evaporator configuration. The result is a modular approach which is effective and convenient to use. A tenth-order nonlinear, dynamic model of a double-effect pilot plant evaporator was derived using this approach and then simplified and linearized to produce a fifth-order state-space model which gave generally good comparisons with experimental open-loop responses. Lower-order linear models were also developed, but gave satisfactory results only for specific applications. The performance of models in the design and experimental implementation of conventional, inferential, feedforward, multivariable optimal, and state-driving control systems was also examined. The schematic diagram of the double-effect pilot plant evaporator at the University of Alberta is shown in Figure 2.

At Kansas State University, the undergraduate laboratories begin with experiments in Transport Phenomena [7], which are done in Chemical Engineering Laboratory I (spring semester, junior year) and Chemical Engineering Laboratory II (fall semester, senior year). The experiments begin with momentum transport; the students determine the viscosity of newtonian liquids, the velocity profiles in steady state turbulent flow, the friction factor in circular tubes, and the efflux time for a tank with exit pipe. The energy transport experiments include the determination of the thermal conductivity of solids, the temperature profiles in solids, the heat-transfer coefficient in circular tubes, heating liquids in tank storage, and the operation of a double-pipe heat exchanger. The

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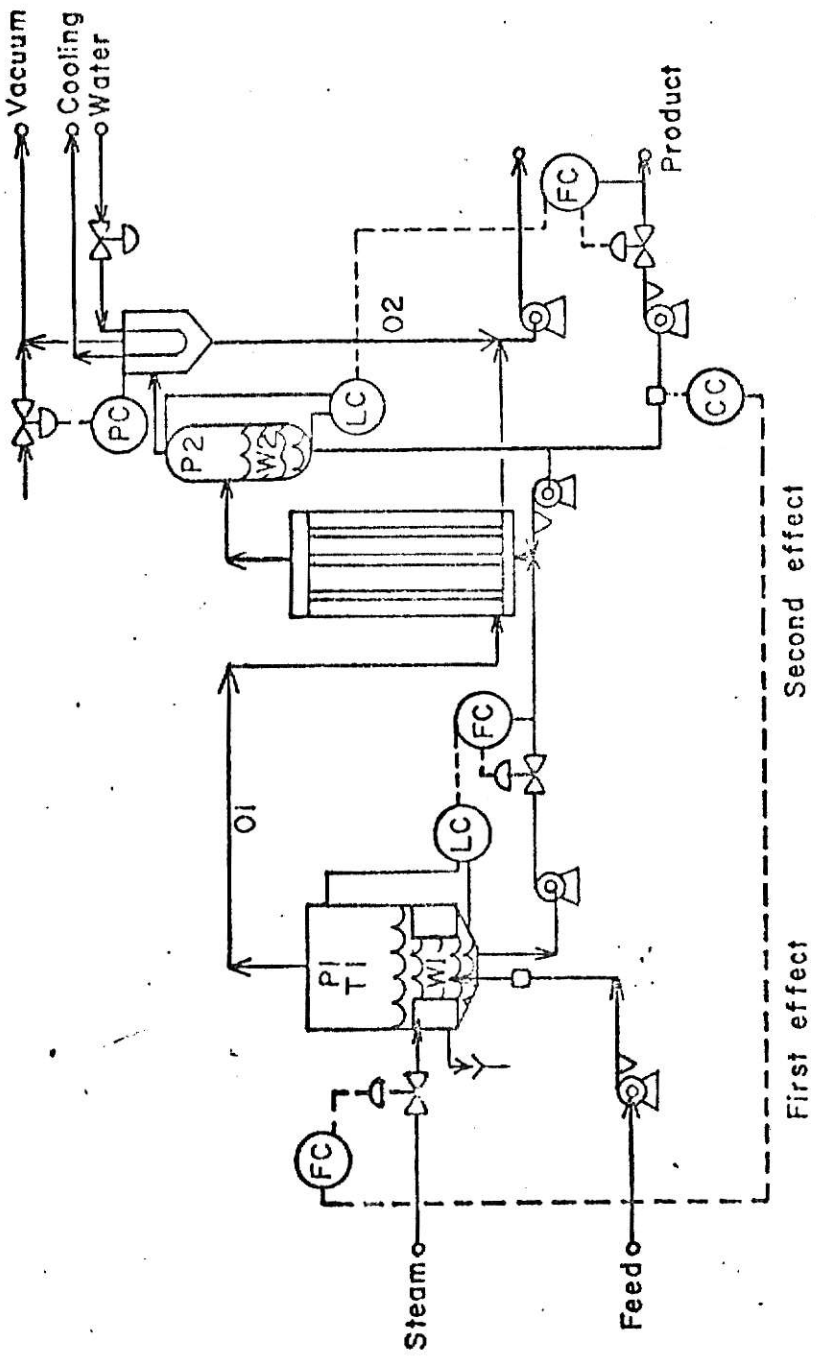


Figure 2. Schematic Diagram of the Double-effect, Pilot Plant Evaporator

determination of mass diffusivity for gases, concentration profiles in a stagnant film, mass transfer coefficient in circular tubes, and the heating value of a fuel gas are the four mass transport experiments. The theoretical background for those experiments has previously been obtained in Introduction to Process Analysis and Transport Phenomena I and II.

Chemical Engineering Laboratory III (spring semester, senior year) is mostly a Unit Operations Laboratory. It includes fractional distillation (isopropanol-water), gas absorption (water-sulfur dioxide-air), solvent extraction (isopropanol-benzene-water), solid drying, and a kinetic experiment for the determination of the activation energy and the heat of reaction for the sodium thiosulfate and hydrogen peroxide exothermic reaction in an adiabatic batch reactor.

Also in Chemical Process Dynamic and Control (spring semester, senior year), the students run three experiments which are: the Analog/Digital Simulation, the Level Control for Two Tanks, and the Dynamics and Control of a Tubular Heat Exchanger.

The laboratory sequence at Kansas State is probably about typical of most universities. The experiment at the University of Alberta is more complex than what is available at most universities.

B) Chlorination of Benzene

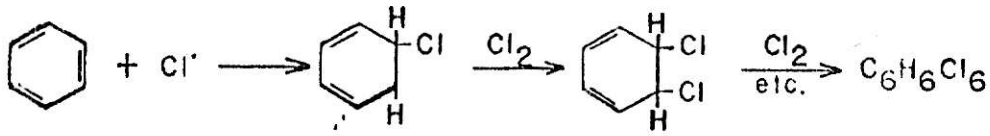
The chlorination of benzene is a very well-known industrial process. The chlorinated benzene compounds are widely produced all over the world as they are the starting raw materials for numerous industrial products such as solvents (phenols and aniline), insecticides (D.D.T.), and pesticides.

In 1920, F. Bourion [3] studied the chlorination of benzene and found that the reaction products were not affected by the rate of feeding chlorine to the reactor after a specific chlorination level. The products of the reaction were considered to contain benzene, monochlorobenzene, and

polychlorinated compounds which were separated by distillation into four principal groups depending on temperatures.

The chlorination of benzene from an organic chemistry point of view was given by L. T. Finar in 1953 [9]. He explained the addition and direct halogenation of benzene. The addition reaction mechanism is as follows:

$$Cl_2 \xrightarrow{h\nu} 2Cl^{\cdot}$$



Hexachlorocyclohexane can exist in eight stereoisomeric forms. Until recently only seven of these were known: α, β, γ, δ, ε, η and θ. The γ isomer is a powerful insecticide which is very stable and acts more quickly than dichloro-diphenyl-trichloroethane (D.D.T.)

$$C_6H_6 + Cl_2 \xrightarrow{U.V.} C_6H_6Cl_6 \quad (\alpha, \beta, \gamma, \text{ and } \delta) \qquad \gamma(12\text{-}14\%)$$

The separation may be accomplished by fractional crystallization from various organic solvents. In direct halogenation, the chlorination of benzene is carried out at ordinary temperatures in the presence of iron or aluminum amalgam catalyst.

$$C_6H_6 + Cl_2 \xrightarrow{Fe} C_6H_5Cl + HCl \quad (90\%)$$

$$C_6H_5Cl + Cl_2 \xrightarrow{Fe} C_6H_4Cl_2 + HCl \qquad o + p \text{ (predominating)}$$

The amount of substitution depends on the amount of halogen used. Monochlorobenzene is also produced commercially by the Raschig process in which a mixture of benzene vapor, air and hydrogen chloride is passed over a catalyst (copper chloride)

$$C_6H_6 + HCl + \tfrac{1}{2}O_2 \longrightarrow C_6H_5Cl + H_2O$$

Buehler and Pearson [4] noted that the percentage of dichloro-or trichloro-benzene isomers may be changed by the following two reactions:

1) o-, m-, or p- $C_6H_4Cl_2$ $\xrightarrow[160°C,\ 30\ hr\ or\ more]{AlCl_3\ (.27\ moles)}$ 54%m, 30%p and 16%o $C_6H_4Cl_2$

2) any $C_6H_3Cl_3$ + $AlCl_3$ + $MgSO_4$ $\xrightarrow[5\ hr]{200°c}$ 73% 1, 2, 4-, 24% 1, 3, 5-, and 3% 1, 2, 3-$C_6H_6Cl_3$

1 mole .34 mole .6 mole

J. S. Sconce [23], in his book, discussed the chemical reaction and the product distribution of the chlorinated benzene. The liquid phase chlorination in the absence of metals, but in presence of molecules activated by U.V., produces additive products such as hexachlorocyclohexane. The gas phase chlorination, with or without catalyst, substitutes one or more hydrogen atom of the benzene ring with chlorine. The substitution in the liquid phase, which dissolves a Friedel-Craft catalyst, by gaseous chlorine, is the major commercial process in use today for the production of chlorinated benzene. The results obtained by liquid phase chlorination of individual benzenes with anhydrous ferric chloride as the catalyst at temperatures in the range of 50° to 150°C are shown in Figure 3.

The chlorination of benzene as a unit process has been described by Groggins [12]. The industrial preparation of monochlorobenzene is generally carried out in tall narrow tanks, jacketed or surface-cooled. They are provided with a reflux condenser and may have external circulation through a cooler. Chlorine is introduced through an iron distributor pipe near the base of the reactor. Dried benzene is charged to the chlorinator along with a small quantity of anhydrous ferric chloride (0.1 - 0.5 percent).

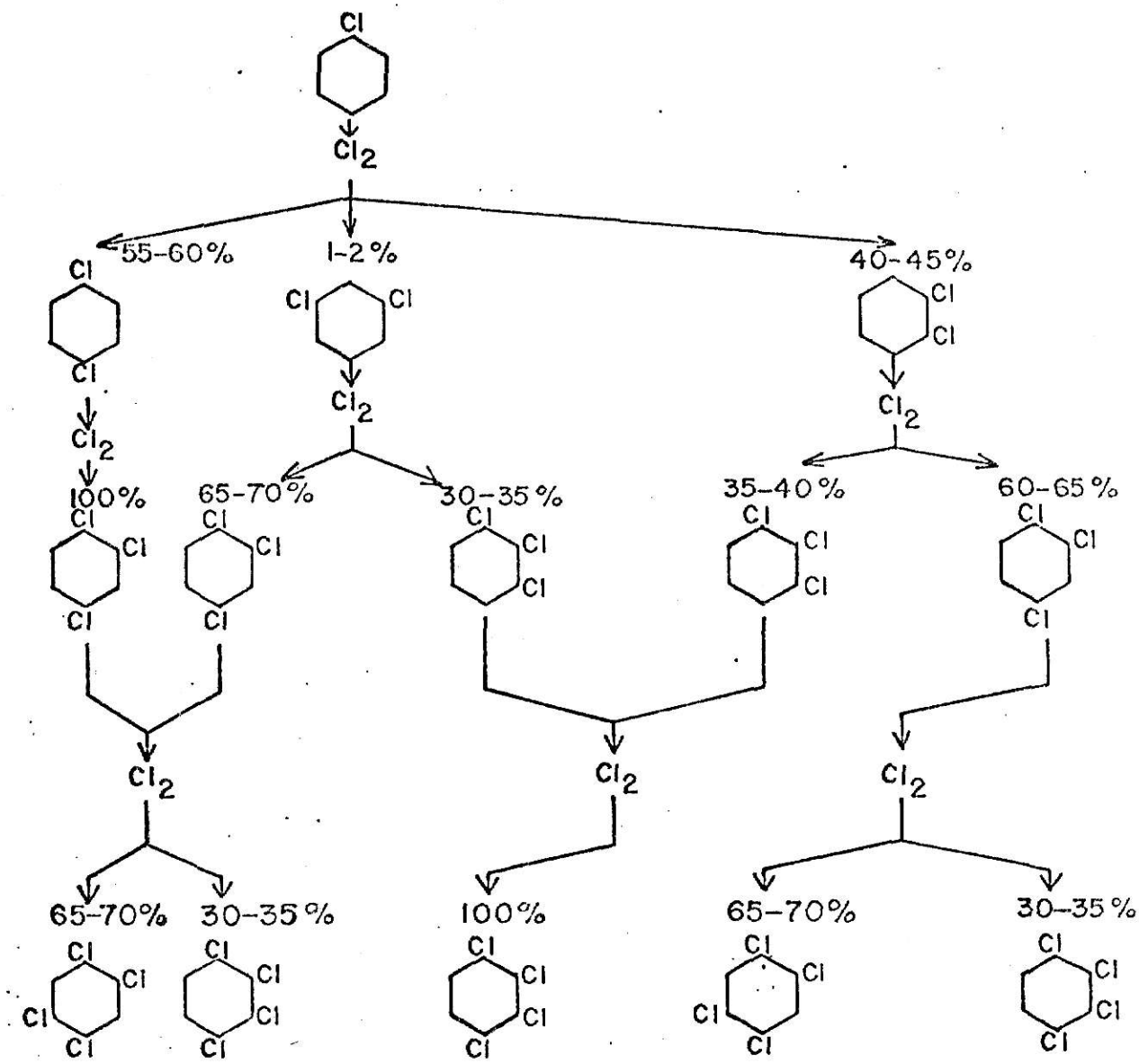


Figure 3. Distribution of Isomers in the Reaction Products [23]

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The operation ceases when the density is 1.28 at 15°C (≈6 hr). The separation of the chlorinated compound is done by distillation. The chlorination of benzene plant assembly is shown in Figure 5. In the industrial preparation of hexachlorocyclohexane, benzene is chlorinated in the liquid phase in the presence of an activation agent such as light, gamma rays, or elemental fluorine. A mixture of five isomers of hexachlorocyclohexane is produced. The commercial reactor consists or 13 reactor tubes in the recycle section and five tubes in the cleanup section. Each reactor tube consist of a concentric arrangement of a two-inch Pyrex tube into which are inserted two 40-watt fluorescent lamps, a four-inch Karbate tube enclosing the reactor section and an eight-inch steel pipe enclosing the cooling section as shown in the following flowsheet (Figure 4).

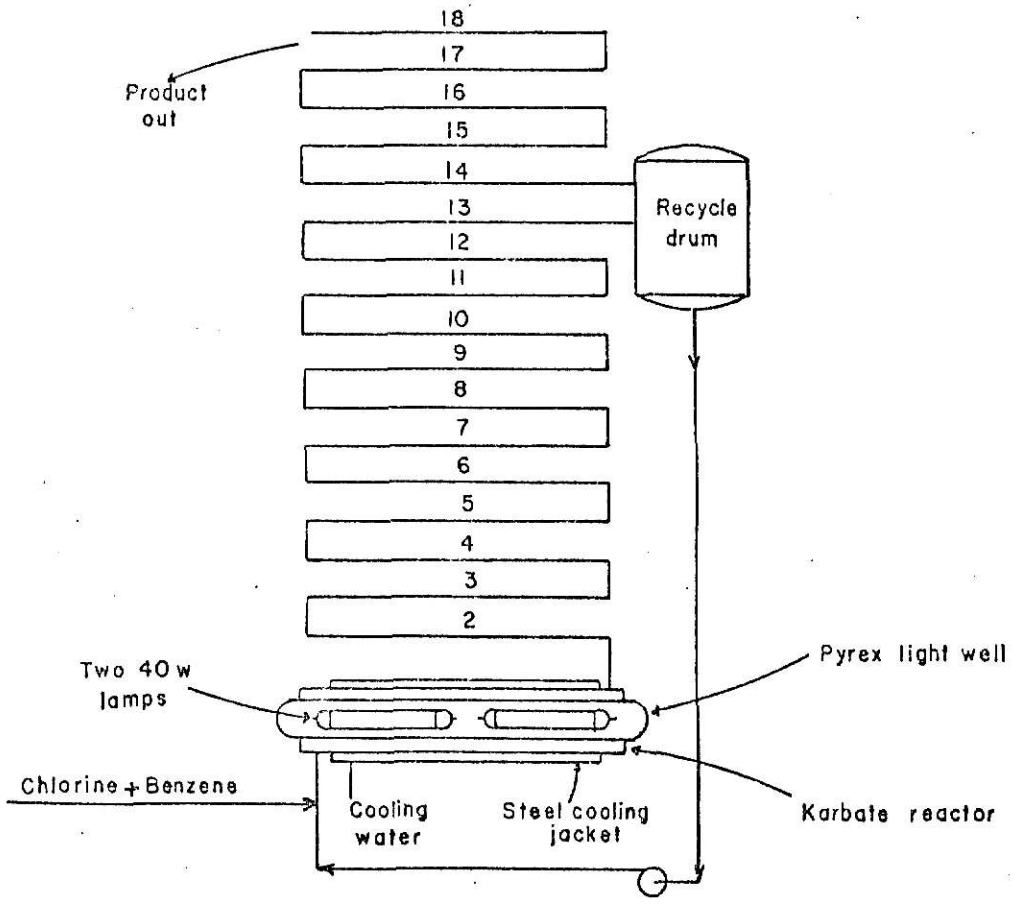

Figure 4 Two-Stage Hexacyclohexane Photochemical Reactor [12]

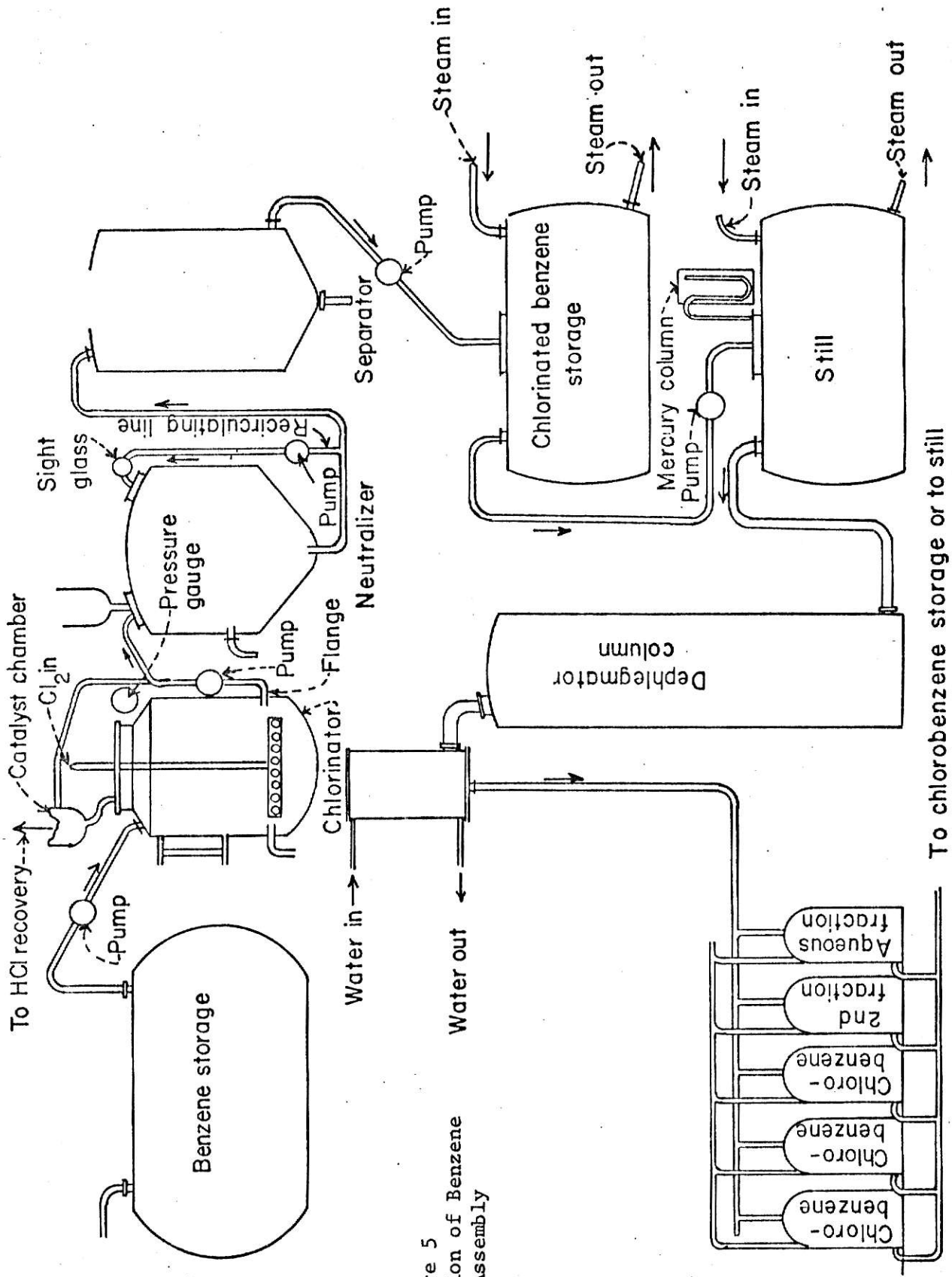

Figure 5
Chlorination of Benzene
Plant Assembly

Smith [24] in his chemical engineering kinetics book, showed by an example of how to determine the composition of the reaction mixture as a function of the number of moles of chlorine (from 0 to 2.1) added per mole of benzene charged.

The results section of the "Analog Computer Study of a Semi-Batch Reactor" [2] gave a very interesting and important graph from which the value of k (rate constant) was deduced and used for the design of the reactor. The graph represents the reduced concentrations versus time for benzene, monochlorobenzene, dichlorobenzene, and trichlorobenzene as shown in Figure 6.

W. Donahue [8] concluded from his results that the aluminum chloride catalyzed batch reaction of chlorine and benzene was shown to be second order overall, being first order with respect to each reacting species. The reaction rate constant varied from 2.26×10^{-4} to 6.92×10^{-4} liter/mole/second over the temperature range 25°C to 45°C; the activation energy of the reaction was calculated to be 10.3 Kcal/mole.

The reaction of chlorine was found to obey the rate expression

$$-r_{Cl_2} = K\, C_{Cl_2}\, C_{FeCl_3}$$

for constant volume and ferric chloride catalyst where

C_{Cl_2} = liquid phase free chlorine concentration, g-mole/liter

C_{FeCl_3} = ferric chloride concentration g/liter and the reaction rate constant, K, is given by

$$\ln K = (-2.45 \times 10^4/RT) = 42.3$$

with T = absolute temperature, °K,

and K = rate constant, $(g/liter)^{-1}\ (min)^{-1}$ [22]

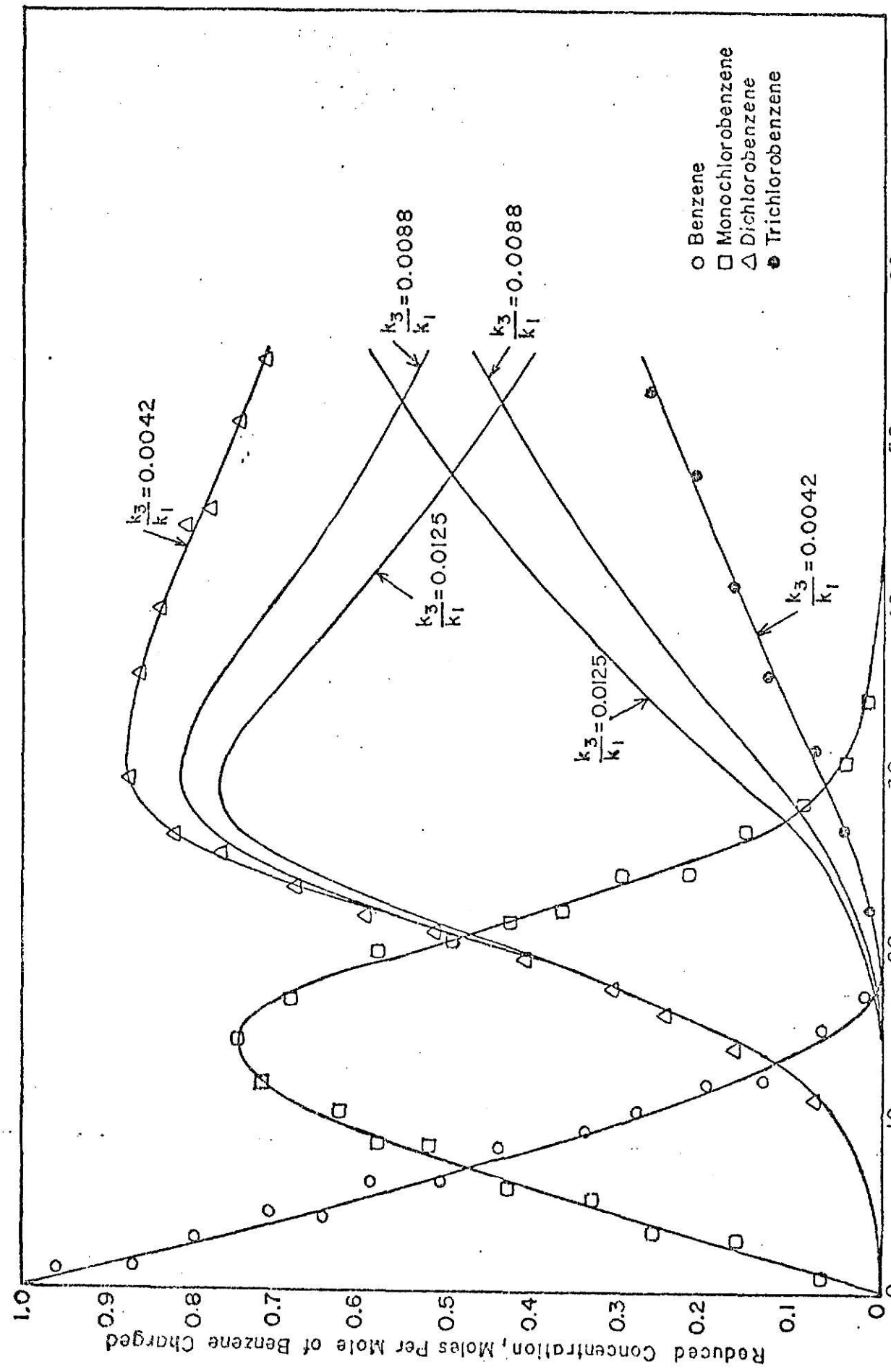

Figure 6. Reduced Concentrations Versus Time For the Chlorination of Benzene [2]

III DEVELOPMENT OF THE UNDERGRADUATE EXPERIMENT BASED ON CHLORINATION OF BENZENE

A) Development of the Experiment

In this experiment, the major purpose will be to obtain a reasonable amount of the chlorinated compounds, mostly monochlorobenzene. The maximization of monochlorobenzene yield, which is desirable for industrial purposes, is not required and, in fact, is undesirable since it would greatly increase the operating costs. A small reactor will also help reduce the operating cost by requiring a small flow rate of benzene. A sufficient reaction will have to be obtained to allow measurement and monitoring of the different streams. Generally a 10 to 20% reaction conversion would be desirable - this being large enough for measurement purposes, but still small from financial considerations. A small residence time is also preferred - approximately 1 to 1 1/2 minutes - so that the process will reach steady state in a reasonably short time, thus allowing plenty of time for several experimental investigations at steady state during a laboratory period. The rate of reaction depends on the concentration of benzene and dissolved chlorine. The solubility of chlorine in benzene may be increased by decreasing the temperature as shown in Figure 7 and/or by increasing the pressure. An increased chlorine concentration will, of course, increase the rate of reaction. The effect of changing the temperature has little effect on the rate of reaction due to the opposing results of changing rate constant and chlorine solubility. From the graph representing the concentration versus time, which is shown in Figure 6 (page 17) the rate constant was obtained by taking the slope of the curve representing the reduced concentration of benzene. For the operating conditions: $t = 55°C$ and $P = 2$ atmospheres, the value of k obtained was:

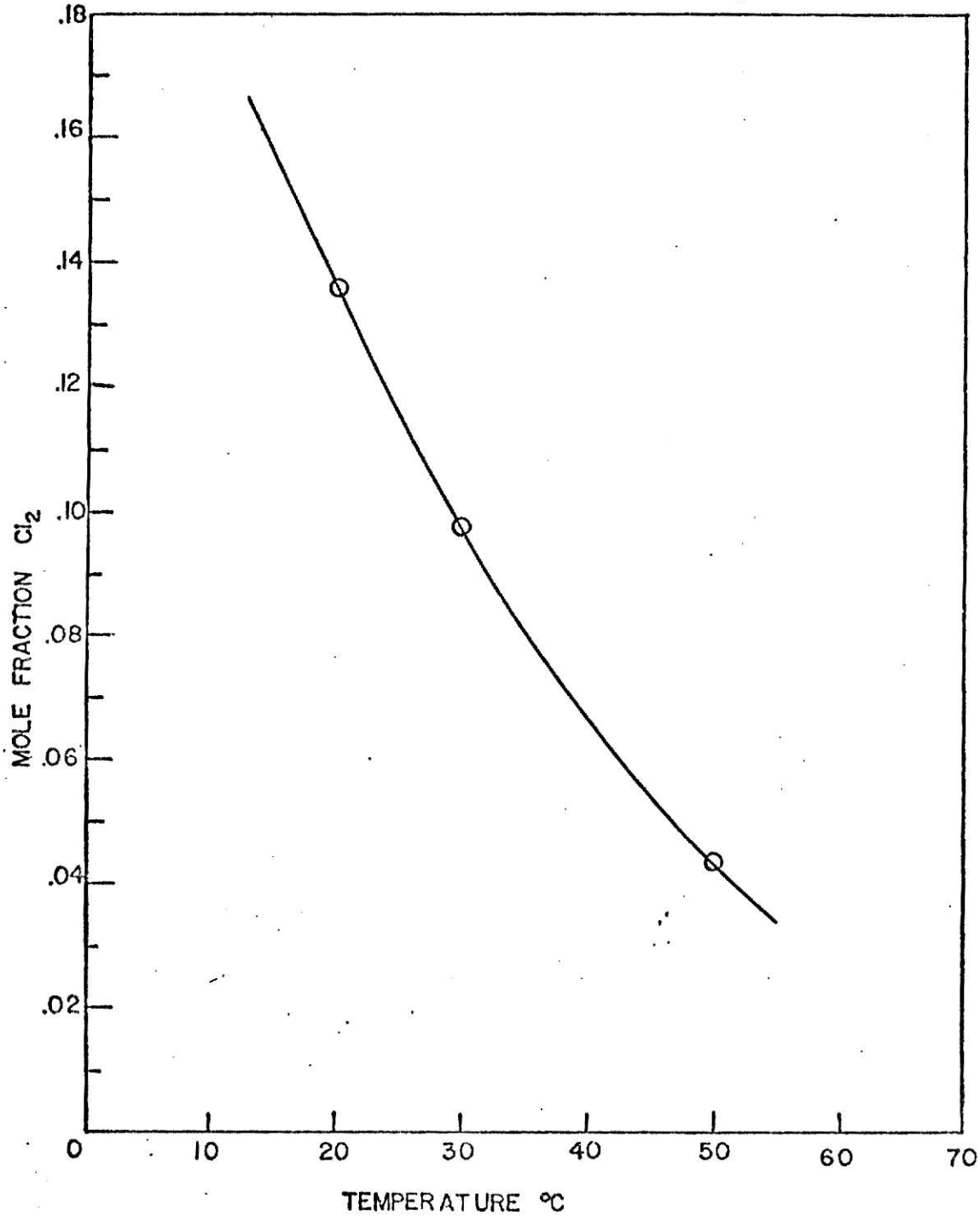

Figure 7. Solubilty of Chlorine in Benzene at Total Pressure of 1 Atmosphere [8]

$$.07 \quad \frac{\text{moles of benzene reacted/liter}}{(\text{moles of benzene charged/liter})\ (\text{minute})}$$

Due to the lack of information about the relationship between the rate constant and the pressure of the reaction, it was assumed that the rate constant is directly proportional to the pressure since an increase in the pressure will increase the solubility of chlorine and therefore the rate of reaction. The value of k obtained indicates that operating at atmospheric pressure will decrease the benzene conversion percentage from 10-20% to 3 - 4%.

The heat of reaction may be calculated as follows:

$$C_6H_{6(1)} + Cl_{2(g)} \xrightarrow{298°K} C_6H_5Cl_{(1)} + HCl_{(g)}$$

1) heat of formation at 298°K

$\Delta H_{C_6H_{6(1)}}$ = + 11.718 Kcal/g mole [21]

$\Delta H_{HCl_{(g)}}$ = - 22.063 Kcal/g mole [21]

$\Delta H_{C_6H_5Cl_{(1)}}$ = + 2.58 Kcal/g mole [26]

$\Delta H_{Cl_{2(g)}}$ = 0

2) $\Delta H_R\ (298°K) = \Sigma\ \Delta H_{f(\text{Product})} - \Sigma\ \Delta H_{f(\text{Reactant})}$

= -31.201 Kcal/g mole

The temperature of benzene feed from the feed tank and chlorine gas from a compressed gas cylinder will be room temperature (assumed to be 25°C). The presssure and temperature of the catalytic reactor will depend on the operating conditions. Due to the exothermic reaction, the reactor will be

cooled to maintain a constant temperature. The pressure of the reactor products, which will be benzene, monochlorobenzene, hydrogen chloride, and chlorine gas will be two to five atmospheres; a flash tank will be used to reduce the pressure to one atmosphere and to separate most of the gases from the liquid products. The gases will be absorbed by water in a packed column. The liquid products may be stored in a reactor product tank or will be separated to benzene and monochlorobenzene by a distillation column with a total condenser. The distillation feed will be preheated to its saturation temperature. The distillation column will consist of several sieve trays. The reboiler will be heated by steam and the bottom product as well as the distillate, will be cooled to 25° C and will be stored in product tanks. Full details of the design of each piece of equipment is included in the following pages and a flow-sheet of the entire process is shown in Figure 8 .

In the design of the reactor, the formation of monochlorobenzene was the only reaction considered due to the limited amount of conversion. The concentration of chlorine will be assumed constant because a 50% excess chlorine will be introduced into the reactor. The reaction was considered first order depending on benzene concentration only. The equations for a steady state stirred tank flow reactor are:

$$qC_{Ao} - qC_A = - Vr = - VkC_A \qquad (1)$$

$$C_A = C_{Ao}/(1 + k\tau) \qquad (2)$$

$$\text{mole fraction of benzene} = C_A/C_{Ao} = 1/(1 + k\tau) \qquad (3)$$

$$\text{conversion} = k\tau/(1 + k\tau) \qquad (4)$$

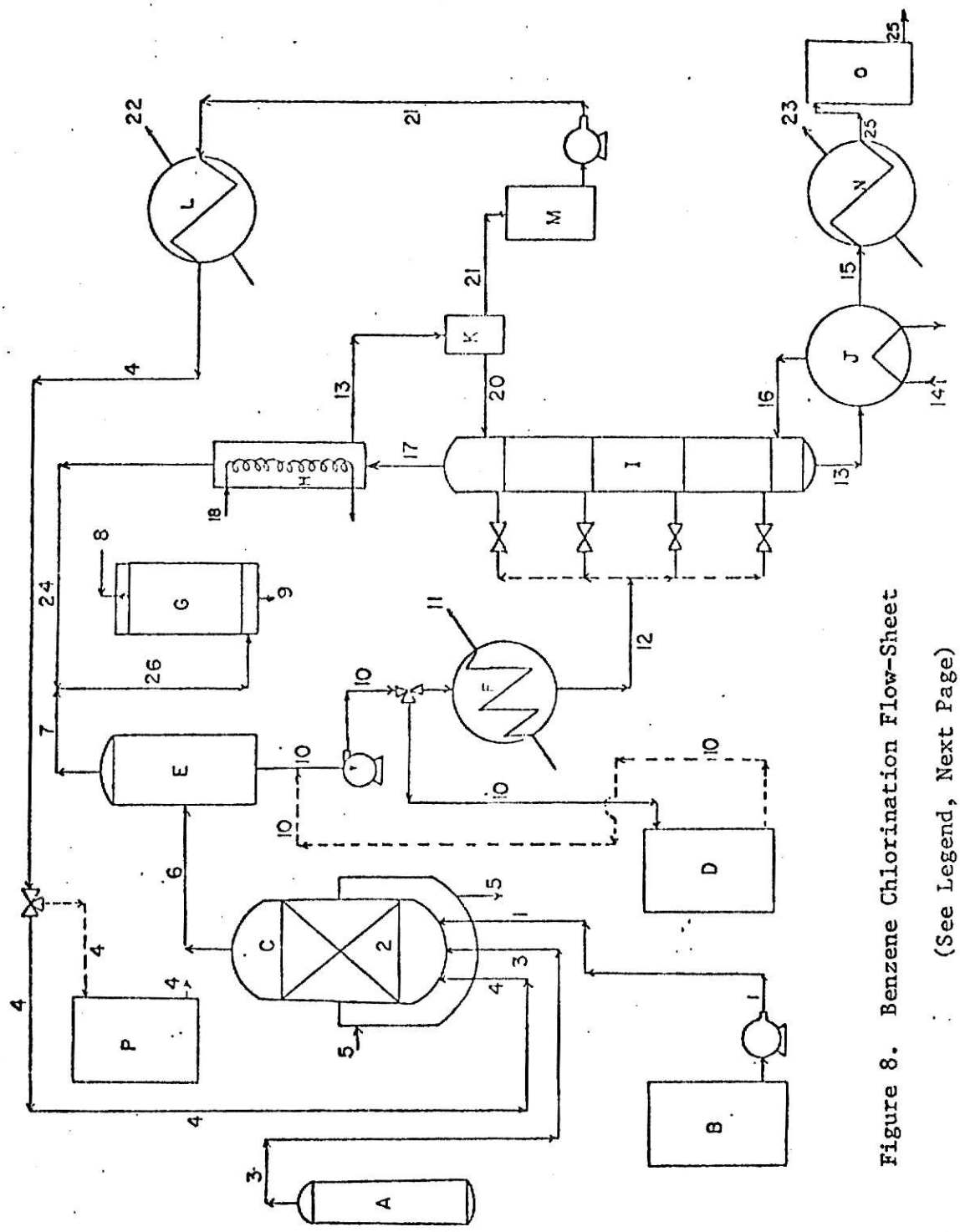

Figure 8. Benzene Chlorination Flow-Sheet

(See Legend, Next Page)

LEGEND FOR FIGURE 8

A	Chlorine Cylinder
B	Benzene Feed Tank
C	Reactor
D	Product Tank
E	Flash Tank
F	Heater
G	HCl and Cl_2 Absorber
H	Condenser
I	4-Plate Distillation Column
J	Reboiler
K	Reflux Splitter
L	Distillate Cooler
M	Reflux Storage Tank
N	Bottom Product Cooler
O	Bottom Product Tank
P	Distillate Storage Tank

Generally, either a jacket or a cooling coil would be sufficient to operate the reactor isothermally, but to have more flexibility in the control, both will be used. The reacting solution will be mixed by a magnetic stirrer - perfect mixing has been assumed for calculations.

The capacity of all the tanks (B,D,O, and P) excluding the reflux storage tank (M) were calculated based on the flow rate of fresh benzene (stream #1) and assuming five hours of runs for each laboratory period. A residence time of at least two minutes was assumed in calculating the capacity of the reflux storage tank (M), the flash tank (E) - based on liquid flow rate -, and also the absorber (G) for which no special interest was given to design due to the small amount of absorbed gases. Two positive displacement, metering pumps were choosen to increase the pressure of the fresh benzene feed (stream 1), and the recycled stream #4, to a slightly higher pressure than the reactor pressure; a centrifugal pump was used to circulate the liquid products from the flash tank.

Water flowing in a 1/8" O.D. coil will be used for cooling purposes in the reactor (C) and the two coolers (L) and (N). The assumed overall heat transfer coefficients in $Kcal/m^2/sec/°K$

1) for coolers and reactors = .163
2) for condenser = .081
3) for reboiler and heater using steam at 50 psig = .500

The heat transfer area was calculated from the following equation:

$$\text{heat transfer area} = \frac{\text{(heat added or removed)}}{\text{(overall heat transfer coefficient)} \quad \text{(average temperature difference)}}$$

The distillation feed will be heated by electric heat instead of steam due to the small amount of heat required.

For the distillation column, sieve trays were selected because of the difficulties in manufacturing small-sized bubble-cap trays. The McCabe and Thiele method, which will be described in the computer program, was used due to its simplicity in determining the tray to tray composition. For the determination of the column diameter, first the flooding constant was calculated, then it, together with the vapor flow rate, was used to obtain the superficial gas velocity and to calculate the diameter of the column [29]

B) Computer Program (Steady-State)

A digital computer (PDP 11/10) was used to calculate the steady state, to obtain the conditions and results for each stream in the flowsheet, and to evaluate the column diameter. The computer program contains three major divisions: the main program, EXPT, and two groups of subroutines, SUB1 and SUB2.

The main program is divided into three parts:

1) The steady state calculations were obtained by using an iterative procedure. Figure 9 shows a simplified flow diagram which is used to describe the iterations.

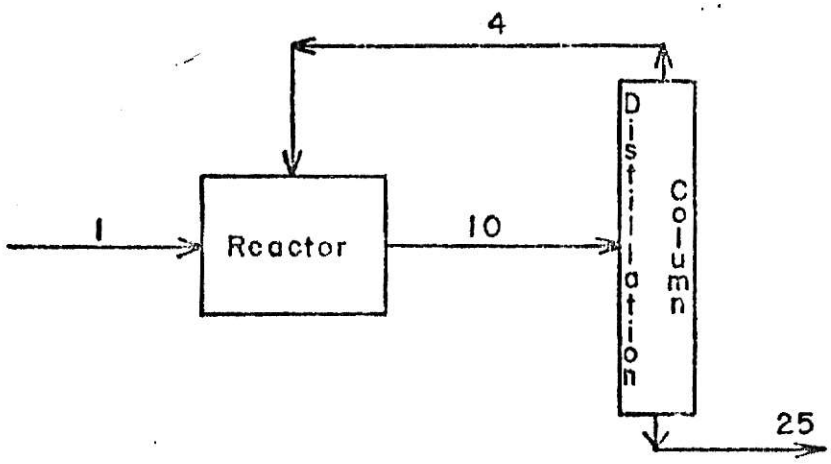

Figure 9. Simplified Diagram for the Process

From the concentration of stream 1 and the kinetic equations cited earlier in this section, the concentration and mole fraction of stream 10 was determined. The subroutine D1SB was used to calculate the composition of stream 4 and 25. Then the recycled stream 4 was considered, and the feed stream to the reactor was determined in this second iteration. The same procedure was used to determine the new concentration of streams 10, 4, 25 in the following iterations until the steady state was reached when the difference between the mole fraction of stream 10 for two successive iterations was $\leq .01$.

2) Detailed calculations and specifications were made for each stream, including the phase, mole fraction of benzene, volumetric flow rate, mass flow rate, molar flow rate, temperature, pressure, and heat transfer area for coolers, heaters, the condenser, and the reboiler.

3) Finally, the diameter of the distillation column was calculated.

Polynomial regression analyses were used to correlate the different physical and thermodynamic properties in the subroutine SUB1. The values used in the program are given in the tables shown in Appendix C. The results obtained are as follows:

1) Subroutine DMVSB (table 26) calculates the density (RO) of liquid mixture in Kg/dm^3 at any benzene mole fraction (P) at 298°K.

$$RO = .8729273 + .2600657P - .0355391P^2 + .003671427P^3$$

2) Subroutine TVSPB (table 29) determines the saturated liquid temperature (T) in degrees Kelvin at any benzene mole fraction (P) as shown in Figure 10.

$$T = 404.4375 - 97.58154P + 73.29699P^2 - 27.22487P^3$$

3) The heat required (HB and HC) in Kcal/Kg to rise the temperature of liquid benzene and monochlorobenzene from a reference temperature (TR) to a desired temperature (T) is given by the subroutine HBCVST (table 27).

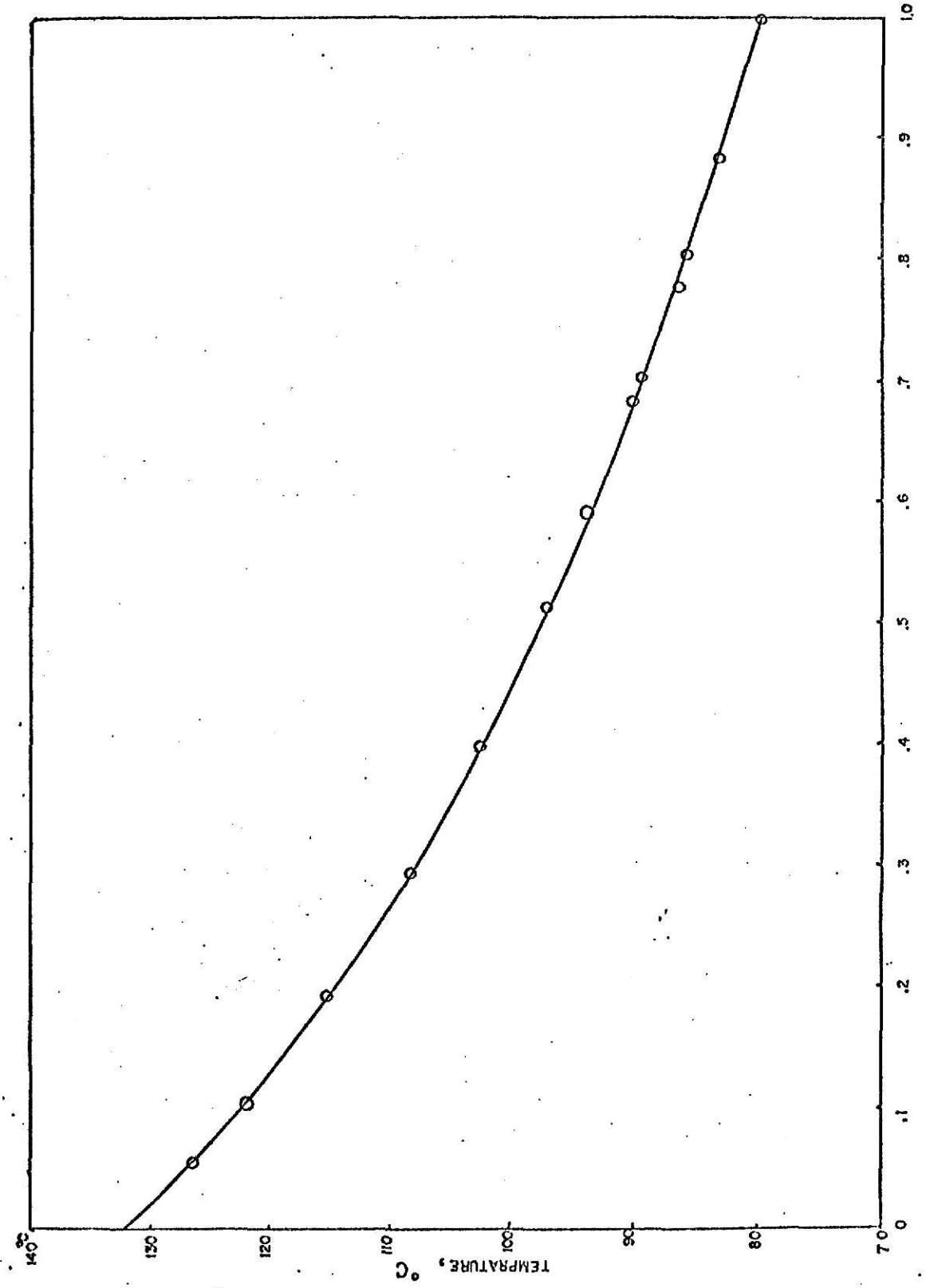

Figure 10. Equilibrium Temperature Curve
Benzene-Chlorobenzene
(atmospheric pressure) [10]

For benzene: $HB = .1036839\ (T - TR) + .1006199 \times 10^{-2}\ (T^2 - TR^2)/2 + .488006 \times 10^{-7}\ (T^3 - TR^3)/3$

For monochlorobenzene: $HC = .05277707\ (T - TR) + .9172735 \times 10^{-3}\ (T^2 - TR^2)/2 - .1490487 \times 10^{-6}\ (T^3 - TR^3)/3$

4) Subroutine VAVST (table 27) gives the relation between the heats of vaporization (HVB and HVC) in Kcal/Kg of benzene and monochlorinebenzene, and the temperature (T).

For benzene: $HVB = -1987.427 + 16.43142T - .04277849T^2 + .3665559 \times 10^{-4}T^3$

For monochlorobenzene: $HVC = 205.3619 - .5364947T + .4994191 \times 10^{-3}T^2$

5) Subroutine DBCVST (table 28) is used to calculate the densities (DB and DC) in Kg/dm^3 of liquid benzene and monochlorobenzene at any temperature (T).

For benzene: $DB = 1.44717 - .3507709 \times 10^{-2}T + .773703 \times 10^{-3}T^2 - .8148148 \times 10^{-8}T^3$

For monochlorobenzene: $DC = 1.654298 - .3245143 \times 10^{-2}T + .6698303 \times 10^{-5}T^2 - .6854954 \times 10^{-8}T^3$

SUB2 contains two subroutines. In the first, LIXY, the liquid-vapor equilibrium curve (table 29), shown in Figure 11, was fitted by linear interplotation to obtain the corresponding equilibrium values of X versus Y or vice-versa. The second subroutine, DISB, calculates the tray to tray composition in the distillation column at a given reflux ratio, feed composition, and number of trays. An iterative method was used in the computation. First, a top distillation mole fraction was assumed half-way between the feed composition and X = 1.0 which will be equal to: (benzene mole fraction of feed + 1.0)/2.0; and from the feed mole fraction and its conditions along with the reflux ratio and the assumed distillate

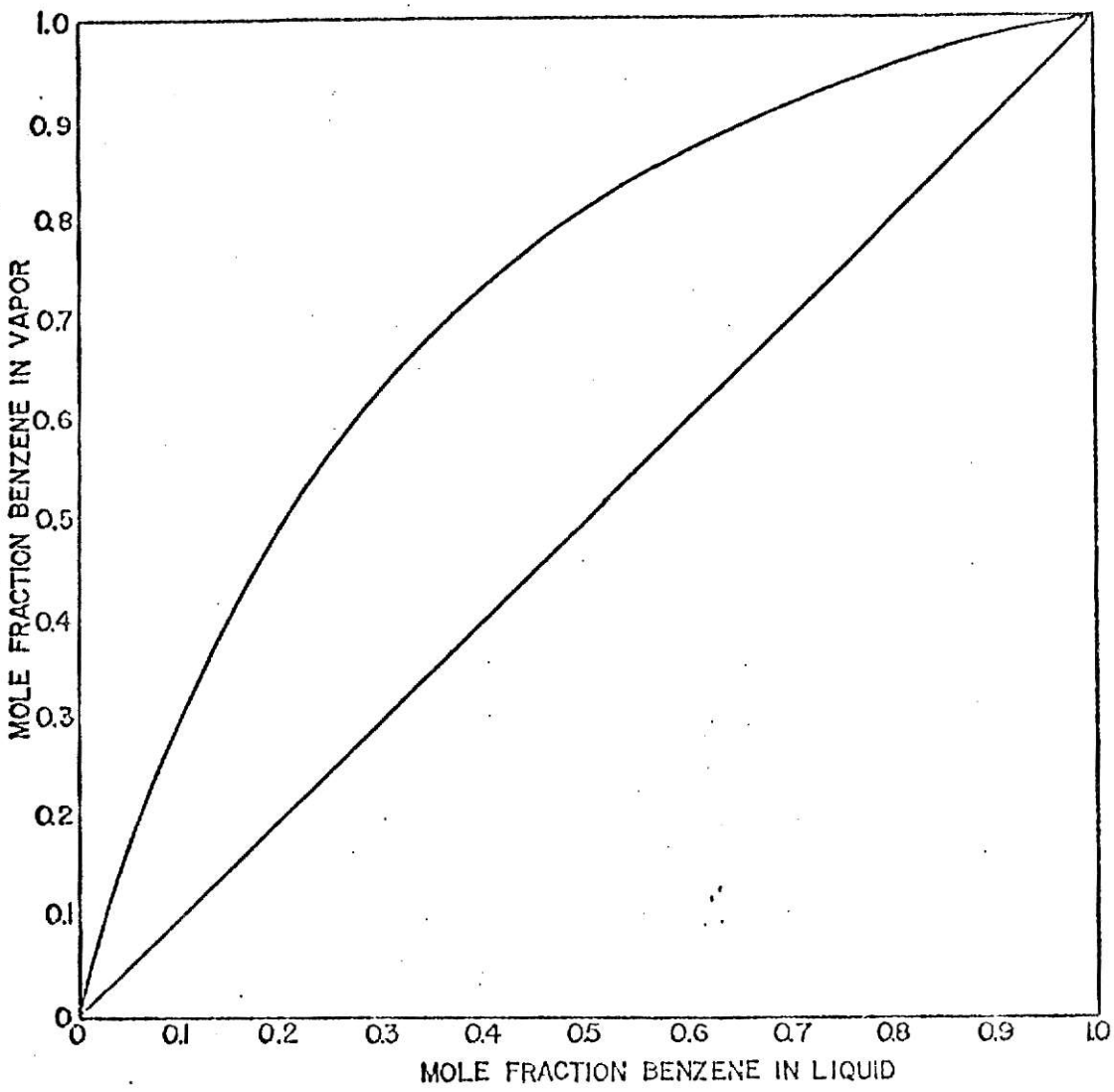

Figure 11. Vapor-Liquid Equilibrium Diagram
Benzene-Chlorobenzene
(atmospheric pressure) [10]

mole fraction, the equation of the operating line in the enriching section was determined. Then the McCabe and Thiele method was used to determine a calculated distillate mole fraction by knowing the number of trays in that section and by starting the computation at the feed tray. The calculated and assumed distillate mole fraction were compared; and if the difference between them was >.001, another trial was made until the difference was $\leq$ .001. The same method was used to calculate the mole fraction of the bottom product where the starting value was equal to: (benzene mole fraction of feed)/2.0. Table 1 shows the input and output quantities for each subroutine.

Table 1. Subroutine Specifications

Subroutine	Input Quantity	Output Quantity
DMVSPB	benzene mole fraction at 298°K	density of mixture (Kg/cubic dm)
TVSPB	benzene mole fraction	saturated liquid temperature (°K)
HBCVST	temperature (°K)	heat needed for heating C_6H_6 and C_6H_5Cl (Kcal/Kg)
VAVST	temperature (°K)	heat of vaporization of C_6H_6 and C_6H_5Cl (Kcal/Kg)
DBCVST	temperature (°K)	density of pure C_6H_6 and C_6H_5Cl (Kg/cubic dm)
DISB	reflux ration, feed mole fraction, fraction of feed which is vapor, and number of plate in the rectifying and stripping section	liquid and vapor composition for each plate in the column
LIXY	vapor or liquid benzene mole fraction	liquid or vapor benzene mole fraction

The next several pages are the actual program described above.

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      C     CONTINUOUS CHLORINATION OF BENZENE
      C
      C     THE KNOWN QUANTITIES ARE:
      C    1)THE BENZENE FLOW RATE (CUBIC CM/SEC)
      C    2)THE TEMPERATURE OF THE REACTOR(DEGREE KELVIN)
      C    3)THE NUMBER OF PLATES IN THE STRIPPING AND RECTIFYING SECTION
      C    4)THE TRAY SPACING (CM) AND THE VALUE OF Q
      C    5)THE VOLUME OF THE REACTOR (CUBIC DM)
      C    6)THE REACTION'S RATE CONSTANT AND THE REACTION PRESSURE(N/SQUARE M.)
      C    7)THE WEIGHT OF THE CATALYST ADDED AT THE STARTING POINT
      C    8)THE HEAT OF THE REACTION (KCAL/KG MOLE OF BENZENE)
      C    9)THE REFLUX RATIO
      C    10)THE ACCURACY NEEDED IN THE FEED STREAM(AA)
      C     THIS PROGRAM CALCULATES:
      C     PART ONE:THE STEADY STATE CONDITIONS
      C     PART TWO:DETAILED CALCULATIONS FOR EACH STREAM IN THE FLOWSHEET
      C     PART THREE:THE DIAMETER OF THE DISTILLATION COLUMN
      C     NOTATION:
      C     A=RESIDENCE TIME (SEC)
      C     AA=THE ALLOWED DIFFERENCE IN THE MOLE FRACTION IN STREAM#10 (AT S.S.
      C       AND BEFORE S.S.)
      C     AAP=ACTIVE AREA OF TRAY
      C     AF$=AREA (FEET SQUARE)
      C     AH=HOLE AREA PER TRAY
      C     AR$=AREA (CENTIMETER SQUARE)
      C     B=CONVENSION
      C     C=CONCENTRATION OF BENZENE IN STREAM #12 (KG MOLE/CUBIC DM)
      C     C$=CONCENTRATION OF BENZENE
      C     CB=CONCENTRATION OF BENZENE IN STREAMS ONE AND FOUR
      C     CC=CONCENTRATION OF CHLOROBENZENE
      C     CF=FLOADING CONSTANT
      C     D=DIAMETER OF THE DISTILLATION COLUMN (CM)
      C     F$=MASS FLOW RATE (KG/SEC)
      C     G=GAS PHASE
      C     HB$=HEAT REQUIRED TO RISE THE TEMPERATURE OF LIQUID BENZENE FROM
      C       TR TO T (KCAL/KG)
      C     H$=HEAT REMOVED OR ADDED (KCAL/SEC)
      C     HC$=SAME AS HB$ BUT FOR CHLOROBENZENE
      C     HR=HEAT OF REACTION AT 298 DEGREE KELVIN (KCAL/KG MOLE)
      C     HS$=HEAT OF VAPORIZATION OF STEAM (KCAL/KG)
      C     HTS=OVERALL HEAT TRANFER COEFFICIENT FOR REBOILER AND HEATER
      C     HVB$=HEAT OF VAPORIZATION OF BENZENE (KCAL/KG)
      C     HVC$=HEAT OF VAPORIZATION OF CHLOROBENZENE
      C     HWG=OVERALL HEAT TRANSFER COEFFICIENT FOR CONDENSER
      C     HWM=OVERALL HEAT TRANFER COEFFICIENT FOR COOLERS AND REACTOR
      C     L=LIQUID PHASE
      C     N=NUMBER OF PLATES
      C     NB=NUMBER OF PLATES IN THE STRIPPING SECTION
      C     NT=NUMBER OF PLATES IN THE RECTIFYING SECTION
      C     P=BENZENE MOLE FRACTION IN STREAM#12
      C     P$=BENZENE MOLE FRACTION
      C     PR$=PRESSURE IN BAR
      C     PRR=PRESSURE OF THE REACTION(BAR)
      C     Q=FRACTION OF FEED WHICH IS VAPOR=0.0
      C     QG$=FLOW RATE OF GAS (CUBIC FEET/SEC)
      C     QL$=FLOW RATE OF LIQUID (CUBIC FEET/SEC)
      C     R=RATE CONSTANT AT PRR(KG MOLE/KG MOLE BENZENE CHARGED/SEC)
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      C     RAA=RATE CONSTANT AT 2 BAR AND 328 DEGREE KELVIN
      C     RAA=.0011666666 (KG MOLE/KG MOLE OF BENZENE CHARGED/SEC)
```

```
      C     ROB$=DENSITY OF LIQUID BENZENE AT T DEGREE KELVIN
      C          (KG/CUBIC DM)
      C     ROC$=DENSITY OF LIQUID CHLOROBENZENE AT T DEGREE KELVIN
      C     ROG$=DENSITY OF GAS MIXTURE (LB/FEET CUBE)
      C     ROL$=DENSITY OF LIQUID MIXTURE
      C     ROM$=DENSITY OF LIQUID MIXTURE AT 298 DEGREE KELVIN
      C          (KG/CUBIC DM)
      C     RR=REFLUX RATIO
      C     S=MOLAR FLOW RATE OF STREAM#12 (KG MOLE/SEC)
      C     S$=MOLAR FLOW RATE
      C     SIG=SURFACE TENSION (DYNE/CENTIMETER)
      C     S=SOLID PHASE(IN TABLE 1)
      C     T$=TEMPERATURE IN DEGREE KELVIN
      C     TI$=INLET TEMPERATURE OF COOLING WATER
      C     TO$=OUTLET TEMPERATURE OF COOLING WATER
      C     TRR=TEMPERATURE OF THE REACTOR
      C     V$=VOLUMETRIC FLOW RATE (CUBIC CM/SEC)
      C     V=VAPOR PHASE
      C     VF=SUPERFICIAL VELOCITY OF GAS (FEET CUBE/SEC)
      C     VFA=ACTUAL SUPERFICIAL VELOCITY OF GAS
      C     VR=VOLUME OF REACTOR (CUBIC DM)
      C     WA$=AVERAGE MOLECULAR WEIGHT
      C     WT$=POWER IN KILOWATT
      C     Z$=VOLUMETRIC FLOW RATE OF LIQUID (CUBIC DM/SEC)
      C     ZB=VOLUMETRIC FLOW RATE OF STREAMS ONE AND FOUR (CUBIC DM/SEC)
      C     ZM=COMPRESSIBILITY  FACTOR
      C
      C
      C     MAIN PROGRAM
      C
      C
0001        DIMENSION F4(25),S4(25),B(25),P(25),A(25),R(25),C(25),Z(25),
           1    ZB(25),CB(25),Z4(25),S(25)
0002        WRITE(5,80)
0003  80    FORMAT(5X,'WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)',
           1    /,' THE REACTOR VOLUME(VR IN CUBIC DM)',
           2  /,' THE PRESSURE IN THE REACTOR(PRR IN BAR)',
           3  /,' THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)',
           4  /,' THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)',
           5  /,' AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?')
0004        READ(5,83) V1,VR,PRR,TRR,RAA,HR
0005  83    FORMAT(6(F17.10/))
0006        WRITE(5,81)
0007  81    FORMAT(5X,'WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZN
           1B)',/,' THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)',
           2    /,' THE REFLUX RATIO(RR)',
           3  /,' THE ACCURACY NEEDED IN THE FEED STREAM(AA)',
           4  /,' AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?')
0008        READ(5,85) ZNB,ZNT,RR,AA,F2
0009  85    FORMAT(5(F15.10/))
0010        NB=ZNB
0011        NT=ZNT
0012        Q=0.0
      C
      C
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      C     PART ONE:THE STEADY STATE CONDITIONS
      C
      C
      C    1)WITHOUT RECYCLE
0013        Z1=V1/1000.
0014        T1=298.
0015        A(1)=VR/Z1
0016        CALL  DBCVST (T1,ROB1,ROC1)
      D     WRITE(5,1000)
```

```
0017   1000   FORMAT(5X,'1000')
0018          C1=ROR1/78.12
0019          R(1)=RAA*PRR/2.0
       D      RRR=R(1)
       D      WRITE(5,3020)C1,RRR
0020   3020   FORMAT(2(F15.10,2X))
       C      BASIS ONE SECOND
0021   112    SS1=C1*Z1
0022          S(1)=SS1
0023          C(1)=C1/(1.+R(1)*A(1))
0024          P(1)=1./(1.+R(1)*A(1))
0025          B(1)=1.-P(1)
       D      BBB=B(1)
       D      CCC=C(1)
       D      PPP=P(1)
       D      WRITE(5,3030)CCC,PPP,BBB
0026   3030   FORMAT(3(F15.10,2X))
       C     2)WITH RECYCLE
       D      WRITE(5,1001)
0027   1001   FORMAT(5X,'1001')
0028          JDUM=2
0029          DO 120 I=1,20
0030          PJ=P(I)
0031          CALL  DISB (PJ,RR,P4,P15,P13,P16,NB,NT,Q,JDUM)
0032          CALL DMVSPB (P4,ROM4)
0033          S4(I)=S(I)*(P(I)-P15)/(P4-P15)
0034          F4(I)=S4(I)*(P4*78.12+(1.-P4)*112.554)
0035          Z4(I)=F4(I)/ROM4
0036          ZB(I)=Z1+Z4(I)
0037          CB(I)=(SS1+S4(I)*P4)/ZB(I)
0038          R(I+1)=RAA*PRR/2.0
0039          A(I+1)=VR/ZB(I)
0040          C(I+1)=CB(I)/(1.+R(I+1)*A(I+1))
0041          B(I+1)=R(I+1)*A(I+1)/(1.+R(I+1)*A(I+1))
0042          S(I+1)=SS1+S4(I)
0043          P(I+1)=(SS1+S4(I)*P4)*(1.-B(I+1))/S(I+1)
0044          P12=P(I+1)
0045          C12=C(I+1)
0046          S12=S(I+1)
0047          CON=B(I+1)*100.
0048          CETA=A(I+1)
0049          SS4=S4(I)
0050          FF4=F4(I)
0051          ZZ4=Z4(I)
0052          IF((P(I+1)-P(I))-AA) 130,130,120
0053   120    CONTINUE
0054   130    JDUM=1
0055          CALL  DISB (PJ,RR,P4,P15,P13,P16,NB,NT,Q,JDUM)
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0056          WRITE(5,135) I,CON,CETA
0057          WRITE(5,140) S12,C12,P12,P4
0058          WRITE(5,145) SS4,FF4,ZZ4,P15
0059   135    FORMAT(//,2X,'#OF ITERATION=',I3,2X,'CONVERSION % =',F7.2,2X,
              1 'RESIDENCE TIME=',F7.2)
0060   140    FORMAT(//,2X,'S12=',E10.3,2X,'C12=',E10.3,2X,'P12=',F9.4,2X,
              1 'P4=',F9.4)
0061   145    FORMAT(//,2X,'S4=',E10.3,2X,'F4=',E10.3,2X,'Z4=',E10.3,2X,'P15=',
              1 F9.4)
       C
       C      PART TWO:DETAILED CALCULATIONS FOR EACH STREAM IN THE FLOWSHEET
       C      STREAM#1
0062          F1=SS1*78.12
0063          PR1=5.0
0064          P1=1.
       D      WRITE(5,2000)SS1,T1,F1
```

```
0065  2000  FORMAT(3(F15.10,2X))
      C     STEAM#4
0066        T4=298.
0067        V4=ZZ4*1000.
      C     STREAM#21
0068        P21=P4
0069        F21=FF4
0070        S21=SS4
0071        CALL  TVSPB (P21,T21)
0072        V21=V4
      D     WRITE(5,2001) P21,T21,V21
0073  2001  FORMAT(3(F15.10,2X))
      C     STREAM#22 (COOLING WATER)
0074        CALL  HRCVST (T21,T4,HR21,HC21)
      C     H22=HEAT REMOVED BY COOLER (KCAL/SEC)
0075        H22=S21*(P21*78.12*HR21+(1.-P21)*112.556*HC21)
0076        TI22=293.
0077        TO22=303.
0078        F22=H22/10.
0079        T22D=(T21-TO22+T4-TI22)/2.
      C     HWM=162.852E-7(KCAL/SEC/SQUARE CM/DEGREE KELVIN)
0080        HWM=162.852E-7
      C     AR22=AREA OF COOLER
0081        AR22=H22/HWM/T22D
      D     WRITE(5,5000)T22D,H22,HWS,AR22
0082  5000  FORMAT(10X,'#22',4(E10.3,2X))
      C     STREAM#10
0083        P12=P(I+1)
0084        P10=P12
0085        S10=S12
0086        F10=S10*(P10*78.12+(1.-P10)*112.556)
      C     ASSUMING THAT T10=298. (NO CHANGE IN TEMPERATURE DUE TO
      C     EXPANSION)
0087        T10=TRR
0088        CALL  DMVSPB (P10,ROM10)
0089        V10=F10/ROM10*1000.
      D     WRITE(5,2003) T10,P10,V10,F12
0090  2003  FORMAT(4(F15.10,2X))
      C     STREAM#12 (SATURATED LIQUID)
0091        CALL  TVSPB (P12,T12)
      D     WRITE(5,2004)P12,T12
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0092  2004  FORMAT(2(F15.10))
0093        V12=V10
0094        F12=F10
      C     STREAM#11 (STEAM OR ELECTRICITY)
0095        CALL  HRCVST (T12,T10,HR12,HC12)
      C     H11=HEAT ADDED BY HEATER (KCAL/SEC)
0096        H11=S12*(P12*78.12*HR12+(1.-P12)*112.556*HC12)
0097        WT11=H11*3600.*1.163/1000.
      C     USING STEAM AT ONE BAR AND 373 DEGREE KELVIN
      C     HS11=539.42488 (KCAL/KG)
0098        HS11=539.42488
0099        F11=H11/HS11
0100        T11=373.
0101        T11D=(2.*T11-T10-T12)/2.
      C     HTS=500.E-7(KCAL/SEC/SQUARE CM/DEGREE KELVIN)
0102        HTS=500.E-7
0103        AR11=H11/HTS/T11D
      C     STREAM#15(SATURATED LIQUID)
0104        S15=S12-S21
0105        CALL  TVSPB (P15,T15)
0106        F15=S15*(P15*78.12+(1.-P15)*112.556)
0107        CALL  DRCVST (T15,ROR15,ROC15)
0108        Z15=S15*(P15*78.12/ROR15+(1.-P15)*112.556/ROC15)
```

```
0109          V15=Z15*1000.
      C       STREAM#25 (RESIDUE)
0110          T25=298.
0111          P25=P15
0112          V25=V15
0113          F25=F15
0114          S25=S15
      C       STREAM#23 (COOLING WATER)
0115          CALL HBCVST (T15,298.,HBB15,HBC15)
      C       H23=HEAT REMOVED BY COOLER (KCAL/SEC)
0116          H23=S15*(P15*78.12*HBB15+(1.-P15)*112.556*HBC15)
0117          TI23=293.
0118          TO23=313.
0119          F23=H23/20.
0120          T23D=(T15-TO23+298.-TI23)/2.
      C       AR23=AREA OF COOLER
0121          AR23=H23/HWR/T23D
      D       WRITE(5,5100) T23D,H23,HWG,AR23
0122  5100    FORMAT(10X,'#23',4(E10.3,2X))
      C       STREAM#7
0123          S7=S10*(1.-P10)-SS4*(1.-P4)
0124          P7=0.0
0125          T7=TRR
0126          F7=S7*36.5
0127          PR7=1.0
0128          V7=S7*T7*8314.3/PR7*10.
      C       STREAM#8 (WATER FOR ABSORPTION)
      C      67.3 KG OF (HCL) ARE DISSOLVED IN 100 KG OF WATER (SAFETY
      C       FACTOR=2.)
0129          F8=F7/67.3*100.*2.
0130          V8=F8*1000.
0131          T8=298.
      C       STREAM#9 (DILUTE (HCL))
0132          F9=F7+F8
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0133          V9=V8
      C       ASUMING NEGLIGEIBLE HEAT OF SOLUTION
0134          T9=T8
      C       STREAM#6
0135          F6=F7+F10
0136          PR6=4.0
0137          T6=TRR
0138          V6=V10+V7/4.
0139          S6=S7+S10
0140          P6=P10
      C       STREAM#3 (CHLORINE GAS)
      C       A 50% EXCESS CHLORINE IS USED
0141          S3=S7*1.5
0142          F3=S3*71.
0143          T3=298.
0144          PR3=5.0
0145          P3=0.0
0146          V3=S3*T3/PR3*8314.3*10.
      C       STREAMS#19 AND 20
      C       RR=S20/S21
0147          S20=RR*S21
0148          S19=S20+S21
0149          P20=P21
0150          P19=P21
0151          F20=S20*(P20*78.12+(1.-P20)*112.556)
0152          F19=F20+F21
0153          T19=T21
0154          T20=T21
0155          V19=V21*(1.+RR)
0156          V20=V19-V21
```

```
      C     STREAM#17
0157        F17=F19
0158        P17=P19
0159        S17=S19
0160        PR17=1.0
0161        T17=T19
      C     ZM17=1.
0162        V17=S17*T17*8314.3/PR17*10.
      C     STREAM#18 (COOLING WATER)
0163        CALL VAVST (T17,HVB17,HVC17)
      C     H18=HEAT REMOVED BY CONDENSER (KCAL/SEC)
0164        H18=S17*(P17*78.12*HVB17+(1.-P17)*112.556*HVC17)
      D     WRITE(5,3010) T17,HVB17,HVC17,H18
0165  3010  FORMAT(4(F15.8,2X))
0166        TI18=293.
0167        TO18=303.
0168        F18=H18/10.
0169        T18D=(T17*2.-TI18-TO18)/2.
      C     HWG=81.426E-7(KCAL/SEC/SQUARE CM/DEGREE KELVIN)
0170        HWG=81.426E-7
      C     AR18=AREA OF CONDENSER
0171        AR18=H18/HWG/T18D
0172        V18=F18*1000.
      D     WRITE(5,5001)T18D,H18,AR18
0173  5001  FORMAT(10X,'*18',3(E10.3,2X))
      C     STREAM#14
      C     HEAT BALANCE ON THE DISTILLATION COLUMN
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      C     H14=HEAT ADDED TO THE REBOILER (KCAL/SEC)
      C     BASIS:T12 (TEMPERATURE)
      C     H14+H12=H18+H21+H15
0174        CALL  HBCVST (T21,T12,HB21,HC21)
0175        H21=S21*(HB21*78.12*P21+(1.-P21)*112.556*HC21)
0176        CALL  HBCVST (T15,T12,HB15,HC15)
0177        H15=S15*(HB15*78.12*P15+(1.-P15)*112.556*HC15)
0178        H12=0.0
0179        H14=H18+H21+H15
      D     WRITE(5,3011) HB21,HC21,H21,HB15,HC15,H15,H14
0180  3011  FORMAT(7(F13.5,2X))
0181        WT14=H14*3600.*1.163/1000.
      C     USING STEAM AT 50 PSI AND 411.3 DEGREE KELVIN
0182        T14=411.3
      C     HS14=513.6516(KCAL/KG)
0183        HS14=513.6516
0184        F14=H14/HS14
0185        T16=T15
0186        CALL TVSPB (P13,T13)
0187        T14D=(2.*T14-T13-T16)/2.
0188        AR14=H14/HTS/T14D
      C     STREAMS#13 AND 16
0189        S16=S15*(P13-P15)/(P16-P13)
0190        S13=S16+S15
0191        PR16=1.0
      C     ZM16=1.
0192        V16=S16*T16*8314.3/PR16*10.
0193        CALL  DBCVST (T13,ROB13,ROC13)
0194        Z13=(P13*78.12/ROB13+(1.-P13)*112.556/ROC13)*S13
0195        V13=Z13*1000.
0196        F13=S13*(P13*78.12+(1.-P13)*112.556)
0197        F16=F13-F15
      C     STREAM#2 (FERRIC CHLORIDE)
      C     F2=WEIGHT OF CATALYST ADDED AT THE STARTING POINT (GM)
0198        T2=298.
      C     STREAM#5 (COOLING WATER)
0199        TI5=291.
```

```
0200          TO5=301.
      C       BB=NUMBER OF KG MOLES OF BENZENE CONVERTED TO CHLOROBENZENE
0201          BB=S7
      C       REFERENCE TEMPERATURE=298.
      C       H5=HEAT REMOVED BY COOLER
0202          CALL HBCVST (TRR,298.,HB10,HC10)
0203          H10=S10*(P10*78.12*HB10+(1.-P10)*112.556*HC10)
      C       THE MEAN MOLAR HEAT CAPACITY OF HCL FROM 298 TO 360 DEGREE
      C       KELVIN IS 6.95(KCAL/KG MOLE/DEGREE KELVIN)
0204          H7=S7*6.95*(TRR-298.)
0205          H5=HR*BB-H10-H7
0206          F5=H5/(TO5-TI5)
0207          V5=F5*1000.
0208          T5D=(2.*TRR-TO5-TI5)/2.
      C       AR5=AREA OF REACTOR COOLING COILS
0209          AR5=H5/HWM/T5D
      D       WRITE(5,5002)H5,AR5,H10,H7
0210  5002    FORMAT(10X,'H5',4(E10.3,2X))
      C       COMMENTS ON THE RESULTS (TABLES)
      C       PHASE:LIQUID=L,GAS=G,VAPOR=V AND SOLID=S
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      C       VOLUMETRIC FLOW RATE:(CUBIC CM/SEC)
      C       MASS FLOW RATE:(KG/SEC)
      C       TEMPERATURE:(DEGREE KELVIN)
      C       PRESSURE:(BAR)
      C       POWER:(KW)
      C
      C
      C       THE WRITE STATEMENTS
      C
      C
0211          WRITE(5,158)
0212  158     FORMAT(/////////,46X,'TABLE 1(MATERIAL BALANCE)')
0213          WRITE(5,160)
0214  160     FORMAT(/,2X,'STREAM #',2X,'PHASE',2X,'MOLE FRACTION OF BENZENE',
             12X,'VOLUMETRIC FLOW RATE',2X,'MASS FLOW RATE',2X,
             2'MOLAR FLOW RATE',2X,'TEMPERATURE',2X,'PRESSURE')
0215          WRITE(5,161)
0216  161     FORMAT(48X,'(CUBIC CM/SEC)',8X,'(KG/SEC)',5X,'(KG MOLE/SEC)',
             1 4X,'(D. KELVIN)',3X,'(BAR)')
0217          WRITE(5,162)P1,V1,F1,SS1,T1,PR1
0218  162     FORMAT(6X,'1',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1,4X,F6.1)
0219          WRITE(5,164)F2,T2
0220  164     FORMAT(6X,'2',7X,'S',8X,'FERRIC CHLORIDE',30X,E10.3,'*',22X,F7.1)
0221          WRITE(5,166)V3,F3,S3,T3,PR3
0222  166     FORMAT(6X,'3',7X,'G',8X,'(CHLORINE GAS)',13X,E10.3,8X,E10.3,
             1 8X,E9.2,6X,F7.1,4X,F6.1)
0223          WRITE(5,168)P4,V4,FF4,SS4,T4
0224  168     FORMAT(6X,'4',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0225          WRITE(5,170)P6,V6,F6,S6,T6,PR6
0226  170     FORMAT(6X,'6',6X,'L,G',4X,F9.4,1X,'AND HCL GAS',9X,E10.3,8X,
             1 E10.3,8X,E9.2,6X,F7.1,4X,F6.1)
0227          WRITE(5,172)V7,F7,S7,T7,PR7
0228  172     FORMAT(6X,'7',7X,'G',9X,'HYDROCHLORIC ACID',9X,E10.3,8X,
             1 E10.3,8X,E9.2,6X,F7.1,4X,F6.1)
0229          WRITE(5,174)V8,F8,T8
0230  174     FORMAT(6X,'8',7X,'L',13X,'WATER',17X,E10.3,8X,E10.3,23X,F7.1)
0231          WRITE(5,176)V9,F9,T9
0232  176     FORMAT(6X,'9',7X,'L',12X,'HCL DILUTE',13X,E10.3,8X,E10.3,23X,
             1 F7.1)
0233          WRITE(5,178)P10,V10,F10,S10,T10
0234  178     FORMAT(5X,'10',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
```

```
0235          WRITE(5,180)P12,V12,F12,S12,T12
0236    180   FORMAT(5X,'12',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0237          WRITE(5,182)P13,V13,F13,S13,T13
0238    182   FORMAT(5X,'13',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0239          WRITE(5,184)P15,V15,F15,S15,T15
0240    184   FORMAT(5X,'15',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0241          WRITE(5,186)P16,V16,F16,S16,T16,PR16
0242    186   FORMAT(5X,'16',7X,'V',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1,4X,F6.1)
0243          WRITE(5,188)P17,V17,F17,S17,T17,PR17
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0244    188   FORMAT(5X,'17',7X,'V',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1,4X,F6.1)
0245          WRITE(5,190)P19,V19,F19,S19,T19
0246    190   FORMAT(5X,'19',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0247          WRITE(5,192)P20,V20,F20,S20,T20
0248    192   FORMAT(5X,'20',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0249          WRITE(5,194)P21,V21,F21,S21,T21
0250    194   FORMAT(5X,'21',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0251          WRITE(5,195)P25,V25,F25,S25,T25
0252    195   FORMAT(5X,'25',7X,'L',11X,F9.4,15X,E10.3,8X,E10.3,8X,E9.2,
             1 6X,F7.1)
0253          WRITE(5,191)
0254    191   FORMAT(/,2X,'* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY')
0255          WRITE(5,196)
0256    196   FORMAT(2X,'STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOR   '
             1OBENZENE) AND GAS (HCL)')
0257          WRITE(5,197)
0258    197   FORMAT(2X,'STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLO
             1RINE) COMING FROM THE CONDENSER')
0259          WRITE(5,198)
0260    198   FORMAT(2X,'STREAM#26 IS COMPOSED OF STEAM#24 AND 7')
0261          WRITE(5,199)
0262    199   FORMAT(//,40X,'TABLE 2(HEAT BALANCE)')
0263          WRITE(5,200)
0264    200   FORMAT(/,2X,'STREAM #',2X,'INLET TEMPERATURE',2X,'OUTLET TEMPERA
             1TURE',2X,'COOLING  WATER',6X,'STEAM',10X,'AREA',6X,'POWER')
0265          WRITE(5,201)
0266    201   FORMAT(50X,'MASS FLOW RATE',2X,'MASS FLOW RATE')
0267          WRITE(5,202)
0268    202   FORMAT(12X,'(DEGREE KELVIN)',4X,'(DEGREE KELVIN)',7X,'(KG/SEC)',
             1 8X,'(KG/SEC)',5X,'(SQUARE CM)',3X,'(KW)')
0269          WRITE(5,203)TI5,TO5,F5,AR5
0270    203   FORMAT(6X,'5',8X,F7.1,12X,F7.1,10X,E10.3,22X,E10.3)
0271          WRITE(5,204)F11,AR11,WT11
0272    204   FORMAT(5X,'11',60X,E10.3,6X,E10.3,2X,F6.2)
0273          WRITE(5,206)F14,AR14,WT14
0274    206   FORMAT(5X,'14',60X,E10.3,6X,E10.3,2X,F6.2)
0275          WRITE(5,208)TI18,TO18,F18,AR18
0276    208   FORMAT(5X,'18',8X,F7.1,12X,F7.1,10X,E10.3,22X,E10.3)
0277          WRITE(5,210)TI22,TO22,F22,AR22
0278    210   FORMAT(5X,'22',8X,F7.1,12X,F7.1,10X,E10.3,22X,E10.3)
0279          WRITE(5,211) TI23,TO23,F23,AR23
0280    211   FORMAT (5X,'23',8X,F7.1,12X,F7.1,10X,E10.3,22X,E10.3)
0281          WRITE(5,212)
0282    212   FORMAT(/,4X,'HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY
             1 ELECTRIC POWER')
          C
          C
```

```
      C
      C     PART THREE:THE DIAMETER OF THE DISTILLATION COLUMN (CM)
      C
      C
      C     USING A SIEVE TRAY [29].
      C     STREAM#17 IS THE DISTILLATE
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      C     STREAM#13 IS THE RESIDUE
      C     STREAM#12 IS THE FEED
      C     BASIS ONE HOUR
0283        WA17=78.12*P17+(1.-P17)*112.556
0284        WA13=78.12*P13+(1.-P13)*112.556
0285        ROG17=WA17*273./359./T17
0286        ROL13=F13/Z13*62.4
0287        QG17=V17/1000./28.316
0288        QL13=Z13/28.316
      D     WRITE(5,3100) ROG17,ROL13,QG17,QL13
0289  3100  FORMAT(//,4(F15.8,2X))
0290        WRITE(5,217)
0291  217   FORMAT(//,5X,'WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?')
0292        READ(5,218) TS
0293  218   FORMAT(F10.5)
0294        ZZ=QL13/QG17*SQRT(ROL13/ROG17)
0295        IF(ZZ-.1)300,300,312
0296  300   ZZ=.1
0297        TS1=TS/2.54
0298  312   AK=.0062*TS1+.0385
0299        BK=.00253*TS1+.05
      C     CF=(AK*ALOG(1./ZZ)+BK)*((SIG/20.)**.2)*(5.*AH/AAB+.5)
      C     SIG IS ASSUMED TO BE 22.5 (DYNE/CM)
      C     AH/AAB IS ASSUMED TO BE .1275
0300        CF=(AK*ALOG(1./ZZ)+BK)*((22.5/20.)**.2)*(5.*.1275+.5)
      D     WRITE(5,3101)AK,BK,CF
0301  3101  FORMAT(3(F15.9,2X))
0302        VF=CF*SQRT(ROL13/ROG17-1.)
      C     USING 80% OF FLOODING
0303        VFA=.8*VF
0304        AF=QG17/VFA
0305        D=12.*SQRT(AF*4./3.1415926)*2.54
0306        N=NB+NT
0307        WRITE(5,320)D,TS,N
0308  320   FORMAT(5X,'TOWER DIAMETER=',F7.2,'(CM)',4X,'TRAY SPACING=',
     1  F8.3,'(CM)',4X,'NUMBER OF PLATES=',I3)
0309        STOP
0310        END
*^C
```

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      C     SUBROUTINES USED IN THIS PROGRAM
0001        SUBROUTINE DMVSPB (P,RO)
      C     FOR CALCULATING THE DENSITY OF LIQUID MIXTURE AT CERTAIN BENZENE
      C     MOLE FRACTION AT 298. DEGREE KELVIN(KG/CUBIC DM)
      D     WRITE(5,1002)
0002  1002  FORMAT(5X,'DMVSPB')
0003        D2=P*P
0004        D3=D2*P
0005        RO=.8729273+.2600657*P-.0355391*D2+.00371427*D3
0006        RETURN
0007        END
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0001        SUBROUTINE TVSPB (P,T)
      C     FOR CALCULATING THE SATURATED LIQUID TEMPERATURE AT A CERTAIN
      C     BENZENE MOLE FRACTION
      D     WRITE(5,1003)
0002  1003  FORMAT(5X,'TVSPB')
0003        PA2=P*P
0004        PA3=PA2*P
0005        T=404.4375-97.58154*P+73.29699*PA2-27.22487*PA3
0006        RETURN
0007        END
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0001        SUBROUTINE HBCVST (T,TR,HB,HC)
      C     FOR CALCULATING THE HEAT NEEDED FOR HEATING LIQUID BENZENE
      C     AND LIQUID CHLOROBENZENE FROM TR TO T DEGREE KELVIN(KCAL/KG)
      D     WRITE(5,1004)
0002  1004  FORMAT(5X,'HBCVST')
0003        TA2=T/100.*T
0004        TR2=TR/100.*TR
0005        TA3=TA2/100.*T
0006        TR3=TR2/100.*TR
0007        HB=.1036839*(T-TR)+.1006199*(TA2-TR2)/2.
           1 +.488006E-3*(TA3-TR3)/3.
0008        HC=.05277707*(T-TR)+.09172735*(TA2-TR2)/2.
           1 -.1409487E-2*(TA3-TR3)/3.
0009        RETURN
0010        END
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0001        SUBROUTINE VAVST (T,HVB,HVC)
      C     FOR CALCULATING THE HEAT OF VAPORIZATION OF BENZENE AND
      C     CHLOROBENZENE AT T DEGREE KELVIN (KCAL/KG)
      D     WRITE(5,1005)
0002  1005  FORMAT(5X,'VAVST')
0003        TK2=T/100.*T
0004        TK3=TK2/100.*T
0005        HVB=-1987.429+16.43142*T-4.277849*TK2+.3665559*TK3
0006        HVC=205.3619-.5364947*T+.04994191*TK2
0007        RETURN
0008        END
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0001        SUBROUTINE DBCVST (T,DB,DC)
      C     FOR CALCULATING THE DENSITIES OF LIQUID BENZENE AND LIQUID
      C     CHLOROBENZENE AT T DEGREE KELVIN (KG/CUBIC DM)
      D     WRITE(5,1007)
0002  1007  FORMAT(5X,'DBCVST')
0003        TD2=T/100.*T
```

```
0004          TD3=TD2/100.*T
0005          DB=1.44717-.003507709*T+.773703E-3*TD2-.8148148E-4*TD3
0006          DC=1.654298-.003245143*T+.6698303E-3*TD2-.6854954E-4*TD3
0007          RETURN
0008          END
*


 DX1:SUB2,TT:=DX1:SUB2/L:1/W


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0001          SUBROUTINE DISB (XF,R,P4,P15,P13,P16,NB,NT,F,JDUM)
      C       FOR CALCULATING THE MOLE FRACTION OF THE BOTTOM PRODUCT AND
      C       THE DISTILLATE COMPOSITION
      C       BINARY DISTILLATION USING MC CABE-THIELE ASSUMPTIONS
      C       PURPOSE:
      C       THE DISTILLATE COMPOSITION IS DETERMINED USING A TRIAL AND ERROR
      C       TECHNIQUE.THEN THE BOTTOM COMPOSITION IS DETERMINED BY ANOTHER
      C       TRIAL AND ERROR CALCULATION.RESULTS FOR EACH PLATE ARE PRINTED
      C       DESCRIPTION OF IMPORTANT VARIABLES:
      C       D:          USED IN THE TRIAL AND ERROR CALCULATION TO REPRESENT
      C       THE ERROR IN THE FINAL RESULT AFTER EACH TRIAL.THE OBJECTIVE
      C       IS TO DRIVE THIS VARIABLE TO ZERO.IN THE RECTIFYING SECTION IT
      C       REPRESENTS THE DIFFERENCE BETWEEN THE COMPUTED DISTILLATE COMP.
      C       AND THE ASSUMED DISTILLATE COMP.IN THE THE STRIPPING SECTION,IT
      C       IS THE DIFFERENCE BETWEEN THE COMPUTED BOTTOM COMP. AND THE
      C       ASSUMED BOTTOM COMPOSITION.
      C       F:          THE FRACTION OF THE FEED WHICH IS VAPOR.
      C       NB:         NUMBER OF IDEAL PLATES IN THE STRIPPING SECTION(BOT.)
      C       NT:         NUMBER OF IDEAL PLATES IN THE RECTIFYING SECTION(TOP)
      C       R:          REFLUX RATIO
      C       SL:         SLOPE OF THE OPERATING LINE IN THE STRIPPING SECTION.
      C       X AND AX: AN ARRAY TO REPRESENT THE LIQUID COMPOSITION LEAVING
      C       THE PLATES.
      C       XB:   RESIDUE COMPOSITION.
      C       XD:       COMPOSITION OF THE OVERHEAD PRODUCT.
      C       XF:       MOLE FRACTION OF THE LIGHT COMPONENT IN THE FEED.
      C       XS:        THE X-COORDINATE OF THE INTERSECTION OF THE FEED
      C       LINE AND THE OPERATING LINES.
      C       Y AND YY:  AN ARRAY TO REPRESENT THE VAPOR COMPOSITION LEAVING
      C       THE PLATES.
      C       OUTPUT:
      C      1. ECHO PRINT OF INPUT VARIABLES (R,XF,F,NB,NT).
      C      2. VALUES OF THE GUESSED VARIABLE (RECTIFYING SECTION:XD;
      C         STRIPPING SECTION: XB, AND THE ERROR FOR EACH TRIAL.)
      C      3. THE LIQUID AND VAPOR COMPOSITION FOR EACH PLATE.
      C       LIMITATIONS: THE TOLERANCE FOR D HAS BEEN SET TO .001
      C       MAIN PROGRAM:
0002          DIMENSION X(50),Y(50),XD(50),AX(50),YY(50),C(50),XB(50),
             1    XX(50),SL(50),D(50)
      D       WRITE(5,1008)
0003  1008    FORMAT(5X,'DISB')
0004  2       FORMAT(/19H1RECTIFYING SECTION/)
0005  3       FORMAT(41HOOPERATING LINE INTERSECTS FEED LINE AT =,F7.4)
0006  4       FORMAT(18HODISTILLATE COMP.:,F10.4,4X,6HERROR:,F10.5)
0007  5       FORMAT(18HOPLATE    X       Y,/,(I4,F9.4,F9.4))
0008  6       FORMAT(/19H1STRIPPING SECTION/)
0009  7       FORMAT(13HOBOTTOM COMP:,F10.4,4X,6HERROR:,F10.5)
0010  8       FORMAT(/10H1DATA ECHO/5H  R =,F7.4,3X,4HXF =,F7.4,/5H  F =,F6.3,
             1 /5H  NB=,I3,7X,4HNT =,I3)
```

```
0011          IF(JDUM-2) 56,57,57
0012    56    WRITE(5,8) R,XF,F,NB,NT
0013    57    CONTINUE
      C       RECTIFYING SECTION
0014          IF(JDUM-2) 58,59,59
0015    58    WRITE(5,2)
0016    59    CONTINUE
0017          XD(1)=1.
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0018          XD(2)=(1.+XF)/2.
0019          DO 41 J=1,50
0020          Y(NT)=XD(J+1)
      C       THE NEXT STATEMENT CHECKS F. IF IT IS ZERO THEN XS IS SET
      C       EQUAL TO XF AND TRANSFER IS MADE TO STATEMENT 15. THIS AVOIDS
      C       DIVISION BY ZERO IN STATEMENT 14.
0021          IF(F) 14,10,14
0022    10    XS=XF
0023          GO TO 15
0024    14    XS=(XF/F-XD(J)/(R+1.))/(R/(R+1.)+(1.-F)/F)
0025    15    IF(JDUM-2) 60,61,61
0026    60    WRITE(5,3) XS
0027    61    CONTINUE
0028          X(1)=XS
      C       NEXT STATEMENTS PERFORM CALCULATIONS UP THE PLATES IN THE
      C       RECTIFYING SECTION.
0029          DO 20 I=1,NT
      C       THE EQUILIBRIUM RELATION:
0030          XKK=X(I)
0031          CALL LIXY (XKK,YYY,0)
0032          Y(I)=YYY
      C       FOLLOWING STATEMENT IS:EQUATION FOR RECTIFYING OPER. LINE
0033          X(I+1)=Y(I)*(R+1.)/R-XD(J+1)/R
0034    20    CONTINUE
0035          XX(J+1)=XD(J+1)-XS
0036          D(1)=XX(2)
0037          D(J+1)=X(NT+1)-XD(J+1)
0038          IF(ABS(D(J+1))-0.001) 27,27,25
0039    25    IF(JDUM-2) 62,63,63
0040    62    WRITE(5,4) XD(J+1),D(J+1)
0041    63    CONTINUE
0042          A=XD(J+1)-XD(J)
0043          AA=ABS(A)
0044          IF(XX(J+1)+D(J+1)) 98,98,99
0045    98    XD(J+2)=XD(J+1)+AA/2.
0046          GO TO 38
0047    99    IF(D(J+1)-1.) 111,112,112
0048    112   GO TO 42
0049    111   CONTINUE
0050          IF(D(J+1)) 95,95,97
0051    95    XD(J+2)=XD(J+1)-AA/2.
0052          GO TO 38
0053    97    XD(J+2)=XD(J+1)+AA/2.
0054    38    IF(XD(J+2)-1.) 41,42,42
0055    42    XD(J+2)=(1.+XD(J+1))/2.
0056    41    CONTINUE
0057    27    IF(JDUM-2) 64,65,65
0058    64    WRITE(5,5) (I,X(NT-I+1),Y(NT-I+1),I=1,NT)
0059    65    CONTINUE
0060          P4=XD(J+1)
      C
      C
      C       STRIPPING SECTION
0061          IF(JDUM-2) 66,67,67
0062    66    WRITE(5,6)
0063    67    CONTINUE
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```
0064          AX(1)=XS
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0065          XB(1)=0.0
0066          XB(2)=XF/2.
0067          YT=R/(R+1.)*AX(1)+XD(J+1)/(R+1.)
0068          DO 52 J=1,50
0069    40    SL(J)=(YT-XB(J+1))/(XS-XB(J+1))
      C       NEXT STATEMENTS PERFORM CALCULATIONS DOWN THE PLATES IN THE
      C       STRIPPING SECTION.
0070          DO 45 I=1,NB+1
      C       NEXT STATEMENT:THE EQUATION OF THE STRIPPING OPERATING LINE
0071.         YY(I+1)=AX(I)*SL(J)+XB(J+1)*(1.-SL(J))
      C       THE EQUILIBRIUM RELATION:
0072          YYK=YY(I+1)
0073          CALL LIXY (AXK,YYK,1)
0074          AX(I+1)=AXK
0075    45    CONTINUE
0076          C(J)=AX(NB+1)-XB(J+1)
0077          IF(ABS(C(J))-.001) 55,55,50
0078    50    IF(JDUM-2)68,69,69
0079    68    WRITE(5,7) XB(J+1),C(J)
0080    69    CONTINUE
0081          B=XB(J+1)-XB(J)
0082          BB=ABS(B)
0083          IF(C(J)-XB(2)) 130,131,131
0084    131   GO TO 120
0085    130   CONTINUE
0086          IF(C(J)) 120,120,121
0087    120   XB(J+2)=XB(J+1)-BB/2.
0088          GO TO 52
0089    121   XB(J+2)=XB(J+1)+BB/2.
0090    52    CONTINUE
0091    55    ISTART=NT+1
0092          IEND=NB+NT
0093          IF(JDUM-2) 71,72,72
0094    71    WRITE(5,5) (I,AX(I-NT+1),YY(I-NT+1),I=ISTART,IEND)
0095    72    CONTINUE
0096          P15=XB(J+1)
0097          P16=YY(NB+1)
0098          P13=AX(NB)
0099          WRITE(5,75) XF,P4,P15
0100    75    FORMAT(//,2X,'FEED COMPOSITION =',F8.4,2X,'XD=P4=',F8.4,2X,
             1 'XB=P15=',F8.4)
0101          RETURN
0102          END
RT-11 FORTRAN IV          V01B-08                                    PAGE 001

0001          SUBROUTINE LIXY (XE,YE,K)
0002          DIMENSION X(25),Y(25)
0003          X(1)=-100.
0004          X(2)=0.
0005          X(3)=.053
0006          X(4)=.103
0007          X(5)=.15
0008          X(6)=.192
0009          X(7)=.25
0010          X(8)=.296
0011          X(9)=.35
0012          X(10)=.399
0013          X(11)=.45
0014          X(12)=.514
0015          X(13)=.55
0016          X(14)=.591
0017          X(15)=.63
0018          X(16)=.684
```

```
0019          X(17)=.703
0020          X(18)=.786
0021          X(19)=.804
0022          X(20)=.884
0023          X(21)=.95
0024          X(22)=1.0
0025          X(23)=100.
0026          Y(1)=-100.
0027          Y(2)=0.0
0028          Y(3)=.175
0029          Y(4)=.31
0030          Y(5)=.45
0031          Y(6)=.48
0032          Y(7)=.57
0033          Y(8)=.629
0034          Y(9)=.69
0035          Y(10)=.731
0036          Y(11)=.777
0037          Y(12)=.819
0038          Y(13)=.84
0039          Y(14)=.865
0040          Y(15)=.883
0041          Y(16)=.906
0042          Y(17)=.914
0043          Y(18)=.943
0044          Y(19)=.951
0045          Y(20)=.973
0046          Y(21)=.991
0047          Y(22)=1.0
0048          Y(23)=100.
0049          IF(K) 1,1,2
0050    1     DO 110 J=1,21
0051          IF(XE-X(J)) 112,111,110
0052    110   CONTINUE
0053    111   YE=Y(J)
0054          GO TO 300
0055    112   IF((XE-X(J-1))-.001) 10,10,11
0056    10    YE=Y(J-1)
0057          GO TO 300
RT-11 FORTRAN IV          V01B-08                                    PAGE 002

0058    11    YE=Y(J-1)+(Y(J)-Y(J-1))/(X(J)-X(J-1))*(XE-X(J-1))
0059          GO TO 300
0060    2     DO 210 J=1,21
0061          IF(YE-Y(J)) 212,211,210
0062    210   CONTINUE
0063    211   XE=X(J)
0064          GO TO 300
0065    212   IF((YE-Y(J-1))-.001) 20,20,21
0066    20    XE=X(J-1)
0067          GO TO 300
0068    21    XE=X(J-1)+(X(J)-X(J-1))/(Y(J)-Y(J-1))*(YE-Y(J-1))
0069    300   RETURN
0070          END
*
```

C) Results of Computer Simulation

The results obtained, from the mini-computer, for the different investigated computer runs, are shown in the next pages, and followed by Table 2 which represents a summary of operating conditions and results for those runs. In the result we have:

1) The input data presented as questions;
2) The feed, distillate, and bottom product compositions given for each iteration;
3) The trial and error procedure, for determining the composition of the enriching and stripping section, presented with the final tray to tray composition at steady state;
4) The distillation feed, distillate, and bottom product composition given with the number of iterations, conversion per cent, residence time, concentration, and mass flow rate of stream 4 and 12 at steady state;
5) The material and heat balance, which describe each stream in the flowsheet, shown in Table 1 and 2, respectively;
6) Finally, the tower diameter given with the tray spacing and the number of plates - including the reboiler.

RUN 1

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNP)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
3.
2.
.25
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  1.0000  XB=P15=  0.0000

 FEED COMPOSITION =  0.7463  XD=P4=  0.9559  XB=P15=  0.3309

 FEED COMPOSITION =  0.7676  XD=P4=  0.9607  XB=P15=  0.3416

 FEED COMPOSITION =  0.7890  XD=P4=  0.9658  XB=P15=  0.3693

 FEED COMPOSITION =  0.8045  XD=P4=  0.9702  XB=P15=  0.3960

 FEED COMPOSITION =  0.8157  XD=P4=  0.9723  XB=P15=  0.4031
DATA ECHO
 R = 0.2500    XF = 0.8157
 F = 0.000
 NR=  3        NT =  2
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:    0.9079    ERROR:   0.46067

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:    0.9539    ERROR:   0.23033
```

```
OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:     0.9770     ERROR:  -0.04034

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:     0.9654     ERROR:   0.07230

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:     0.9712     ERROR:   0.01209

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:     0.9741     ERROR:  -0.01811

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:     0.9726     ERROR:  -0.00300

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

DISTILLATE COMP.:     0.9719     ERROR:   0.00456

OPERATING LINE INTERSECTS FEED LINE AT = 0.8157

PLATE     X        Y
  1    0.8820    0.9724
  2    0.8157    0.9542
STRIPPING SECTION

BOTTOM COMP:     0.4079     ERROR:  -0.00594

BOTTOM COMP:     0.2039     ERROR:   0.22740

BOTTOM COMP:     0.3059     ERROR:   0.11390

BOTTOM COMP:     0.3569     ERROR:   0.05506

BOTTOM COMP:     0.3824     ERROR:   0.02488

BOTTOM COMP:     0.3951     ERROR:   0.00956

BOTTOM COMP:     0.4015     ERROR:   0.00184

BOTTOM COMP:     0.4047     ERROR:  -0.00204

PLATE     X        Y
  3    0.7802    0.9410
  4    0.6574    0.8947
  5    0.4030    0.7346

 FEED COMPOSITION =  0.8157  XD=P4=  0.9723  XB=P15=  0.4031

 #OF ITERATION=  6  CONVERSION % =  16.00  RESIDENCE TIME=  86.57

 S12= 0.297E-04  C12= 0.106E-01  P12=  0.8242  P4=  0.9723

 S4= 0.202E-04  F4= 0.160E-02  Z4= 0.146E-02  P15=  0.4031
```

RUN 1 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.347E 02	0.497E-03	0.70E-05	298.0	5.0
4	L	0.9723	0.146E 01	0.140E-02	0.20E-04	298.0	
6	L,G	0.8242 AND HCL GAS	0.332E 02	0.267E-02	0.34E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.123E 03	0.170E-03	0.47E-05	318.0	1.0
8	L	WATER	0.506E 00	0.505E-03		298.0	
9	L	HCL DILUTE	0.506E 00	0.677E-03		298.0	
10	L	0.8242	0.235E 01	0.250E-02	0.30E-04	318.0	
12	L	0.8242	0.235E 01	0.250E-02	0.30E-04	358.6	
13	L	0.6574	0.414E 01	0.367E-02	0.41E-04	364.2	
15	L	0.4031	0.101E 01	0.938E-03	0.95E-05	375.2	
16	V	0.7346	0.977E 03	0.273E-02	0.31E-04	375.2	1.0
17	V	0.9723	0.744E 03	0.200E-02	0.25E-04	353.8	1.0
19	L	0.9723	0.183E 01	0.200E-02	0.25E-04	353.8	
20	L	0.9723	0.365E 00	0.400E-03	0.51E-05	353.8	
21	L	0.9723	0.146E 01	0.160E-02	0.20E-04	353.8	
25	L	0.4031	0.101E 01	0.938E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.125E-01		0.349E 03	
11				0.901E-04	0.249E 02	0.18
14				0.371E-03	0.917E 02	0.80
18	293.0	303.0	0.188E-01		0.413E 03	
22	293.0	303.0	0.387E-02		0.851E 02	
23	293.0	313.0	0.137E-02		0.500E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 3.66(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 5
STOP --

RUN 2

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.

    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
3.
2.
.5
.01
.0015


 FEED COMPOSITION =  0.6589  XD=P4=  0.9464  XB=P15=  0.1802

 FEED COMPOSITION =  0.7296  XD=P4=  0.9625  XB=P15=  0.2052

 FEED COMPOSITION =  0.7714  XD=P4=  0.9701  XB=P15=  0.2230

 FEED COMPOSITION =  0.7988  XD=P4=  0.9756  XB=P15=  0.2403

 FEED COMPOSITION =  0.8187  XD=P4=  0.9791  XB=P15=  0.2575

 FEED COMPOSITION =  0.8335  XD=P4=  0.9815  XB=P15=  0.2719

 FEED COMPOSITION =  0.8450  XD=P4=  0.9830  XB=P15=  0.2806
DATA ECHO
```

```
 R = 0.5000    XF = 0.8450
 F = 0.000
 NB=  3        NT =  2
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8450

DISTILLATE COMP.:     0.9225     ERROR:    0.23247

OPERATING LINE INTERSECTS FEED LINE AT = 0.8450

DISTILLATE COMP.:     0.9613     ERROR:    0.11623

OPERATING LINE INTERSECTS FEED LINE AT = 0.8450

DISTILLATE COMP.:     0.9806     ERROR:    0.01114

OPERATING LINE INTERSECTS FEED LINE AT = 0.8450

DISTILLATE COMP.:     0.9903     ERROR:   -0.03376

OPERATING LINE INTERSECTS FEED LINE AT = 0.8450

DISTILLATE COMP.:     0.9855     ERROR:   -0.01131

OPERATING LINE INTERSECTS FEED LINE AT = 0.8450

PLATE     X        Y
  1    0.9207    0.9830
  2    0.8450    0.9623
STRIPPING SECTION

BOTTOM COMP:      0.4225     ERROR:   -0.15962

BOTTOM COMP:      0.2113     ERROR:    0.07602

BOTTOM COMP:      0.3169     ERROR:   -0.03924

BOTTOM COMP:      0.2641     ERROR:    0.01885

BOTTOM COMP:      0.2905     ERROR:   -0.01007

BOTTOM COMP:      0.2773     ERROR:    0.00442

BOTTOM COMP:      0.2839     ERROR:   -0.00281

PLATE     X        Y
  3    0.7689    0.9370
  4    0.5640    0.8486
  5    0.2814    0.6102

 FEED COMPOSITION =  0.8450  XD=P4=  0.9830  XB=P15=  0.2806

 #OF ITERATION=  7  CONVERSION % =  13.48  RESIDENCE TIME=  70.84

 S12= 0.370E-04  C12= 0.112E-01  P12=   0.8543  P4=   0.9830

 S4= 0.275E-04  F4= 0.217E-02  Z4= 0.197E-02  P15=   0.2806
```

RUN 2 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.366E 02	0.525E-03	0.74E-05	298.0	5.0
4	L	0.9830	0.197E 01	0.217E-02	0.28E-04	298.0	
6	L,G	0.8543 AND HCL GAS	0.355E 02	0.326E-02	0.42E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.130E 03	0.180E-03	0.49E-05	318.0	1.0
8	L	WATER	0.535E 00	0.535E-03		298.0	
9	L	HCL DILUTE	0.535E 00	0.715E-03		298.0	
10	L	0.8543	0.297E 01	0.308E-02	0.37E-04	318.0	
12	L	0.8543	0.287E 01	0.308E-02	0.37E-04	357.6	
13	L	0.5640	0.699E 01	0.631E-02	0.68E-04	367.8	
15	L	0.2806	0.103E 01	0.978E-03	0.95E-05	382.2	
16	V	0.6102	0.185E 04	0.534E-02	0.58E-04	382.2	1.0
17	V	0.9830	0.121E 04	0.325E-02	0.41E-04	353.5	1.0
19	L	0.9830	0.296E 01	0.325E-02	0.41E-04	353.5	
20	L	0.9830	0.987E 00	0.108E-02	0.14E-04	353.5	
21	L	0.9830	0.197E 01	0.217E-02	0.28E-04	353.5	
25	L	0.2806	0.103E 01	0.978E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.129E-01		0.359E 03	
11				0.969E-04	0.297E 02	0.22
14				0.606E-03	0.172E 03	1.30
18	293.0	303.0	0.306E-01		0.678E 03	
22	293.0	303.0	0.522E-02		0.115E 03	
23	293.0	313.0	0.152E-02		0.505E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 4.67(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 5
STOP --

RUN 3

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
3.
2.
.75
.01
.0015


 FEED COMPOSITION =  0.6589  XD=P4=  0.9547  XB=P15=  0.1274

 FEED COMPOSITION =  0.7332  XD=P4=  0.9682  XB=P15=  0.1375

 FEED COMPOSITION =  0.7769  XD=P4=  0.9756  XB=P15=  0.1533

 FEED COMPOSITION =  0.8058  XD=P4=  0.9810  XB=P15=  0.1873

 FEED COMPOSITION =  0.8263  XD=P4=  0.9834  XB=P15=  0.2017

 FEED COMPOSITION =  0.8412  XD=P4=  0.9851  XB=P15=  0.2152

 FEED COMPOSITION =  0.8530  XD=P4=  0.9868  XB=P15=  0.2266
DATA ECHO
 R = 0.7500    XF = 0.8530
 F = 0.000
 NB=  3        NT =  2
```

```
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9265     ERROR:    0.17152

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9632     ERROR:    0.08576

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9816     ERROR:    0.01653

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9908     ERROR:   -0.01270

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9862     ERROR:    0.00192

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9885     ERROR:   -0.00539

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

DISTILLATE COMP.:     0.9874     ERROR:   -0.00174

OPERATING LINE INTERSECTS FEED LINE AT = 0.8530

PLATE     X        Y
  1    0.9347    0.9868
  2    0.8530    0.9645
STRIPPING SECTION

BOTTOM COMP:      0.4265     ERROR:   -0.21903

BOTTOM COMP:      0.2132     ERROR:    0.01506

BOTTOM COMP:      0.3199     ERROR:   -0.09981

BOTTOM COMP:      0.2666     ERROR:   -0.04198

BOTTOM COMP:      0.2399     ERROR:   -0.01338

PLATE     X        Y
  3    0.7472    0.9294
  4    0.5014    0.8108
  5    0.2274    0.5350

 FEED COMPOSITION =   0.8530   XD=P4=   0.9868   XB=P15=   0.2266

 #OF ITERATION=   7   CONVERSION % =   12.86   RESIDENCE TIME=   67.09

 S12= 0.393E-04   C12= 0.114E-01   P12=    0.8627   P4=    0.9868

 S4= 0.298E-04   F4= 0.234E-02   Z4= 0.213E-02   P15=    0.2266
```

RUN 3 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.372E 02	0.533E-03	0.75E-05	298.0	5.0
4	L	0.9868	0.213E 01	0.234E-02	0.30E-04	298.0	
6	L,G	0.8627 AND HCL GAS	0.361E 02	0.344E-02	0.44E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.132E 03	0.183E-03	0.50E-05	318.0	1.0
8	L	WATER	0.543E 00	0.543E-03		298.0	
9	L	HCL DILUTE	0.543E 00	0.725E-03		298.0	
10	L	0.8627	0.303E 01	0.326E-02	0.39E-04	318.0	
12	L	0.8627	0.303E 01	0.326E-02	0.39E-04	357.3	
13	L	0.5014	0.910E 01	0.832E-02	0.87E-04	370.5	
15	L	0.2266	0.104E 01	0.995E-03	0.95E-05	385.8	
16	V	0.5350	0.250E 04	0.733E-02	0.78E-04	385.8	1.0
17	V	0.9868	0.153E 04	0.410E-02	0.52E-04	353.4	1.0
19	L	0.9868	0.373E 01	0.410E-02	0.52E-04	353.4	
20	L	0.9868	0.160E 01	0.176E-02	0.22E-04	353.4	
21	L	0.9868	0.213E 01	0.234E-02	0.30E-04	353.4	
25	L	0.2266	0.104E 01	0.995E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.129E-01		0.361E 03	
11				0.102E-03	0.312E 02	0.23
14				0.765E-03	0.237E 03	1.65
18	293.0	303.0	0.386E-01		0.857E 03	
22	293.0	303.0	0.563E-02		0.125E 03	
23	293.0	313.0	0.160E-02		0.507E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 5.26(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 5
STOP --

RUN 4

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR )IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
3.
2.
1.
.01
.0015


 FEED COMPOSITION =  0.6589  XD=P4=  0.9587  XB=P15=  0.1081

 FEED COMPOSITION =  0.7347  XD=P4=  0.9715  XB=P15=  0.1205

 FEED COMPOSITION =  0.7788  XD=P4=  0.9784  XB=P15=  0.1308

 FEED COMPOSITION =  0.8081  XD=P4=  0.9835  XB=P15=  0.1421

 FEED COMPOSITION =  0.8295  XD=P4=  0.9853  XB=P15=  0.1491

 FEED COMPOSITION =  0.8451  XD=P4=  0.9873  XB=P15=  0.1717
```

```
 FEED COMPOSITION =  0.8574  XD=P4=  0.9889  XB=P15=  0.1943
DATA ECHO
 R = 1.0000    XF = 0.8574
 F = 0.000
 NB=  3        NT =  2
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8574

DISTILLATE COMP.:     0.9287     ERROR:    0.14260

OPERATING LINE INTERSECTS FEED LINE AT = 0.8574

DISTILLATE COMP.:     0.9643     ERROR:    0.07130

OPERATING LINE INTERSECTS FEED LINE AT = 0.8574

DISTILLATE COMP.:     0.9822     ERROR:    0.01721

OPERATING LINE INTERSECTS FEED LINE AT = 0.8574

DISTILLATE COMP.:     0.9911     ERROR:   -0.00548

OPERATING LINE INTERSECTS FEED LINE AT = 0.8574

DISTILLATE COMP.:     0.9866     ERROR:    0.00587

OPERATING LINE INTERSECTS FEED LINE AT = 0.8574

PLATE     X        Y
  1    0.9425    0.9890
  2    0.8574    0.9657
STRIPPING SECTION

BOTTOM COMP:      0.4287     ERROR:   -0.27870

BOTTOM COMP:      0.2143     ERROR:   -0.02102

BOTTOM COMP:      0.1072     ERROR:    0.09192

BOTTOM COMP:      0.1608     ERROR:    0.03568

BOTTOM COMP:      0.1876     ERROR:    0.00739

BOTTOM COMP:      0.2010     ERROR:   -0.00680

PLATE     X        Y
  3    0.7291    0.9231
  4    0.4578    0.7821
  5    0.1946    0.4840

 FEED COMPOSITION =  0.8574  XD=P4=  0.9889  XB=P15=  0.1943

 #OF ITERATION=  7  CONVERSION % =  12.53  RESIDENCE TIME=  65.14

 S12= 0.406E-04  C12= 0.115E-01  P12=  0.8672  P4=  0.9889

 S4= 0.311E-04  F4= 0.244E-02  Z4= 0.222E-02  P15=  0.1943
```

RUN 4 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.375E 02	0.537E-03	0.76E-05	298.0	5.0
4	L	0.9889	0.222E 01	0.244E-02	0.31E-04	298.0	
6	L,G	0.8672 AND HCL GAS	0.365E 02	0.354E-02	0.46E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.133E 03	0.184E-03	0.50E-05	318.0	1.0
8	L	WATER	0.547E 00	0.547E-03		298.0	
9	L	HCL DILUTE	0.547E 00	0.731E-03		298.0	
10	L	0.8672	0.512E 01	0.336E-02	0.41E-04	318.0	
12	L	0.8672	0.313E 01	0.336E-02	0.41E-04	357.2	
13	L	0.4578	0.111E 02	0.102E-01	0.11E-03	372.5	
15	L	0.1943	0.105E 01	0.101E-02	0.95E-05	388.0	
16	V	0.4840	0.307E 04	0.919E-02	0.96E-04	388.0	1.0
17	V	0.9889	0.183E 04	0.488E-02	0.62E-04	353.3	1.0
19	L	0.9889	0.444E 01	0.488E-02	0.62E-04	353.3	
20	L	0.9889	0.222E 01	0.244E-02	0.31E-04	353.3	
21	L	0.9889	0.222E 01	0.244E-02	0.31E-04	353.3	
25	L	0.1943	0.105E 01	0.101E-02	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.130E-01		0.362E 03	
11				0.105E-03	0.320E 02	0.24
14				0.911E-03	0.302E 03	1.96
18	293.0	303.0	0.460E-01		0.102E 04	
22	293.0	303.0	0.587E-02		0.130E 03	
23	293.0	313.0	0.166E-02		0.508E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 5.75(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 5
STOP --

RUN 5

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
2.
1.
.25
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  0.8954  XB=P15=  0.3539

 FEED COMPOSITION =  0.7125  XD=P4=  0.9175  XB=P15=  0.3980

 FEED COMPOSITION =  0.7445  XD=P4=  0.9287  XB=P15=  0.4246

 FEED COMPOSITION =  0.7649  XD=P4=  0.9357  XB=P15=  0.4437

 FEED COMPOSITION =  0.7790  XD=P4=  0.9404  XB=P15=  0.4579

 FEED COMPOSITION =  0.7890  XD=P4=  0.9444  XB=P15=  0.4715
DATA ECHO
 R = 0.2500    XF = 0.7890
 F = 0.000
 NB=  2        NT =  1
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:    0.8945    ERROR:   0.24917
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OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9472     ERROR:  -0.01461

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9209     ERROR:   0.11728

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9341     ERROR:   0.05134

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9406     ERROR:   0.01837

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9439     ERROR:   0.00188

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9456     ERROR:  -0.00636

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

DISTILLATE COMP.:     0.9448     ERROR:  -0.00224

OPERATING LINE INTERSECTS FEED LINE AT = 0.7890

PLATE     X        Y
  1    0.7890   0.9443
STRIPPING SECTION

BOTTOM COMP:      0.3945     ERROR:   0.08747

BOTTOM COMP:      0.5917     ERROR:  -0.14911

BOTTOM COMP:      0.4931     ERROR:  -0.02518

BOTTOM COMP:      0.4438     ERROR:   0.03215

BOTTOM COMP:      0.4685     ERROR:   0.00379

BOTTOM COMP:      0.4808     ERROR:  -0.01061

BOTTOM COMP:      0.4746     ERROR:  -0.00339

PLATE     X        Y
  2    0.7013   0.9133
  3    0.4717   0.7913

 FEED COMPOSITION =  0.7890  XD=P4=  0.9444  XB=P15=  0.4715

 #OF ITERATION=  6  CONVERSION % =  17.43  RESIDENCE TIME=  95.92

 S12= 0.263E-04  C12= 0.101E-01  P12=   0.7964  P4=   0.9444

 S4= 0.168E-04  F4= 0.135E-02  Z4= 0.124E-02  P15=   0.4715
```

RUN 5 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.329E 02	0.471E-03	0.66E-05	298.0	5.0
4	L	0.9444	0.124E 01	0.135E-02	0.17E-04	298.0	
6	L,G	0.7964 AND HCL GAS	0.314E 02	0.240E-02	0.31E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.117E 03	0.161E-03	0.44E-05	318.0	1.0
8	L	WATER	0.480E 00	0.480E-03		298.0	
9	L	HCL DILUTE	0.480E 00	0.641E-03		298.0	
10	L	0.7964	0.212E 01	0.224E-02	0.26E-04	318.0	
12	L	0.7964	0.212E 01	0.224E-02	0.26E-04	359.5	
13	L	0.7013	0.340E 01	0.299E-02	0.34E-04	362.7	
15	L	0.4715	0.994E 00	0.915E-03	0.95E-05	371.9	
16	V	0.7913	0.750E 03	0.207E-02	0.24E-04	371.9	1.0
17	V	0.9444	0.620E 03	0.168E-02	0.21E-04	354.7	1.0
19	L	0.9444	0.154E 01	0.168E-02	0.21E-04	354.7	
20	L	0.9444	0.309E 00	0.337E-03	0.42E-05	354.7	
21	L	0.9444	0.124E 01	0.135E-02	0.17E-04	354.7	
25	L	0.4715	0.994E 00	0.915E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.120E-01		0.334E 03	
11				0.728E-04	0.229E 02	0.16
14				0.309E-03	0.720E 02	0.66
18	293.0	303.0	0.157E-01		0.340E 03	
22	293.0	303.0	0.328E-02		0.710E 02	
23	293.0	313.0	0.130E-02		0.498E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 2.32(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 3
STOP --

RUN 6

```
 RUN DX1:LOAD
    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.95
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
2.
2.
.25
.01
.0015


 FEED COMPOSITION =  0.6589  XD=P4=  1.0000  XB=P15=  0.0000


 FEED COMPOSITION =  0.7463  XD=P4=  0.9559  XB=P15=  0.5422
DATA ECHO
 R = 0.2500    XF = 0.7463
 F = 0.000
 NB=  2        NT =  2
RECTIFYING SECTION


OPERATING LINE INTERSECTS FEED LINE AT = 0.7463
```

```
DISTILLATE COMP.:     0.8731    ERROR:    0.63430

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9366    ERROR:    0.20305

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9683    ERROR:   -0.15006

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9524    ERROR:    0.03673

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9604    ERROR:   -0.04678

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9564    ERROR:   -0.00490

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9544    ERROR:    0.01591

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9554    ERROR:    0.00551

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

PLATE     X        Y
  1    0.8220    0.9560
  2    0.7463    0.9291
STRIPPING SECTION

BOTTOM COMP:      0.3731     ERROR:    0.19515

BOTTOM COMP:      0.5597     ERROR:   -0.02399

BOTTOM COMP:      0.4664     ERROR:    0.09121

BOTTOM COMP:      0.5131     ERROR:    0.03601

BOTTOM COMP:      0.5364     ERROR:    0.00675

BOTTOM COMP:      0.5481     ERROR:   -0.00940

PLATE     X        Y
  3    0.7029    0.9140
  4    0.5414    0.8350

 FEED COMPOSITION =   0.7463  XD=P4=   0.9559  XB=P15=   0.5422

 #OF ITERATION=   2  CONVERSION % =   23.69  RESIDENCE TIME= 141.15

 S12= 0.173E-04  C12= 0.912E-02  P12=    0.7479  P4=    0.9559

 S4= 0.778E-05  F4= 0.619E-03  Z4= 0.567E-03  P15=    0.5422
```

RUN 6 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.298E 02	0.427E-03	0.60E-05	298.0	5.0
4	L	0.9559	0.567E 00	0.619E-03	0.78E-05	298.0	
6	L,G	0.7479 AND HCL GAS	0.280E 02	0.165E-02	0.21E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.106E 03	0.146E-03	0.40E-05	318.0	1.0
8	L	WATER	0.435E 00	0.435E-03		298.0	
9	L	HCL DILUTE	0.435E 00	0.582E-03		298.0	
10	L	0.7479	0.143E 01	0.150E-02	0.17E-04	318.0	
12	L	0.7479	0.143E 01	0.150E-02	0.17E-04	361.1	
13	L	0.7029	0.212E 01	0.186E-02	0.21E-04	362.6	
15	L	0.5422	0.983E 00	0.892E-03	0.95E-05	368.7	
16	V	0.8350	0.355E 03	0.969E-03	0.12E-04	368.7	1.0
17	V	0.9559	0.286E 03	0.774E-03	0.97E-05	354.4	1.0
19	L	0.9559	0.709E 00	0.774E-03	0.97E-05	354.4	
20	L	0.9559	0.142E 00	0.155E-03	0.19E-05	354.4	
21	L	0.9559	0.567E 00	0.619E-03	0.78E-05	354.4	
25	L	0.5422	0.983E 00	0.892E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.113E-01		0.316E 03	
11				0.500E-04	0.161E 02	0.11
14				0.143E-03	0.321E 02	0.31
18	293.0	303.0	0.724E-02		0.158E 03	
22	293.0	303.0	0.150E-02		0.328E 02	
23	293.0	313.0	0.123E-02		0.496E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 1.65(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 4
STOP --

RUN 7

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNS)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
2.
3.
.25
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  1.0000  XB=P15=  0.0000


 FEED COMPOSITION =  0.7463  XD=P4=  0.9649  XB=P15=  0.6034
DATA ECHO
 R = 0.2500    XF = 0.7463
 F = 0.000
 NB=  2        NT =  3
RECTIFYING SECTION


OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.8731     ERROR:    0.63430

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9366     ERROR:    0.31715

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9683     ERROR:   -0.06687

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463
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```
DISTILLATE COMP.:     0.9524     ERROR:    0.23786

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9604     ERROR:    0.10354

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9643     ERROR:    0.01437

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9663     ERROR:   -0.02701

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9653     ERROR:   -0.00708

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9648     ERROR:    0.00205

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

DISTILLATE COMP.:     0.9651     ERROR:   -0.00210

OPERATING LINE INTERSECTS FEED LINE AT = 0.7463

PLATE     X         Y
  1    0.8550    0.9650
  2    0.7859    0.9429
  3    0.7463    0.9291
STRIPPING SECTION


BOTTOM COMP:      0.3731     ERROR:    0.26846

BOTTOM COMP:      0.5597     ERROR:    0.05799

BOTTOM COMP:      0.6530     ERROR:   -0.07662

BOTTOM COMP:      0.6064     ERROR:   -0.00399

BOTTOM COMP:      0.5830     ERROR:    0.02809

BOTTOM COMP:      0.5947     ERROR:    0.01239

BOTTOM COMP:      0.6005     ERROR:    0.00429

PLATE     X         Y
  4    0.7236    0.9212
  5    0.6036    0.8708

 FEED COMPOSITION =  0.7463  XD=P4=  0.9649  XB=P15=  0.6034

 #OF ITERATION=  2  CONVERSION % =  25.26  RESIDENCE TIME= 153.65

 S12= 0.157E-04  C12= 0.891E-02  P12=   0.7370  P4=   0.9649

 S4= 0.623E-05  F4= 0.494E-03  Z4= 0.452E-03  P15=   0.6034
```

RUN 7 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.950E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.291E 02	0.417E-03	0.59E-05	298.0	5.0
4	L	0.9649	0.452E 00	0.494E-03	0.62E-05	298.0	
6	L,G	0.7370 AND HCL GAS	0.272E 02	0.151E-02	0.20E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.104E 03	0.143E-03	0.39E-05	318.0	1.0
8	L	WATER	0.425E 00	0.425E-03		298.0	
9	L	HCL DILUTE	0.425E 00	0.568E-03		298.0	
10	L	0.7370	0.131E 01	0.137E-02	0.16E-04	318.0	
12	L	0.7370	0.131E 01	0.137E-02	0.16E-04	361.4	
13	L	0.7236	0.173E 01	0.151E-02	0.17E-04	361.9	
15	L	0.6034	0.973E 00	0.872E-03	0.95E-05	366.3	
16	V	0.8708	0.236E 03	0.641E-03	0.78E-05	366.3	1.0
17	V	0.9649	0.229E 03	0.618E-03	0.78E-05	354.1	1.0
19	L	0.9649	0.565E 00	0.618E-03	0.78E-05	354.1	
20	L	0.9649	0.113E 00	0.124E-03	0.16E-05	354.1	
21	L	0.9649	0.452E 00	0.494E-03	0.62E-05	354.1	
25	L	0.6034	0.973E 00	0.872E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.111E-01		0.310E 03	
11				0.460E-04	0.149E 02	0.10
14				0.113E-03	0.246E 02	0.24
18	293.0	303.0	0.579E-02		0.127E 03	
22	293.0	303.0	0.120E-02		0.262E 02	
23	293.0	313.0	0.117E-02		0.494E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 1.48(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 5
STOP --

RUN 8

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
3.
3.
.25
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  1.0000  XB=P15=  0.0000

 FEED COMPOSITION =  0.7463  XD=P4=  0.9649  XB=P15=  0.4242

 FEED COMPOSITION =  0.7632  XD=P4=  0.9689  XB=P15=  0.4457

 FEED COMPOSITION =  0.7789  XD=P4=  0.9721  XB=P15=  0.4610

 FEED COMPOSITION =  0.7899  XD=P4=  1.0000  XB=P15=  0.0000

 FEED COMPOSITION =  0.8277  XD=P4=  0.9810  XB=P15=  0.4720
DATA ECHO
 R = 0.2500    XF = 0.8277
 F = 0.000
 NB=  3        NT =  3
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:    0.9138    ERROR:   0.43082

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:    0.9569    ERROR:   0.21541

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277
```

```
DISTILLATE COMP.:     0.9785     ERROR:    0.04500

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:     0.9892     ERROR:   -0.14894

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:     0.9838     ERROR:   -0.05169

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:     0.9812     ERROR:   -0.00334

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:     0.9798     ERROR:    0.02083

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:     0.9805     ERROR:    0.00875

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

DISTILLATE COMP.:     0.9808     ERROR:    0.00270

OPERATING LINE INTERSECTS FEED LINE AT = 0.8277

PLATE     X         Y
  1    0.9130    0.9809
  2    0.8636    0.9674
  3    0.8277    0.9575
STRIPPING SECTION


BOTTOM COMP:      0.4138     ERROR:    0.07464

BOTTOM COMP:      0.6208     ERROR:   -0.21475

BOTTOM COMP:      0.5173     ERROR:   -0.06115

BOTTOM COMP:      0.4656     ERROR:    0.00932

BOTTOM COMP:      0.4914     ERROR:   -0.02511

BOTTOM COMP:      0.4785     ERROR:   -0.00772

PLATE     X         Y
  4    0.8025    0.9503
  5    0.7100    0.9164
  6    0.4729    0.7920

 FEED COMPOSITION =  0.8277  XD=P4=  0.9810  XB=P15=  0.4720

 #OF ITERATION=  6  CONVERSION % =  16.54  RESIDENCE TIME=  90.09

 S12= 0.286E-04  C12= 0.106E-01  P12=  0.8240  P4=  0.9810

 S4= 0.191E-04  F4= 0.150E-02  Z4= 0.137E-02  P15=  0.4720
```

RUN 8 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.347E 02	0.497E-03	0.70E-05	298.0	5.0
4	L	0.9810	0.137E 01	0.150E-02	0.19E-04	298.0	
6	L,G	0.8240 AND HCL GAS	0.331E 02	0.258E-02	0.33E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.123E 03	0.170E-03	0.47E-05	318.0	1.0
8	L	WATER	0.506E 00	0.506E-03		298.0	
9	L	HCL DILUTE	0.506E 00	0.677E-03		298.0	
10	L	0.8240	0.226E 01	0.241E-02	0.29E-04	318.0	
12	L	0.8240	0.226E 01	0.241E-02	0.29E-04	358.6	
13	L	0.7100	0.373E 01	0.326E-02	0.37E-04	362.4	
15	L	0.4720	0.994E 00	0.915E-03	0.95E-05	371.8	
16	V	0.7920	0.852E 03	0.235E-02	0.28E-04	371.8	1.0
17	V	0.9810	0.701E 03	0.188E-02	0.24E-04	353.5	1.0
19	L	0.9810	0.171E 01	0.188E-02	0.24E-04	353.5	
20	L	0.9810	0.342E 00	0.376E-03	0.48E-05	353.5	
21	L	0.9810	0.137E 01	0.150E-02	0.19E-04	353.5	
25	L	0.4720	0.994E 00	0.915E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.126E-01		0.352E 03	
11				0.770E-04	0.239E 02	0.17
14				0.347E-03	0.807E 02	0.75
18	293.0	303.0	0.177E-01		0.391E 03	
22	293.0	303.0	0.362E-02		0.801E 02	
23	293.0	313.0	0.129E-02		0.498E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 2.46(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 6
STOP --

RUN 9

```
 RUN DX1:LOAD
    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HF IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
4.
3.
.25
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  1.0000  XB=P15=  0.0000

 FEED COMPOSITION =  0.7463  XD=P4=  0.9649  XB=P15=  0.2361

 FEED COMPOSITION =  0.7746  XD=P4=  0.9713  XB=P15=  0.2572

 FEED COMPOSITION =  0.7997  XD=P4=  1.0000  XB=P15=  0.0000

 FEED COMPOSITION =  0.8354  XD=P4=  0.9821  XB=P15=  0.2545
DATA ECHO
 R = 0.2500   XF = 0.8354
 F = 0.000
 NB=  4       NT =  3
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:    0.9177    ERROR:   0.41148

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:    0.9589    ERROR:   0.20574

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:    0.9794    ERROR:   0.04759

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354
```

```
DISTILLATE COMP.:     0.9897     ERROR:  -0.13756

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:     0.9846     ERROR:  -0.04476

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:     0.9820     ERROR:   0.00141

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:     0.9833     ERROR:  -0.02168

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:     0.9826     ERROR:  -0.01013

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:     0.9823     ERROR:  -0.00436

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

DISTILLATE COMP.:     0.9822     ERROR:  -0.00147

OPERATING LINE INTERSECTS FEED LINE AT = 0.8354

PLATE     X        Y
  1    0.9173    0.9821
  2    0.8699    0.9691
  3    0.8354    0.9596
STRIPPING SECTION


BOTTOM COMP:      0.4177     ERROR:  -0.20086

BOTTOM COMP:      0.2089     ERROR:   0.05326

BOTTOM COMP:      0.3133     ERROR:  -0.07056

BOTTOM COMP:      0.2611     ERROR:  -0.00835

BOTTOM COMP:      0.2350     ERROR:   0.02268

BOTTOM COMP:      0.2480     ERROR:   0.00723

PLATE     X        Y
  4    0.8103    0.9527
  5    0.7277    0.9226
  6    0.5212    0.8232
  7    0.2540    0.5751

 FEED COMPOSITION =  0.8354  XD=P4=  0.9821  XB=P15=  0.2545

 #OF ITERATION=  5  CONVERSION % =  14.91  RESIDENCE TIME=  79.65

 S12= 0.327E-04  C12= 0.109E-01  P12=   0.8401  P4=   0.9821

 S4= 0.232E-04  F4= 0.182E-02  Z4= 0.166E-02  P15=   0.2545
```

RUN 9 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.357E 02	0.512E-03	0.72E-05	298.0	5.0
4	L	0.9821	0.166E 01	0.182E-02	0.23E-04	298.0	
6	L,G	0.8401 AND HCL GAS	0.343E 02	0.291E-02	0.37E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.127E 03	0.175E-03	0.48E-05	318.0	1.0
8	L	WATER	0.521E 00	0.521E-03		298.0	
9	L	HCL DILUTE	0.521E 00	0.697E-03		298.0	
10	L	0.8401	0.256E 01	0.273E-02	0.33E-04	318.0	
12	L	0.8401	0.256E 01	0.273E-02	0.33E-04	358.0	
13	L	0.5212	0.587E 01	0.535E-02	0.57E-04	369.6	
15	L	0.2545	0.103E 01	0.986E-03	0.75E-05	383.9	
16	V	0.5751	0.150E 04	0.436E-02	0.47E-04	383.9	1.0
17	V	0.9821	0.851E 03	0.228E-02	0.29E-04	353.5	1.0
19	L	0.9821	0.208E 01	0.228E-02	0.29E-04	353.5	
20	L	0.9821	0.415E 00	0.456E-03	0.58E-05	353.5	
21	L	0.9821	0.166E 01	0.182E-02	0.23E-04	353.5	
25	L	0.2545	0.103E 01	0.986E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.128E-01		0.356E 03	
11				0.866E-04	0.267E 02	0.20
14				0.430E-03	0.128E 03	0.92
18	293.0	303.0	0.215E-01		0.475E 03	
22	293.0	303.0	0.439E-02		0.972E 02	
23	293.0	313.0	0.156E-02		0.506E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 4.01(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 7
STOP --

RUN 10

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
3.
3.
.75
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  0.9767  XB=P15=  0.1429

 FEED COMPOSITION =  0.7366  XD=P4=  0.9861  XB=P15=  0.1683

 FEED COMPOSITION =  0.7801  XD=P4=  0.9897  XB=P15=  0.1981

 FEED COMPOSITION =  0.8077  XD=P4=  0.9952  XB=P15=  0.2161

 FEED COMPOSITION =  0.8285  XD=P4=  0.9991  XB=P15=  0.2427

 FEED COMPOSITION =  0.8439  XD=P4=  0.9997  XB=P15=  0.2588

 FEED COMPOSITION =  0.8549  XD=P4=  0.9997  XB=P15=  0.2672
DATA ECHO
 R = 0.7500    XF = 0.8549
 F = 0.000
 NB=  3        NT =  3
RECTIFYING SECTION
```

```
OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9275     ERROR:    0.16923

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9637     ERROR:    0.08462

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9819     ERROR:    0.04231

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9909     ERROR:    0.02115

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9955     ERROR:    0.01058

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9977     ERROR:    0.00529

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9989     ERROR:    0.00264

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

DISTILLATE COMP.:     0.9994     ERROR:    0.00132

OPERATING LINE INTERSECTS FEED LINE AT = 0.8549

PLATE     X         Y
  1    0.9595    1.0000
  2    0.9187    0.9825
  3    0.8549    0.9650
STRIPPING SECTION


BOTTOM COMP:      0.4275     ERROR:   -0.17879

BOTTOM COMP:      0.2137     ERROR:    0.05827

BOTTOM COMP:      0.3206     ERROR:   -0.05851

PLATE     X         Y
  4    0.7707    0.9377
  5    0.5527    0.8416
  6    0.2678    0.5928

 FEED COMPOSITION =   0.8549  XD=P4=   0.9997  XB=P15=   0.2672

 #OF ITERATION=   7  CONVERSION % =   13.61  RESIDENCE TIME=   71.61

 S12= 0.369E-04  C12= 0.114E-01  P12=    0.8637  P4=    0.9997

 S4= 0.274E-04  F4= 0.214E-02  Z4= 0.194E-02  P15=    0.2672
```

RUN 10 CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.373E 02	0.535E-03	0.75E-05	298.0	5.0
4	L	0.9997	0.194E 01	0.214E-02	0.27E-04	298.0	
6	L,G	0.8637 AND HCL GAS	0.360E 02	0.324E-02	0.42E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.133E 03	0.183E-03	0.50E-05	318.0	1.0
8	L	WATER	0.544E 00	0.544E-03		298.0	
9	L	HCL DILUTE	0.544E 00	0.728E-03		298.0	
10	L	0.8637	0.285E 01	0.305E-02	0.37E-04	318.0	
12	L	0.8637	0.285E 01	0.305E-02	0.37E-04	357.3	
13	L	0.5527	0.795E 01	0.720E-02	0.77E-04	368.3	
15	L	0.2672	0.103E 01	0.982E-03	0.95E-05	383.1	
16	V	0.5928	0.215E 04	0.622E-02	0.68E-04	383.1	1.0
17	V	0.9997	0.141E 04	0.374E-02	0.48E-04	382.9	1.0
19	L	0.9997	0.340E 01	0.374E-02	0.48E-04	352.9	
20	L	0.9997	0.146E 01	0.160E-02	0.21E-04	352.9	
21	L	0.9997	0.194E 01	0.214E-02	0.27E-04	352.9	
25	L	0.2672	0.103E 01	0.982E-03	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.131E-01		0.367E 03	
11				0.957E-04	0.292E 02	0.22
14				0.701E-03	0.202E 03	1.51
18	293.0	303.0	0.354E-01		0.792E 03	
22	293.0	303.0	0.513E-02		0.115E 03	
23	293.0	313.0	0.154E-02		0.505E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 5.01(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 6
STOP --

```
 RUN DX1:LOAD

    WHAT IS THE INLET BENZENE FLOW RATE(V1 IN CM CUBE/SEC)
THE REACTOR VOLUME(VR IN CUBIC DM)
THE PRESSURE IN THE REACTOR(PRR IN BAR)
THE TEMPERATURE OF THE REACTOR(TRR IN DEGREE KELVIN)
THE RATE CONSTANT(RAA KG MOLE/KG MOLE BENZENE CHARGED/SEC)
AND THE HEAT OF REACTION(HR IN KCAL/KG MOLE)?
.85
.2
4.
318.
.0011
31201.


    WHAT IS THE NUMBER OF TRAYS IN THE STRIPPING SECTION(ZNB)
THE NUMBER OF TRAYS IN THE RECTIFYING SECTION(ZNT)
THE REFLUX RATIO(RR)
THE ACCURACY NEEDED IN THE FEED STREAM(AA)
AND THE WEIGHT OF CATALYST ADDED AT THE START(F2 IN KG)?
4.
3.
.75
.01
.0015



 FEED COMPOSITION =  0.6589  XD=P4=  0.9767  XB=P15=  0.0553

 FEED COMPOSITION =  0.7400  XD=P4=  0.9863  XB=P15=  0.0694

 FEED COMPOSITION =  0.7858  XD=P4=  0.9904  XB=P15=  0.0737

 FEED COMPOSITION =  0.8158  XD=P4=  0.9967  XB=P15=  0.0860

 FEED COMPOSITION =  0.8387  XD=P4=  0.9997  XB=P15=  0.0950

 FEED COMPOSITION =  0.8556  XD=P4=  0.9997  XB=P15=  0.0986

 FEED COMPOSITION =  0.8679  XD=P4=  0.9997  XB=P15=  0.1017

 FEED COMPOSITION =  0.8780  XD=P4=  0.9998  XB=P15=  0.1029
DATA ECHO
 R = 0.7500    XF = 0.8780
 F = 0.000
 NB=  4        NT =  3
RECTIFYING SECTION

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:     0.9390     ERROR:   0.14237

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780
```

```
DISTILLATE COMP.:    0.9695    ERROR:   0.07118

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:    0.9847    ERROR:   0.03559

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:    0.9924    ERROR:   0.01780

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:    0.9962    ERROR:   0.00890

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:    0.9981    ERROR:   0.00445

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:    0.9990    ERROR:   0.00222

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

DISTILLATE COMP.:    0.9995    ERROR:   0.00111

OPERATING LINE INTERSECTS FEED LINE AT = 0.8780

PLATE     X        Y
  1    0.9688   1.0000
  2    0.9334   0.9865
  3    0.8780   0.9713
STRIPPING SECTION

BOTTOM COMP:     0.4390    ERROR:  -0.36190

BOTTOM COMP:     0.2195    ERROR:  -0.12278

BOTTOM COMP:     0.1097    ERROR:  -0.00760

BOTTOM COMP:     0.0549    ERROR:   0.04930

BOTTOM COMP:     0.0823    ERROR:   0.02069

BOTTOM COMP:     0.0960    ERROR:   0.00669

PLATE     X        Y
  4    0.7963   0.9476
  5    0.5804   0.8585
  6    0.2915   0.6233
  7    0.1024   0.3085

 FEED COMPOSITION =  0.8780  XD=P4=  0.9998  XB=P15=  0.1029

 #OF ITERATION=  8  CONVERSION % =  11.34  RESIDENCE TIME=  58.17

 S12= 0.460E-04  C12= 0.119E-01  P12=  0.8864  P4=  0.9998

 S4= 0.365E-04  F4= 0.285E-02  Z4= 0.259E-02  P15=  0.1029
```

RUN 11 (CONT'D)

TABLE 1(MATERIAL BALANCE)

STREAM #	PHASE	MOLE FRACTION OF BENZENE	VOLUMETRIC FLOW RATE (CUBIC CM/SEC)	MASS FLOW RATE (KG/SEC)	MOLAR FLOW RATE (KG MOLE/SEC)	TEMPERATURE (D. KELVIN)	PRESSURE (BAR)
1	L	1.0000	0.850E 00	0.742E-03	0.95E-05	298.0	5.0
2	S	FERRIC CHLORIDE		0.150E-02*		298.0	
3	G	(CHLORINE GAS)	0.388E 02	0.E55E-03	0.78E-05	298.0	5.0
4	L	0.9998	0.259E 01	0.285E-02	0.36E-04	298.0	
6	L,G	0.8864 AND HCL GAS	0.380E 02	0.396E-02	0.51E-04	318.0	4.0
7	G	HYDROCHLORIC ACID	0.138E 03	0.190E-03	0.52E-05	318.0	1.0
8	L	WATER	0.566E 00	0.566E-03		298.0	
9	L	HCL DILUTE	0.566E 00	0.756E-03		298.0	
10	L	0.8864	0.350E 01	0.377E-02	0.46E-04	318.0	
12	L	0.8864	0.350E 01	0.377E-02	0.46E-04	256.6	
13	L	0.2915	0.125E 02	0.118E-01	0.12E-03	381.5	
15	L	0.1029	0.106E 01	0.104E-02	0.95E-05	395.1	
16	V	0.3085	0.348E 04	0.108E-01	0.11E-03	395.1	1.0
17	V	0.9998	0.187E 04	0.499E-02	0.64E-04	352.9	1.0
19	L	0.9998	0.453E 01	0.499E-02	0.64E-04	352.9	
20	L	0.9998	0.194E 01	0.214E-02	0.27E-04	352.9	
21	L	0.9998	0.259E 01	0.285E-02	0.36E-04	352.9	
25	L	0.1029	0.106E 01	0.104E-02	0.95E-05	298.0	

* STREAM#2 IS THE CATALYST ADDED AT THE START ONLY
STREAM#6 IS COMPOSED OF:LIQUID (BENZENE AND CHLOROBENZENE) AND GAS (HCL)
STREAM#24 IS THE NON-CONDENSABLE GASES(HCL AND CHLORINE) COMING FROM THE CONDENSER
STREAM#26 IS COMPOSED OF STEAM#24 AND 7

TABLE 2(HEAT BALANCE)

STREAM #	INLET TEMPERATURE (DEGREE KELVIN)	OUTLET TEMPERATURE (DEGREE KELVIN)	COOLING WATER MASS FLOW RATE (KG/SEC)	STEAM MASS FLOW RATE (KG/SEC)	AREA (SQUARE CM)	POWER (KW)
5	291.0	301.0	0.132E-01		0.367E 03	
11				0.117E-03	0.352E 02	0.26
14				0.940E-03	0.420E 03	2.02
18	293.0	303.0	0.472E-01		0.106E 04	
22	293.0	303.0	0.683E-02		0.153E 03	
23	293.0	313.0	0.182E-02		0.512E 02	

HEATING IS DONE BY STEAM AT ONE ATMOSPHERE OR BY ELECTRIC POWER

WHAT IS THE VALUE OF THE TRAY SPACING(TS IN CM)?
22.86

TOWER DIAMETER= 5.87(CM) TRAY SPACING= 22.860(CM) NUMBER OF PLATES= 7
STOP --

Table 2 Operating conditions investigated and results*

Run #	Reflux Ratio	NB	NT	Residence Time (sec)	Conversion %	X_F	X_D	X_B	D
1	0.25	3	2	86.6	16	0.8157	0.9723	0.4031	3.66
2	0.5	3	2	70.84	13.48	0.8450	0.9830	0.2806	4.67
3	0.75	3	2	67.09	12.86	0.8530	0.9868	0.2266	5.26
4	1.0	3	2	65.14	12.53	0.8574	0.9889	0.1943	5.75
5	0.25	2	1	95.92	17.43	0.7890	0.9444	0.4715	2.32
6	0.25	2	2	141.15	23.69	0.7463	0.9559	0.5422	2.37
7	0.25	2	3	153.65	25.26	0.7463	0.9649	0.6034	2.13
8	0.25	3	3	90.09	16.54	0.8277	0.9810	0.4720	2.46
9	0.25	4	3	79.65	14.91	0.8354	0.9821	0.2545	4.01
10	0.75	3	3	71.61	13.61	0.8549	0.9997	0.2672	5.01
11	0.75	3	3	58.17	11.34	0.8780	0.9998	0.1029	5.87

*Pressure = 4 atmosphere, temperature = 318° K and fresh benzene flow rate = 85 cm^3/sec

Where

NB = the number of trays in the stripping section

NT = the number of trays in the rectifying section

X_D = the distillate benzene mole fraction

X_B = the bottom product benzene mole fraction

X_F = the benzene mole fraction of the distillation feed

D = diameter of column in cm

From Table 2, it was concluded that runs 5, 6, 7, and 8 have to be rejected due to high benzene mole fraction in the bottom product which means that a large amount of benzene will be lost and therefore the cost per run would be high. Runs 10 and 11 show a distillate benzene mole fraction of approximately one which is undesirable because in that region the concentration measurements by the refractive index will be inaccurate, and also because in the iterative procedure described earlier, if the calculated top composition was > 1.0, the next assumed value will be taken as 1.0. This means that in the proximity of 1.0, the iterative procedure is relatively unefficient and inaccurate. Therefore a four plate column - two in the stripping section and two in the enriching section - seems reasonable for the purpose of this experiment. The results of numerous computer simulation for different operating conditions, were examined carefully to select the appropriate equipment size for the design purposes, which fulfill the requirements cited at the beginning of this section. From those results, a fresh benzene feed flow rate of about 1.0 cm^3/sec was selected, with an approximately 200 cm^3 reactor. Also a 5 cm (2") internal diameter distillation column with a 23 cm (9") tray spacing and four plates,would be appropriate for the selected benzene flow rate and reactor volume. The distillation column will separate the reaction products to approximately a 98% distillate benzene mole fraction which will be recycled. For the assumed five hours run for each laboratory experimental investiagation, 19 dm^3 (5 gal) tanks will be used. For design purposes, a safety factor of at least 1.5 was used in calculating the actual heat transfer area (AHTA), from the average heat transfer area

(HTA) taken from the steady state computer results. Table 3 shows the specifications of the heaters, coolers, condenser, reboiler, and reactor. The effective reactor volume was calculated as follows:

1) volume of cooling coils = 39.849 cubic cm
2) the volume of the accessories in the reactor is assumed to be 15% of the cooling coil's volume, therefore it equals 5.976 cubic cm
3) the total volume of reactor (2.87" I.D., 2.5" height) = 265. cubic cm

Therefore the volume of reactor used for the reaction =

265. - 29.869 - 5.976 = 219.175 approximately 220 cubic cm.

Table 3. Cooling Coils and Heater Specifications

Equipment*	Tube O.D. (cm)	Coil Diameter (cm)	Height (cm)	Number of Turns	HTA (square cm)	AHTA (square cm)
Inner Reactor Coil	0.3175	5.7		13		271.
Outer Reactor Coil	0.3175	6.654		13		232.
Reactor Jacket	7.62		6.35			152.
					362.	655.
Heater	1.7		10.		32.	53.4
Condenser					1020.	3000.
Reboiler					302.	1500.
Distillate Cooler	0.3175	2.54		38	130.	302.4
Bottom Product Cooler	0.3175	2.54		13	50.8	103.

*See Figure 8, Page 22

D) The Transient Equations for the Reactor

Figure 12 shows a simplified diagram for the reactor where the inlet and outlet streams are shown.

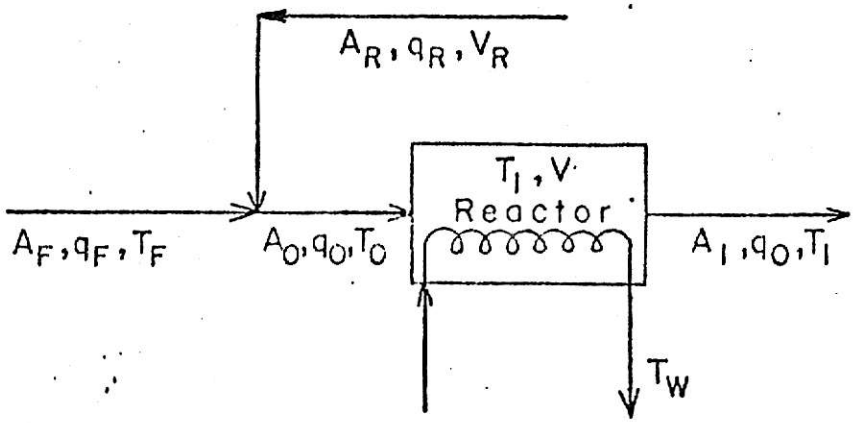


Figure 12 Simplified Diagram for the Reactor

The suffixes R, F, 0, and 1 represent the recycle, the fresh feed, the inlet, and the outlet streams respectively. The transient mass and energy balance are as follows:

1) Mass Balance on Benzene

rate of accumulation = rate in - rate out - rate of consumption

$$\frac{V dA_1}{d\theta} = q_0 A_0 - q_0 A_1 - K A_1 V$$

where

θ = time in seconds

A is the concentration of benzene (gm mole/cm^3)

A_0 = .0118 gm mole/cm^3 at θ = 0 (reactor is full of benzene)

q = flow rate (cm^3/sec)

q_R depends on reflux ratio (R.R.)

q_R = 2.13 cm^3/sec at R.R. = .75

q_R = 2.22 cm^3/sec at R.R. = 1.0

$q_F = .85\ cm^3/sec$

$q_0 = q_F + q_R$

$A_F = .01118\ gm\ mole/cm^3$

$$K = .00117 \frac{(gm\ mole\ benzene/cm^3)}{(gm\ mole\ benzene\ charged/cm^3)\ (seconds)}$$

V = volume of reactor = $200\ cm^3$

The recycled stream is assumed to be pure benzene, which is approximately the case.

2) Energy balance

rate of accum.= (flow in - out) + (generation) + (heat exchange)

$$\rho C_p V \frac{dT_1}{d\theta} = q_0 \rho C_p\ (T_0 - T_1) + (-\Delta H_1)\ KA_1 V - UA(T_1 - T_W)$$

where

T_1 is the temperature of the reactor (^oK)

T_0 is the inlot temperature = 298^o K

T_W is the cooling water temperature

ρ is the density of benzene = $.87\ gm/cm^3$

C_p is the heat capacity of benzene = $.4178\ cal/gm/^oK$

ΔH_1 is the heat of reaction

U is the overall heat transfer coefficient

$= 162.852 \times 10^{-4}\ cal/sec/cm^2/^o$ K

A is the heat transfer area $\sim$ $360\ cm^2$

E) The Transient Equations for Distillation Column [15]

The derivation of the equations that govern the transient behavior of the column is based upon the following equations:

1) Unsteady state total material balance for each tray
2) Unsteady state material balance for the more volatile component on each tray
3) Definition of Murphree tray efficiency
4) Equilibrium vapor composition as a function of liquid composition
5) Liquid reflux flow rate from a tray as a function of tray holdup.

The equations are linearized about an arbitrarily chosen set of steady state operating conditions. All of the dependent variables in the equations, such as tray compositions, liquid and vapor flows, etc., are replaced by their deviations from the steady state. This results in a set of linear differential equations in which all dependent variables are perturbations from a steady state, and in which all coefficients are determined from the steady state operating conditions. The linearized perturbation equations are listed in the next pages, followed by the notation and a simplified diagram (figure 13).

a) Enriching Section

1) component balance

$$\frac{dx_n}{d\theta} = (\bar{x}_{n+1} - \bar{x}_n)(\ell_{n+1} - v_n) + (x_{n+1} - x_n) - \bar{v}(y_n - y_{n-1}) \quad (1)$$

2) total balance

$$\frac{d\ell_n}{d\theta} = \frac{1}{\beta_n}(\ell_{n+1} - \ell_n) \quad (2)$$

3) phase equilibrium

$$y_n = E_n \phi_n' x_n + (1 - E_n) y_{n-1} \quad (3)$$

b) Stripping Section

1) component balance

$$\bar{h}_m \frac{dx_m}{d\theta} = (\bar{x}_{m+1} - \bar{x}_m)\ (\bar{\ell}_{m+1}\ell_{m+1} - \bar{\ell}_m v_m) + \bar{\ell}_m(x_{m+1} - x_m) - \bar{v}_m(y_m - y_{m-1}) \quad (4)$$

2) total balance

$$\frac{d\ell_m}{d\theta} = \frac{1}{\beta_m}(\ell_{m+1} - \ell_m) \quad (5)$$

3) phase equilibrium

$$y_m = E_m \phi_m' x_m + (1 - E_m)\ y_{m-1} \quad (6)$$

c) Feed Tray

1) component balance

$$\bar{h}_F \frac{dx_F}{d\theta} = (\bar{x}_{F+1} - \bar{x}_F)\ \ell_{F+1} + \bar{y}_{F-1}\bar{v}_m v_m - \bar{y}_F \bar{v}_n v_n + (\bar{Z}_F - \bar{q}_F \bar{x}_F)\bar{f} f + (x_{F+1} - \bar{\ell}_m x_F) - (\bar{v}_n y_F - \bar{v}_m y_{F-1}) + \bar{f} Z_F - \bar{x}_F \bar{f} q_F \quad (7)$$

2) total balance

for liquid phase, $\beta_F \bar{\ell}_m \frac{d\ell_F}{d\theta} = \ell_{F+1} - \bar{\ell}_m \ell_F + \bar{q}_F \bar{f} f + \bar{f} q_F$ (8)

for vapor phase, $\bar{v}_n v_n = \bar{v}_m v_m + (1 - \bar{q}_F)\ \bar{f} f - \bar{f} q_F$ (9)

3) phase equilibrium

$$y_F = E_F \phi_F' x_F + (1 - E_F)\ y_{F-1} \quad (10)$$

d) Condenser

1) component balance

$$\frac{dx_{N+1}}{d\theta} = \frac{\bar{v}_n}{\bar{h}_c}(y_N - x_{N+1}) \quad (11)$$

2) total balance

$$\frac{d\ell_c}{d\theta} = \frac{1}{\beta_c} (v_n - \ell_c) \tag{12}$$

e) Reboiler

1) component balance

$$\bar{h}_R \frac{dx_0}{d\theta} = (\bar{x}_1 - \bar{x}_0)\ \bar{\ell}_m \ell_1 - (\bar{y}_0 - \bar{x}_0)\ \bar{v}_m v_m + \bar{\ell}_m x_1 - (\bar{\ell}_R x_0 + \bar{v}_m y_0) \tag{13}$$

2) total balance

$$\bar{\ell}_R \beta_R \frac{d\ell_R}{d\theta} = \bar{\ell}_m \ell_1 - (\bar{v}_m v_m + \bar{\ell}_R \ell_R) \tag{14}$$

3) phase equilibrium

$$y_0 = \phi_0' x_0 \tag{15}$$

Notation

1) Column region is indicated by a subscript: n for enriching section, m for stripping section, N for top tray, F for feed, C and (N+1) for condenser, and R and 0 for reboiler.

2) An overscore indicates a steady state quantity. No superscript indicates a perturbation quantity.

3) $B(L^T)$ = function giving liquid tray hold up H^T in terms of liquid flow rate L^T leaving the tray

B' = $(dB)/(d\bar{L})$ where $H_n = B(L_n)$

E = Murphree tray efficiency

F = feed flow rate (moles/unit time)

f = feed flow rate relative to steady state value = $F/\bar{F}$

$\bar{f}$ = steady state feed flow rate relative to steady state liquid flow in enriching section = $\bar{F}/\bar{L}_n$

H = liquid hold up (moles)

h = liquid hold up relative to steady state liquid flow in enriching section = $H/\bar{H}_n$

$\bar{h}$ = $\bar{H}/\bar{H}_n$

L = liquid flow rate (moles/unit time)

ℓ = liquid flow rate relative to steady state volue = $L/\bar{L}$

$\bar{\ell}$ = $\bar{L}/\bar{L}_n$

q = heat required to convert 1 mole of feed to saturated vapor divided by the molar latent heat of vaporization

V = vapor flow rate (moles/unit time)

v = vapor flow rate relative to steady state value = $V/\bar{V}$

$\bar{v}$ = steady state vapor flow rate relative to steady state liquid flow in enriching section = $\bar{V}/\bar{L}_n$

t = time

x = liquid mole fraction

y = vapor mole fraction

β = $(\bar{L}_n B')/(\bar{H}_n)$

y^* = vapor mole fraction in equilibrium with liquid on sam tray

Z_F = mole fraction of feed

$\phi(x)$ = function giving equilibrium with liquid on same tray y^* in terms of liquid mole fraction x

ϕ' = $(d\phi)/(d\bar{x})$

β = $(\bar{L}_n B')/(\bar{H}_n)$

θ = dimensionless time = $(\bar{L}_n t)/(\bar{H}_n)$

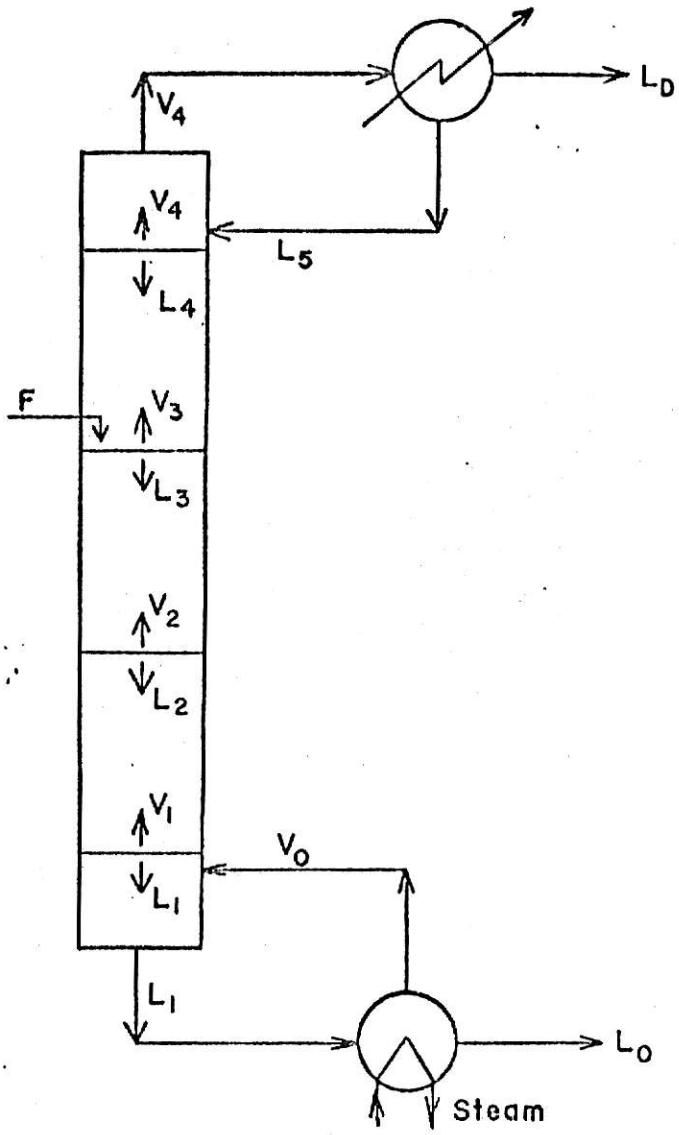


Figure 13. Simplified Diagram for the Distillation Column

From the steady state and mass balance calculations, the following results were obtained where L, V, and F are the molar flow rate(gm/mole/min)for run#3

$L_5 = 1.418$	$X_5 = .9868$	$L_D = 1.891$	$X_D = .9868$
$L_4 = 1.415$	$X_4 = .9347$	$V_4 = 3.309$	$y_4 = .9868$
$L_3 = 5.25$	$X_3 = .853$	$V_3 = 3.306$	$y_3 = .9645$
$L_2 = 5.25$	$X_2 = .7472$	$V_2 = 4.68$	$y_2 = .9294$
$L_1 = 5.25$	$X_1 = .5014$	$V_1 = 4.68$	$y_1 = .8108$
$L_0 = .57$	$X_0 = .2274$	$V_0 = 4.68$	$y_0 = .5350$
$F = 2.34$	$X_F = .853$		

The distillation column was operated at atmospheric pressure with a reflux ratio of .75 and a saturated liquid feed.

Assumptions

1) A linear relationship is assumed between $\bar{L}_n$ and $\bar{H}_n$.

   Therefore $\beta_R = \beta_1 = \beta_2 = \beta_F = \beta_4 = \beta_c = 1$

2) $\bar{h}_c = 2$, $\bar{h}_R = 10$, and $\bar{h}_2 = \bar{h}_1 = 1$

3) $q_F = 0$ (saturated liquid)

4) From figure 14 we have: $\phi_0' = 1.495$, $\phi_1' = .64$, $\phi_2' = .377$,

   $\phi_3' = .292$, and $\phi_4' = .245$

5) Murphree efficiency = 1

By using these assumptions and equations (1) to (15) we get the following differential equations which describe the dynamic characteristics of the distillation column

1) for the condenser

$$\frac{dx_D}{d\theta} = \frac{2.9}{2} (y_4 - x_D) \tag{16}$$

$$\frac{d\ell_c}{d\theta} = v_4 - \ell_c \tag{17}$$

2) enriching section (plate 4)

$$\frac{dx_4}{d\theta} = .0521 (\ell_5 - v_4) + (x_D - x_4) - 2.9 (y_4 - y_3) \tag{18}$$

$$\frac{d\ell_4}{d\theta} = \ell_5 - \ell_4 \tag{19}$$

$$y_4 = .245\, x_4 \tag{20}$$

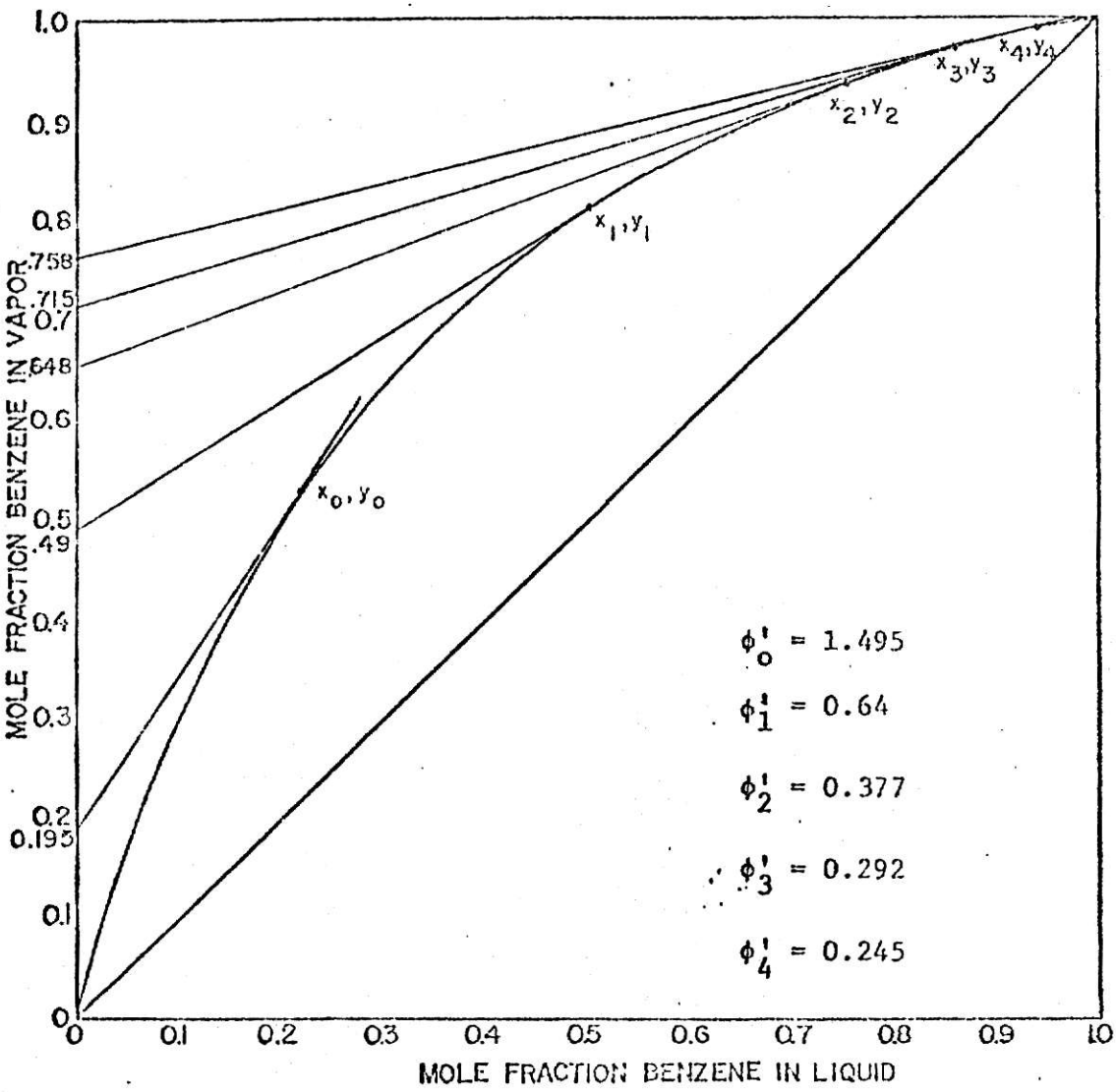


Figure 14. Calculation of Slope at Equilibrium for Run #3

3) feed plate (plate 3)

$$\frac{dx_3}{d\theta} = .0817\ell_4 + 3.074v_2 - 2.334y_3v_3 + 1.411f + (x_4 - 3.71x_3) - (2.337y_3 - 3.307y_2) + 1.654Z_F \quad (21)$$

$$3.71\frac{d\ell_3}{d\ell} = \ell_4 - 3.71\ell_3 \text{ (liquid phase)} \quad (22)$$

$$2.336v_3 = 3.265v_2 + 1.654f \text{ (vapor phase)} \quad (23)$$

$$y_3 = .292x_3 \quad (24)$$

4) stripping section (plate 2 and 1)

$$\frac{dx_2}{d\theta} = .393\ (\ell_3 - v_2) + 3.71\ (x_3 - x_2) - 3.265\ (y_2 - y_1) \quad (25)$$

$$\frac{d\ell_2}{d\theta} = \ell_3 - \ell_2 \quad (26)$$

$$y_2 = .377x_2$$

$$\frac{dx_1}{d\theta} = .912\ (\ell_2 - v_1) + 3.71\ (x_2 - x_1) - 3.265\ (y_1 - y_0) \quad (28)$$

$$\frac{d\ell_1}{d\theta} = \ell_2 - \ell_1 \quad (29)$$

$$y_1 = .64x_1 \quad (30)$$

5) reboiler (plate zero or R)

$$10\frac{dx_0}{d\theta} = 1.017\ell_1 - 1.004v_1 + 3.71x_1 - .403x_0 - 3.265y_0 \quad (31)$$

$$.403\frac{d\ell_R}{d\theta} = 3.71\ell_1 - 3.265v_1 - .403\ell_R \quad (32)$$

$$y_0 = 1.495x_0 \quad (33)$$

Equations 16 to 33 represent the linearized perturbation equations for the transient behavior of the column. In these equations, the six variables that can be perturbed separetely are: the feed composition, the feed flow rate, the feed quality, the distillate composition, the reflux ratio, and the bottom product composition.

IV SUGGESTED EXPERIMENTAL PROCEDURES

Process control and safety considerations are discussed in detail in this section along with their effects on the choice of equipment, accessories, measuring instruments, valves, and controllers. A brief study of optimization aspects will also be presented.

Due to the educational nature of this equipment, the operation and control must be easy to understand and yet it must provide the desired learning experiences - ranging from manual operation to the modern techniques of automatic control and computer simulation and control.

A) MANUAL OPERATION

Each stream may be controlled manually by valves, measuring instruments, and accessories to reach the steady state values already listed in the computer results. Manual operation will be used to study the steady state and the dynamics of the two major pieces of equipment (the reactor and the distillation column); therefore the effect of changing the operating conditions on the operation of the system and on the steady state can be investigated easily. Manual control will provide a way to operate the reactor and the distillation column as one unit or as two separate operations for experimental investigations. The equipment installed for manual operation include the essential and basic equipment in addition to the manually operated, measuring, and controlling equipment and accessories. Even under manual operation, some aspects of the system (liquid level and temperature of the reactor) will be under automatic control at all times; the temperature of the reactor will be kept constant by a feedback control system - a pneumatic valve, an automatic controller, a transducer, and a

valve operator - which will be used to control the flow rate of cooling water in the reactor and the jacket. The reactor, therefore, may be considered to operate at a constant temperature.

The kinetics of the reaction and the dynamics of the reactor can be determined by operating the reactor batchwise or continuously. The distribution of the reaction products with time, or as a function of chlorine concentration, for a batch or continuous reactor may be determined with a comparison between their behavior. The determination of the rate constant for the production of monochlorobenzene and dichlorobenzene at different temperatures and pressures along with the effect of agitation and mixing, can also be obtained. A very interesting and challenging investigation would be to find the effect of catalyst - Fe, $FeCl_3$, $SbCl_3$, $SbCl_5$, $AlCl_3$, or $SnCl_4$ - at different concentrations and temperatures on the product distribution. The methods that can be used to improve one of the dichlorobenzene isomer yields, can be investigated and discussed. In reactor control, the student can determine the effect of the reactor operating conditions - temperature and pressure - on the product distribution; the dynamic characteristics of the different operating valves and the temperature stability can be examined too.

The distillation column is designed to separate the quantities and materials available from the reactor which consist of benzene and chlorinated benzene compounds in a binary or multi-components system, depending on the operating conditions of the reactor. The determination of the effect of feed location and feed quality on the operation of the column, along with

the effect of changing the reflux ratio are classical experimental investigations in distillation. The individual tray and overall efficiencies can be determined easily. A typical process control experiment is the control of the overhead composition by changing the reflux ratio. Also the control of the bottom product or both products may be investigated too.

Many investigations concerning the interaction between the reactor and the distillation column may be planned; for example one may study the manual control of the whole process at steady state, the effect of changing the value of some variable on the stability of the process or for a specific purpose such as minimizing the use of fresh benzene feed and maximizing the monochlorobenzne yield.

The measuring instruments were chosen to give complete information about the most important variables needed in monitoring and controlling each stream in the process during experimental investigations. The temperature and pressure of the reactor with complete information - temperature, flow rate, pressure, and concentration - about the feed streams to the reactor has to be known to predict the kinetics of the reaction and the concentration of the liquid product. Information concerning the gaseous products is not so important except for safety purposes. Check valves will be used to restrict the flow of chlorine and hydrogen chloride to the absorber only. The concentration of the liquid products must be measured along with the temperature and pressure of the ditillation feed. In the distillation column, the temperature of each each tray will be an indirect measurement of the compositions. The flow rate of the distillate, and bottom product, and the reflux ratio are the variables that will be used to control the operation of the column. Electric signals from thermocouples, will be converted to

temperature or concentration readings by a multi-point recorder. The pressures in the process will be measured by gauges and pumps will be used to circulate the various streams at the desired pressures. Rotameters are proposed for measuring the flow because of their simplicity, direct readability, and the moderate pressure used in the system. Generally in the commercial chlorination of benzene process, the concentration is determined by measuring the density or the refractive index of the reactor product; in the proposed experiment, the concentration will be measured by a differential and continuous refractometer which will contain a standard solution in one of the two cells, and its continuous electric signals will be converted to concentration measurements which will be used to control the reactor or the ditillation column. Also samples from the various sampling ports will be analyzed by a gas chromatograph (using 'SE 30' as the stationary phase) for accurate concentration measurements, including that of the isomers. The flow will be regulated by needle valves. Solenoid valves, receiving signals from automatic liquid level controllers, will be used to control the flow of streams 10, 4, and 15 from the flash tank, reflux storage tank, and reboiler respectively. The reflux ratio controller will consist of a round chart temperature controller with proportional and integral control, manual-automatic transfer switch with built-in air pressure regulator, and set point operator. In operation, the controller will operate the reflux splitter on a 12-second repeating cycle, energizing the splitter coil for some portion of each 12-second cycle. When the coil is energized, product will be taken off; when de-energized, reflux will flow back to the column. Figure 15 shows the various valves and measuring instruments which will be used to control each stream manually.

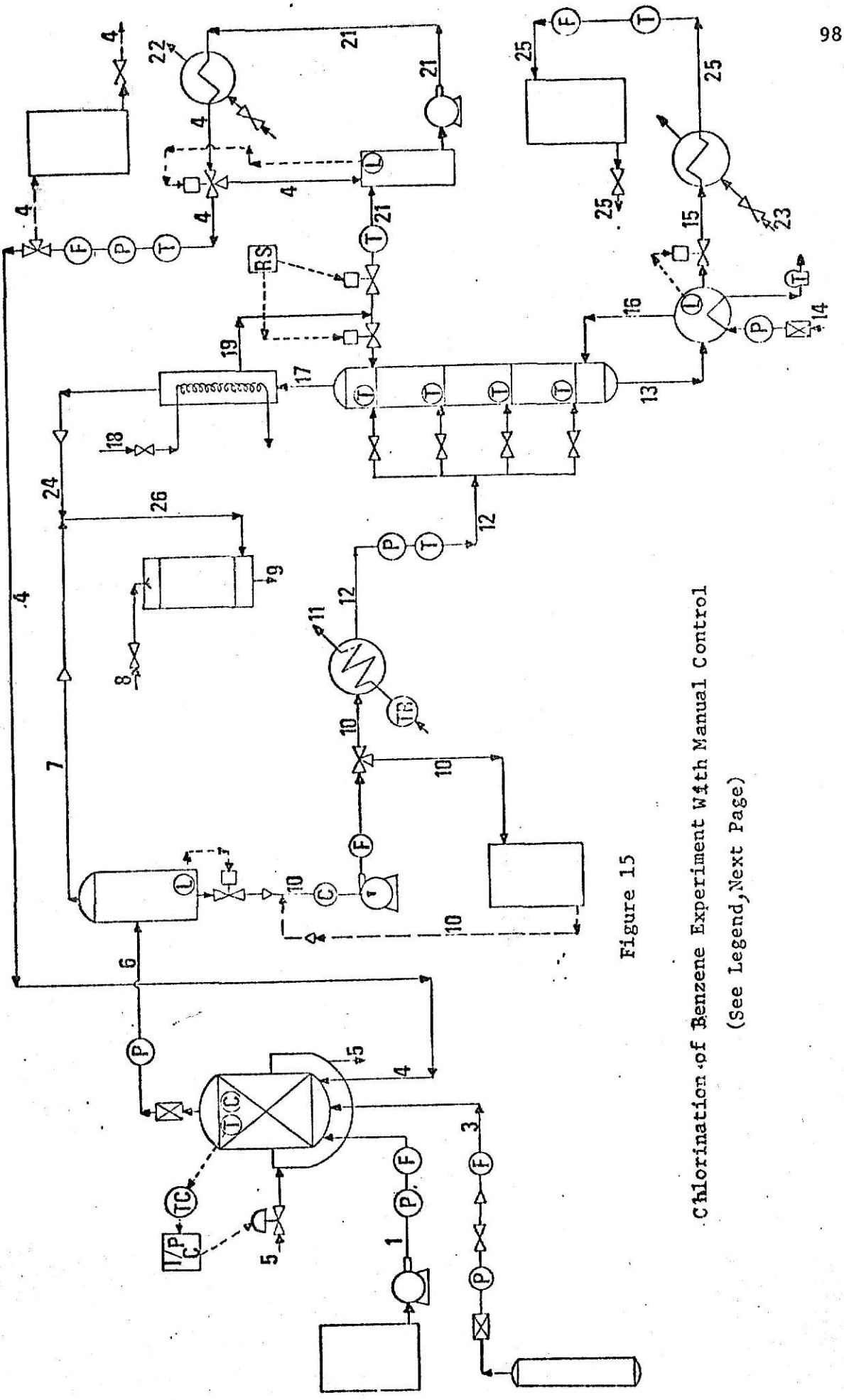


Figure 15

Chlorination of Benzene Experiment With Manual Control

(See Legend, Next Page)

LEGEND FOR FIGURE 15

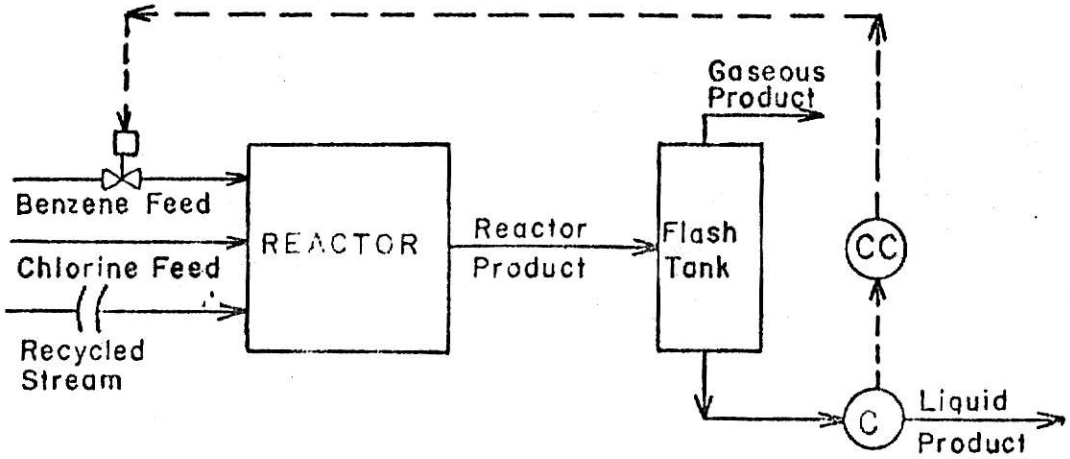
Ⓕ	Flow Measurement
Ⓛ	Liquid Level Measurement
Ⓒ	Concentration Measurement
Ⓟ	Pressure Measurement
Ⓣ	Temperature Measurement
TC	Temperature Controller
TR	Temperature Regulator
RS	Reflux Splitter
I/P	Pneumatic Converter
	Steam Trap
	Pressure Regulator
	Valve
	Check Valve
	3-Way Valve
	Solenoid Valve
	3-Way Solenoid Valve
	Pneumatic Valve

B) Automatic Control

Numerous automatic control investigations can be done with this process, for example the effect of changing the flow rate of fresh benzene on the composition of the reactor product, distillate, and bottom product and also how the changes in reflux ratio can affect the composition of the distillation feed and bottom product, etc. Only three cases concerning the reactor and the distillation column were investigated. The first one demonstrates how to use a feedback control system to maintain the composition of the liquid reactor product constant; the second one shows how a constant distillate composition can be obtained by varying the automatic reflux ratio controller; and finally the last one represents how the changes in the operating conditions of the reactor can be detected by the distillation column. Those three cases cover some control aspects for the reactor, the distillation column, and the interaction between them. The following are the descriptions of the three suggested cases:

1) Feedback control for reactor

The objective of using the feedback control system would be to maintain the composition of the reactor product constant. Generally its composition may change depending on the composition of the recycled stream and its flow rate, on the flow rate of fresh benzene, and on the residence time in the reactor. The concentration should be measured after the liquid-gas products are separated in the flash tank because the refractometer can only analyze liquids and at atmospheric pressure. Figure 16 shows a simplified diagram for the reactor with the feed back control.



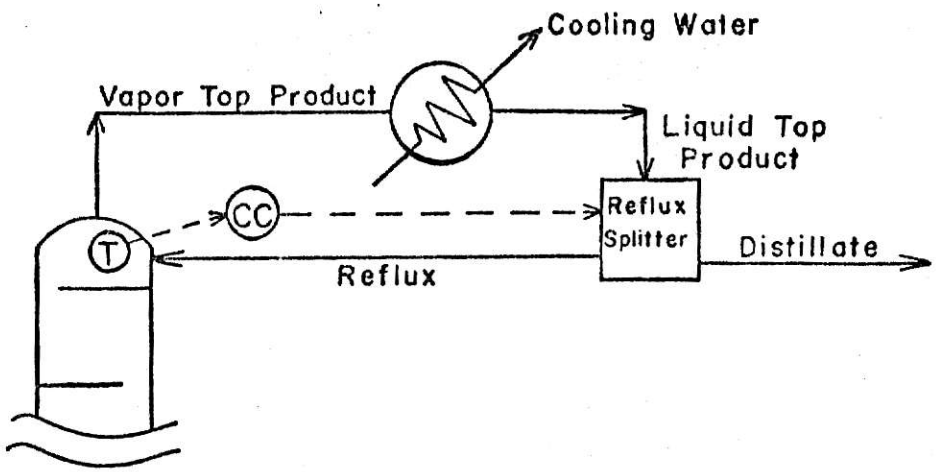
Where (CC) Concentration Controller (3 mode)

(C) Concentration Measurement (Continuous Refractometer)

Figure 16. Feedback Control for Reactor

2) Constant top product composition

The reflux ratio may be adjusted to obtain a constant top product composition. The reflux ratio controller can be operated manually or automatically and the concentration is measured by a thermocouple at the top plate. The reflux ratio controller will energize or de-energize the reflux splitter depending on the corrective action. Figure 17 represents the control of top product composition.



Where (CC) Concentration Controller (Automatic Reflux Ratio Splitter)

(T) Temperature Measurement

Figure 17. Reflux Ratio Control

3) The interaction between the reactor and the distillation column

In this case, the distillate composition will be maintained constant by adjusting the reflux ratio only, but the set point of the reflux ratio controller will be controlled by changes in the composition of the distillation feed which is a function of the operating conditions of the reactor. Figure 18 and 19 show the procedure used to control the distillate composition. The benzene composition will increase when the concentration of the feed stream increases, therefore the temperature will decrease and the reflux ratio set point has to be reduced in order to keep the top product composition constant. Also one can investigate the effect of changing the temperature or pressure of the reactor on the distillate composition by a similar procedure.

The additional equipment needed for automatic control are: air operated needle valves, electric to pneumatic transducers, valve operators, and automatic controllers (3 mode).

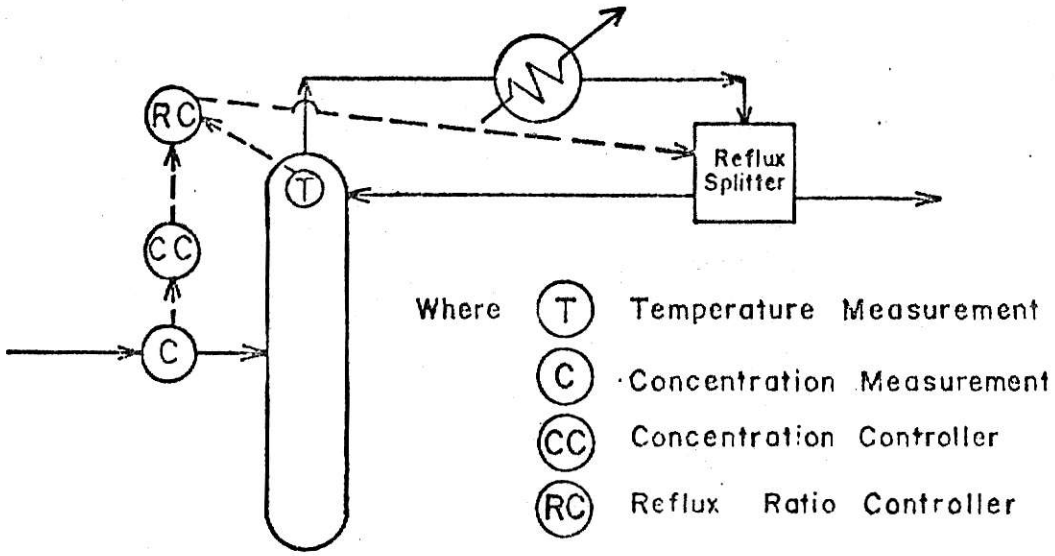
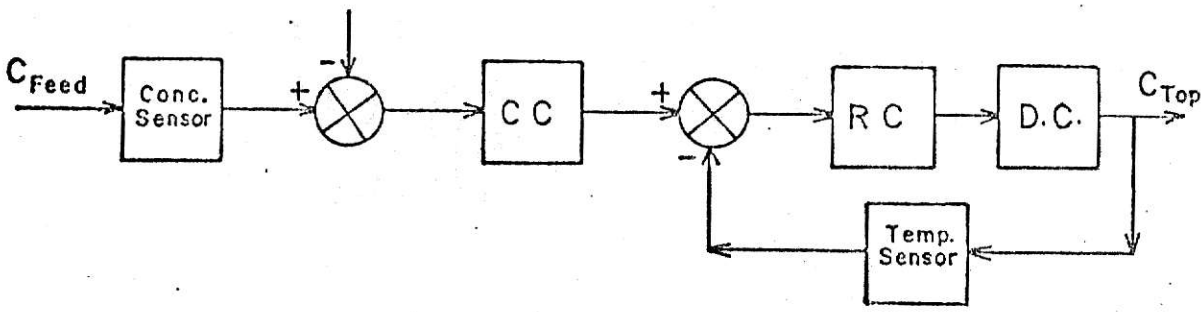


Figure 18. Feedback–Feedforward Combination



Where C_{Feed} Represents the Concentration of Feed Distillate

C_{Top} Represents the Concentration of Top Product

D.C. Represents the Distillation Column

Figure 19. Block Diagram for the Feedback-Feedforward Combination

C) Computer Control.

The PDP 11/10 digital computer, which accepts ± 5 DC volt electric signals, may be used for computer data logging and control. For this reason, amplifiers for the signals from thermocouples, turbine meters, and pressure transducers, have to be installed in order to provide apropriate signals for the computer. The effect of the different variables on the operation of the process can be investigated, with computer control of the whole process. The computer program for the simulation and control of the different streams is beyond the objective of this research, however, the cost of the basic signal conditioners and transducers has been included.

D) Optimization Aspects

The optimization of the design of the proposed process was not considered because the objectives were mostly educational as opposed to commercial production. The three different types of control (manual, automatic, and computer) will be used for teaching purposes as cited earlier.

The optimization of the operating cost will be unrealistic because it will be difficult to calculate the utilities (water, steam, and electricity) cost due to the small amount of raw materials used in the process; and if the utilities cost are assumed, the optimization would be no different than a 'paper-and-pencil' problem. As a result, overall economic optimization experiments will be difficult to plan or investigate with this proposed process.

A reasonable amount of reaction with 10 to 20% benzene conversion, a residence time of one to two minutes, and the use of a small amount of raw materials were the only considerations examined in designing the reactor. No particular concern was given to the yield of any of the other chlorinated compounds (other than monochlorobenzene), but one can optimize the production of a particular component with the present equipment and operating conditions. The following represents some design aspects and procedure used to maximize the production of monochlorobenzene and para-dichlorobenzene:

1) Maximization of Monochlorobenzene Yield

Since monochlorobenzene is the essential intermediate in the production of phenol, aniline, and D.D.T., R. B. MacMullin [18] studied the distribution of the reaction products in benzene chlorination. The fundamental equations are:

$$C_6H_6 + Cl_2 \xrightarrow{K_1} C_6H_5Cl + HCl$$

$$C_6H_5Cl_2 + Cl_2 \xrightarrow{K_2} C_6H_4Cl_2 + HCl$$

$$C_6H_4Cl_2 + Cl_2 \xrightarrow{K_3} C_6H_3Cl_3 + HCl$$

If A is the mole fraction of C_6H_6,

B is the mole fraction of C_6H_5Cl,

C is the mole fraction of $C_6H_4Cl_2$,

D is the mole fraction of $C_6H_3Cl_3$,

x is the total atoms of Cl_2 per mole of benzene constituent,

$r = K_1/K_2$, and $s = K_2/K_3$

therefore $A + B + C + D = 1$ (equation 1)

and $B + 2C + 3D = x$ (equation 2)

The results that he obtained, for the maximization of monochlorobenzene yield, for batch and continuous single stage reactors, are presented in Table 4.

Table 4. Maximization of Monochlorobenzene Yield for Batch and Continuous Reactor

Batch Chlorination	Steady State Single Stage Chlorination
$B_{max.} = r^{-1/(r-1)}$	$B_{max.} = r/(r^{1/2} + 1)^2$
$x = 2 - (1 + 2/r)r^{-1/(r-1)}$	$x = 1 - 1/(r^{1/2} + 1)^2$

Therefore the batch chlorination produces higher yield of C_6H_5Cl as shown in Figure 21(next page). For all values of r between 4 and 32 the maximum occurs within the narrow range of x = 1.05 to 1.07 as shown in Figure 20.

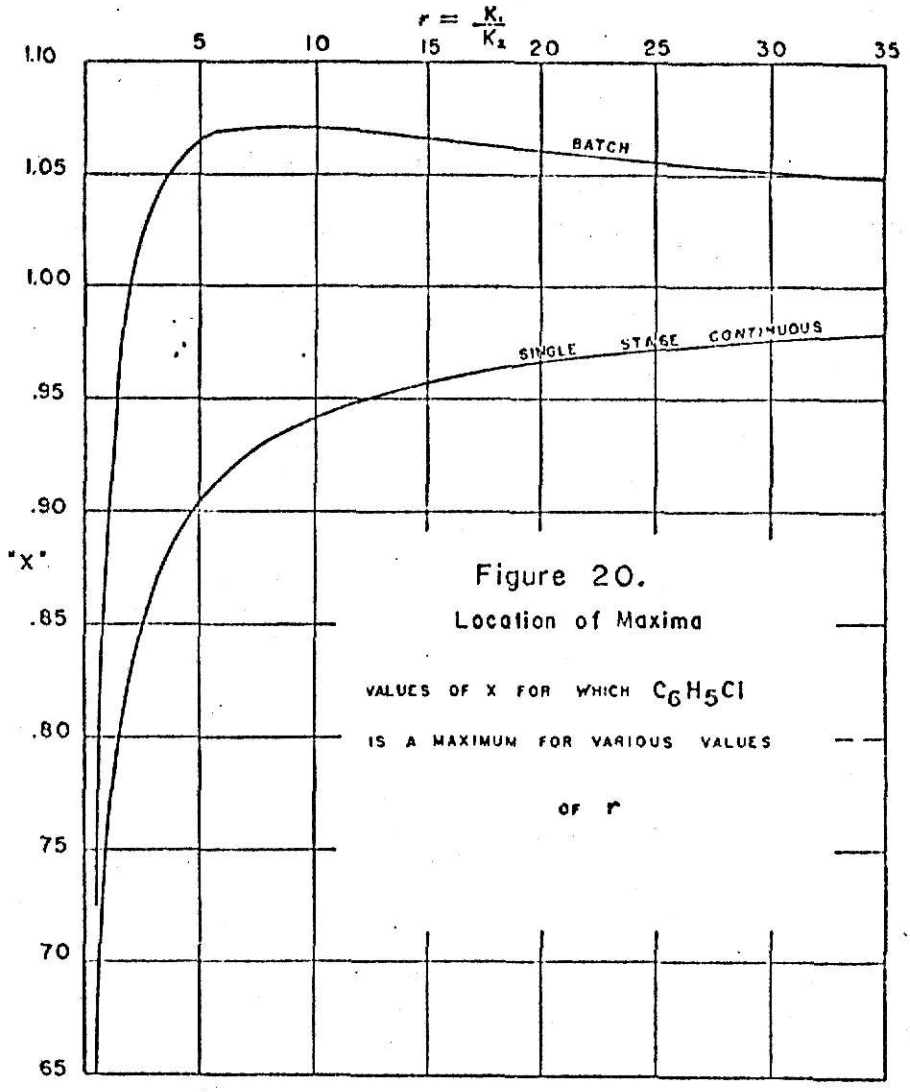


Figure 20.
Location of Maxima

After investigating a two-stage continuous chlorination, he concluded that the greater the number of stages, the closer the approach to batch distribution. The distribution of reaction products for the chlorination of benzene by substitution is given by Figure 22.

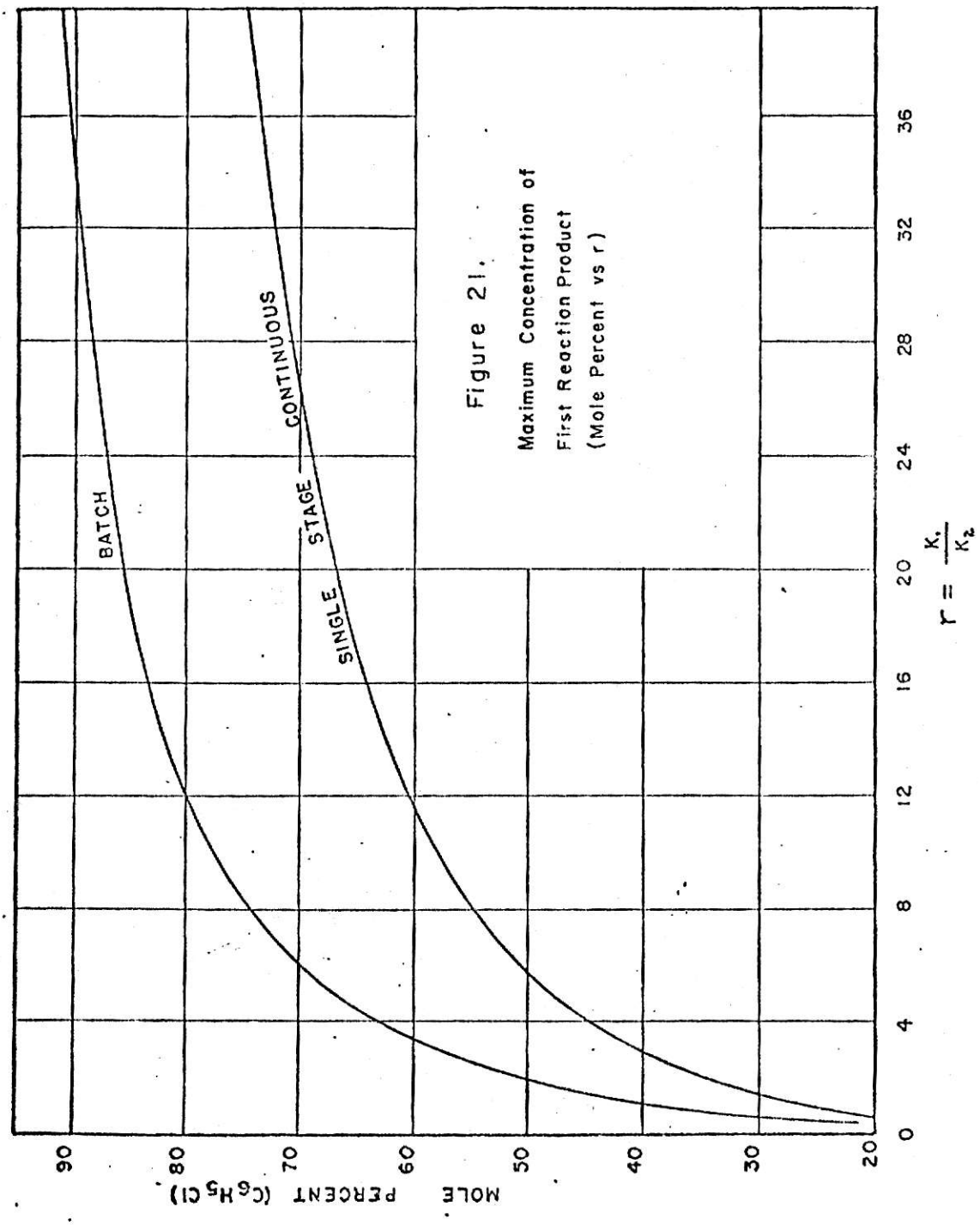


Figure 21.
Maximum Concentration of
First Reaction Product
(Mole Percent vs r)
BATCH
CONTINUOUS
STAGE
SINGLE
MOLE PERCENT (C_6H_5Cl)
90
80
70
60
50
40
30
20
0
4
8
12
16
20
24
28
32
36
$r = \frac{K_1}{K_2}$

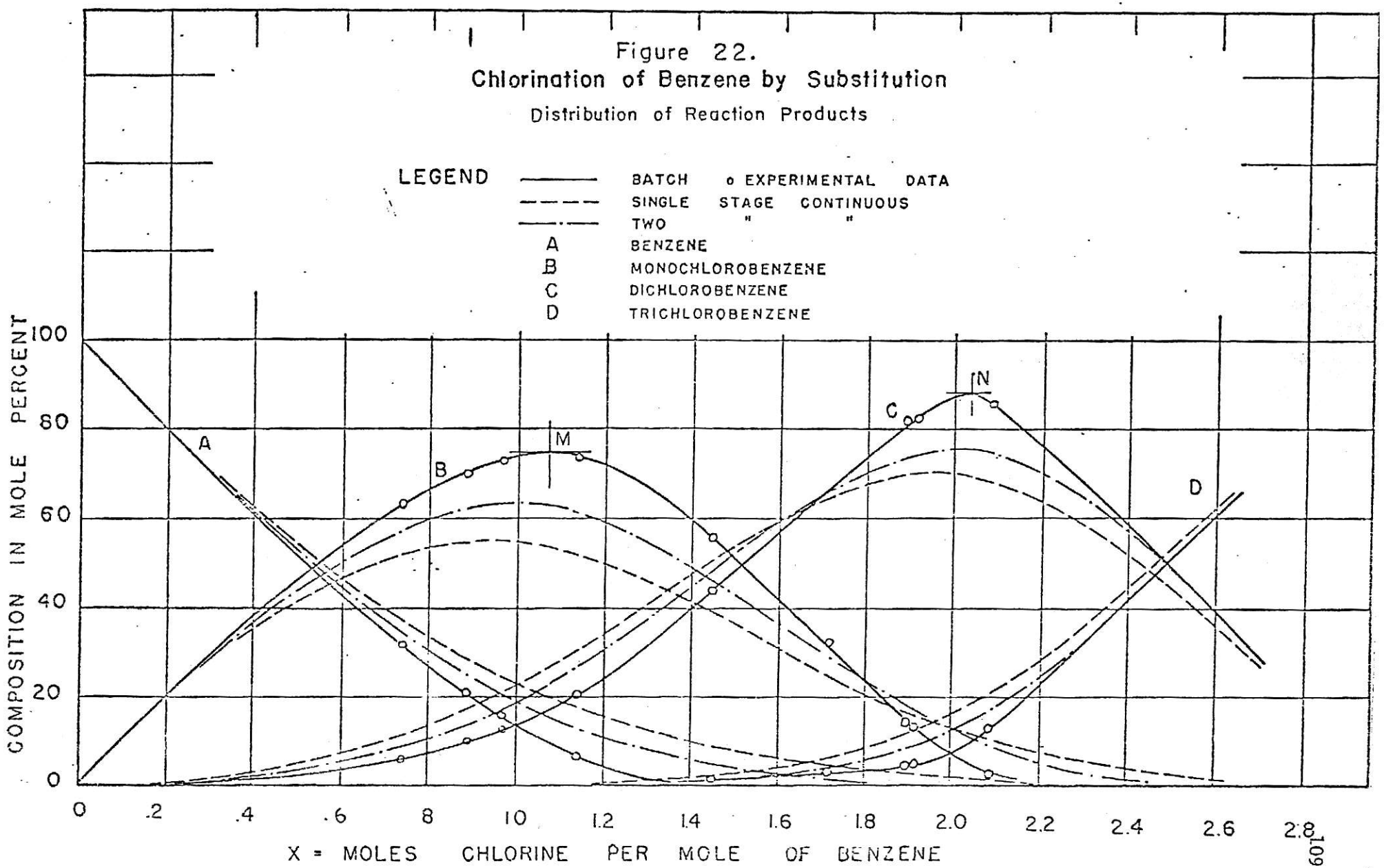


Figure 22.
Chlorination of Benzene by Substitution
Distribution of Reaction Products
LEGEND
BATCH o EXPERIMENTAL DATA
SINGLE STAGE CONTINUOUS
TWO " "
A BENZENE
B MONOCHLOROBENZENE
C DICHLOROBENZENE
D TRICHLOROBENZENE
COMPOSITION IN MOLE PERCENT
100
80
60
40
20
0
M
N
A
B
C
D
0 .2 .4 .6 8 10 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8
X = MOLES CHLORINE PER MOLE OF BENZENE

2) Practical methods used to increase para-dichlorobenzene yield

At present, the para-dichlorobenzene is becoming a valuable byproduct; it is used as solvent, insecticide, and pesticide. Weigandt and Lantos [31] discussed the different practical methods that can be used to improve the p - $C_6H_4Cl_2$ yield. They found that $SbCl_5$ seems to be the best among the catalysts and it is followed by iron (as shown in Figure 23) and the lower the concentration of catalyst, the better the yields percentage of p - $C_6H_4Cl_2$ Figure 24 indicates that the para yield increases at low temperatures (30°C). Higher yields of para are obtained when polar solvents like anhydrous acetic acid (.25% mole), trichloroacetic acid, or ethyl sulfate are present even in small quantities as indicated by Figure 25; it is possible that such compounds influence the orientiation not because of their effect on the dielectric constant of the solution, but by actively entering into the catalyst complex. Adding fresh charges of catalyst during the chlorination has no effect on the yield as shown in Figure 26. From Figure 27, 28 and 29 it can be deduced that adding small amount of o - $C_6H_4Cl_2$ in the feed, increases the p - $C_6H_4Cl_2$ yield. Generally for a given chlorination, at constant temperature, the concentration of para in the dichloro fraction increases as chlorination progresses as indicated by Figure 30. Above chlorination level of two chlorine atoms per benzene molecule, the percentage of para increases even more rapidly, which is due to the fact that the o - $C_6H_4Cl_2$ more rapidly than the para and therefore disappears much faster.

Some optimization problems, concerning the chlorination process, are presented. These problems will help the students to understand the kinetics of the reaction and the process.

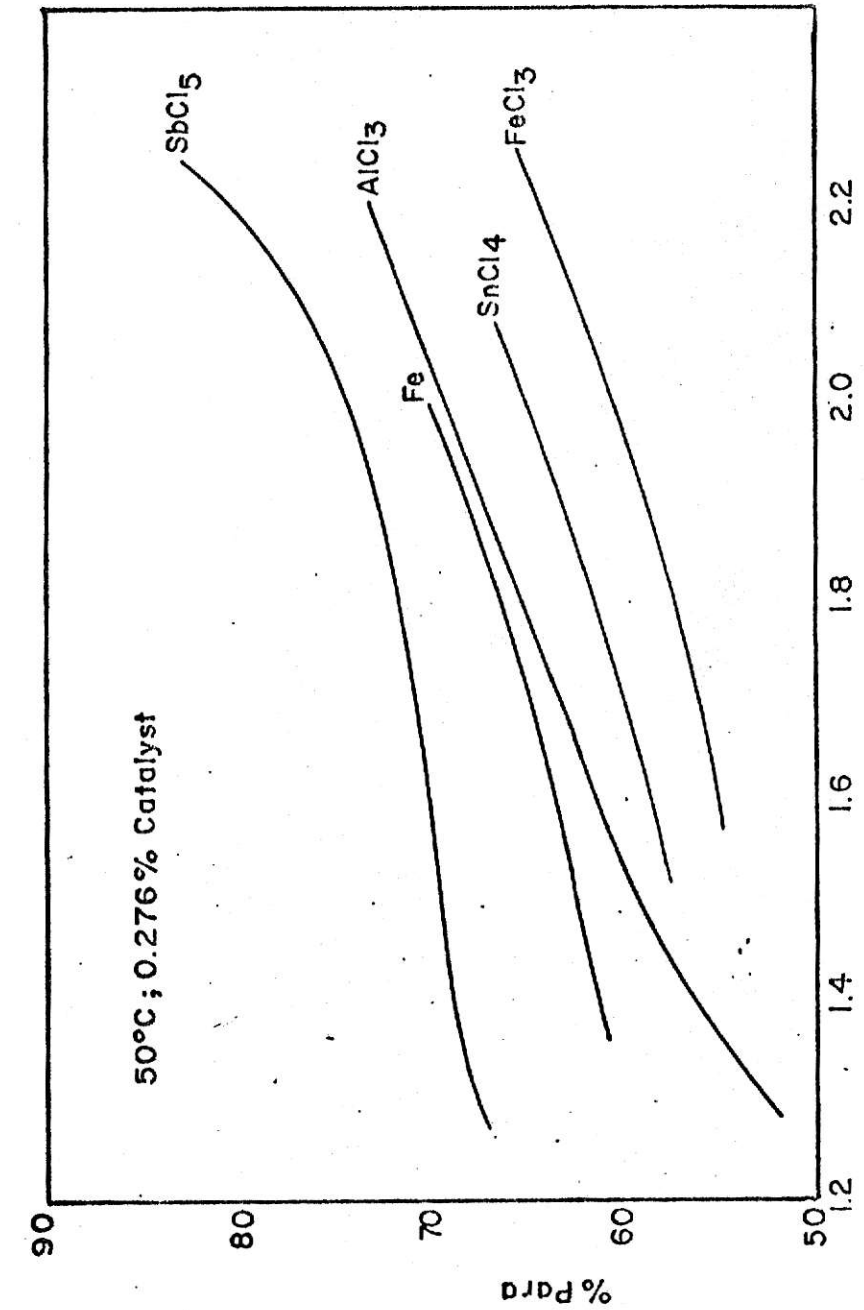


Figure 23. Dichloro Isomer Distribution During Batch Chlorination with Various Catalysts [31].

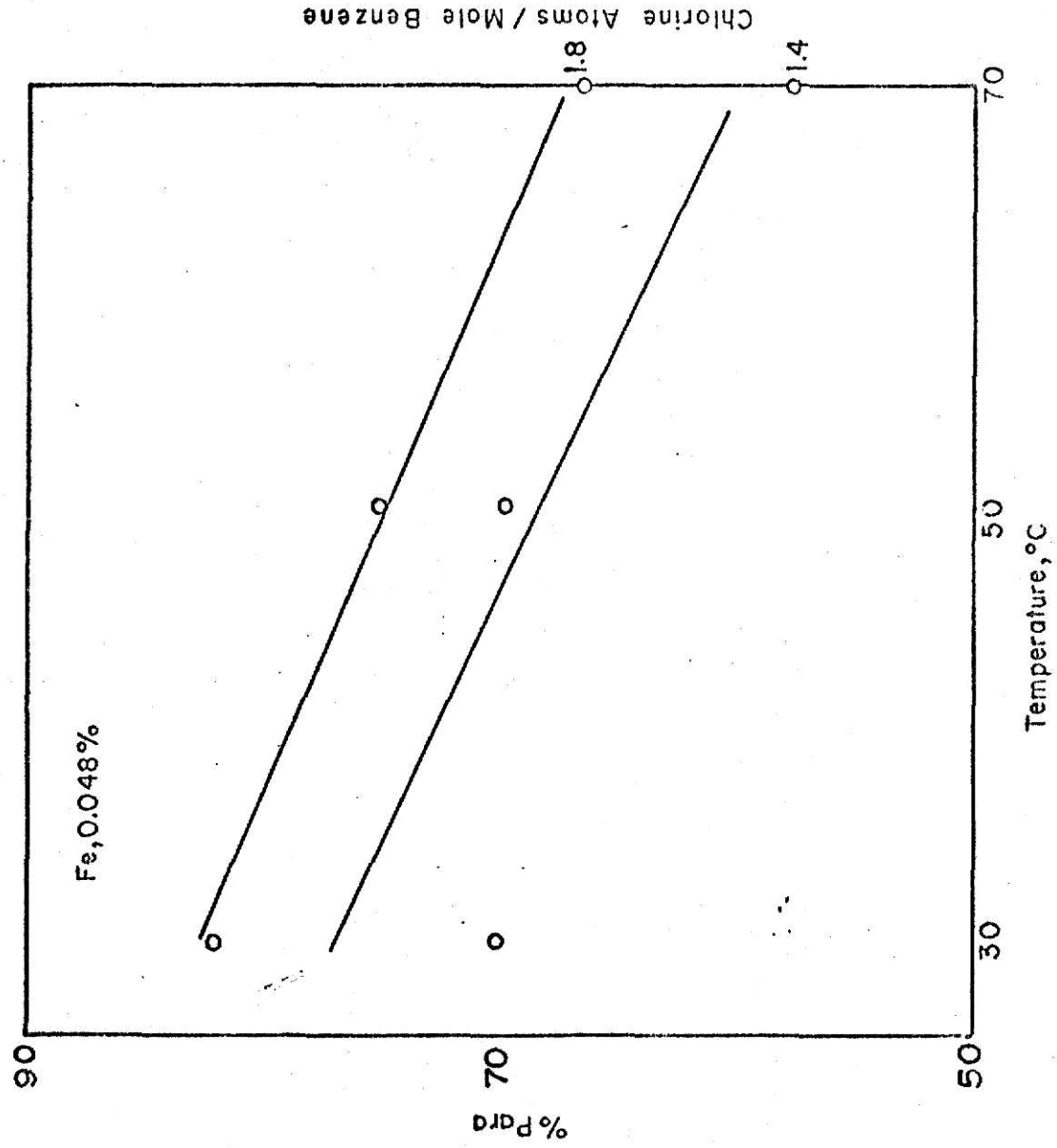


Figure 24. Variation of Dichloro Isomer Distribution with Temperature at Several Chlorination Levels [31].

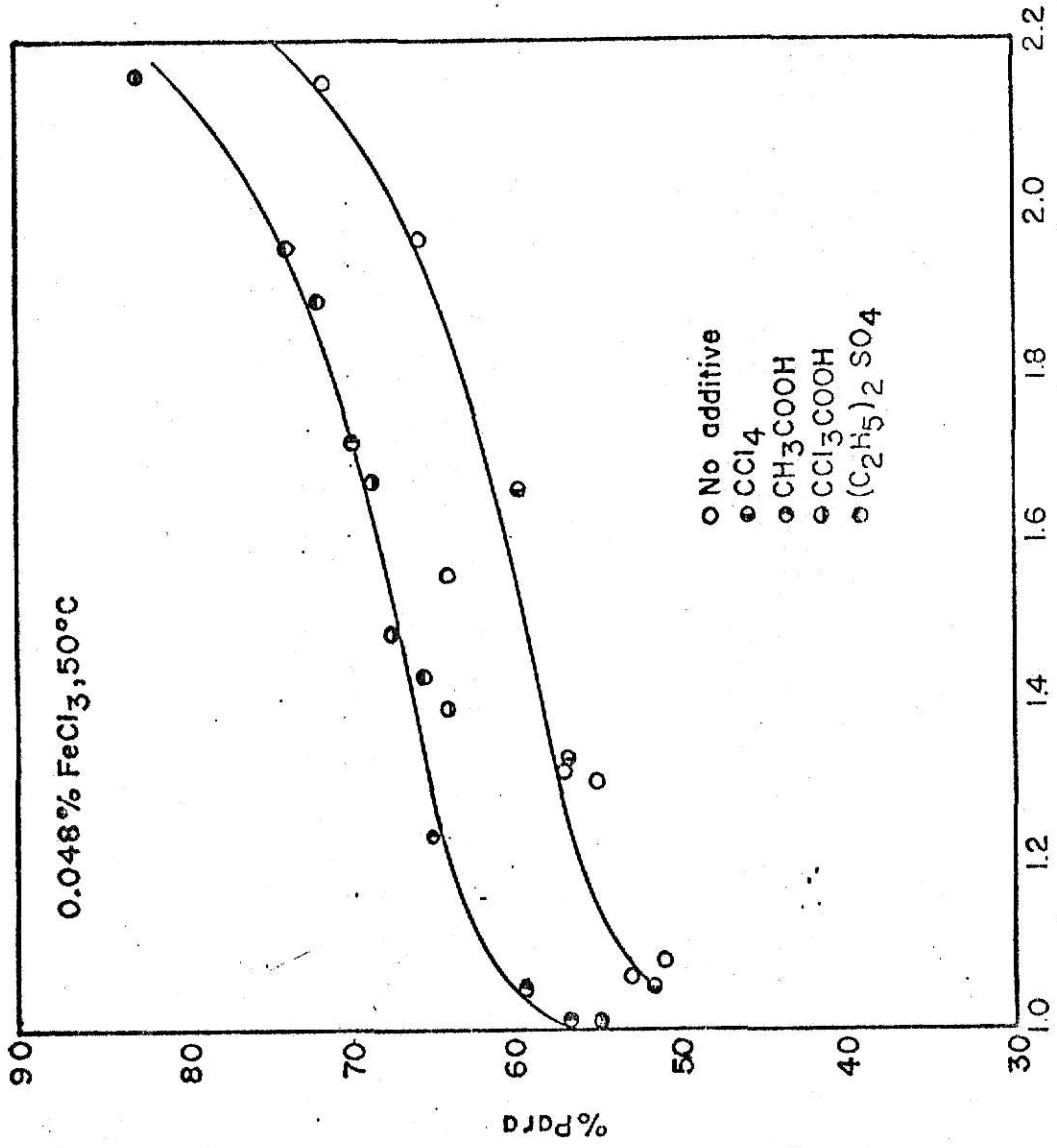


Figure 25. Effect of Polar and Nonpolar Compounds on Distribution of Dichloro Isomers at 50° C [31].

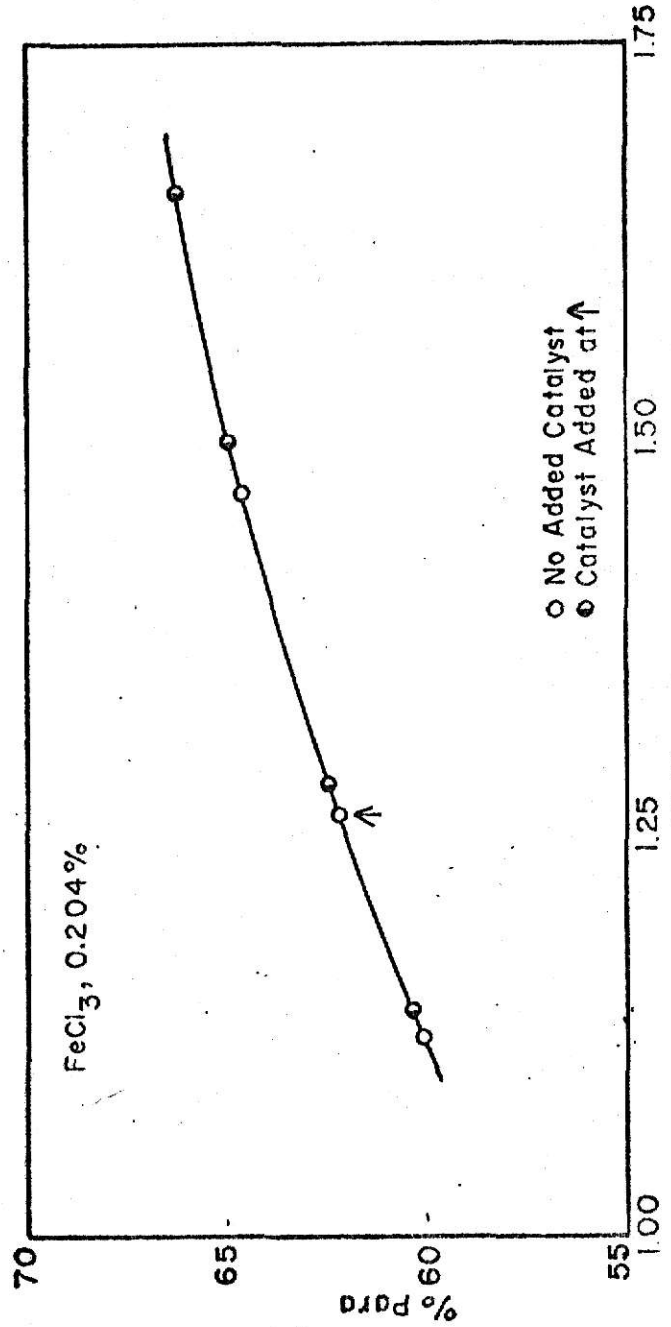


Figure 26. Effect of Adding Fresh Catalyst During Batch Chlorination on Distribution of Dichloro Isomers [31].

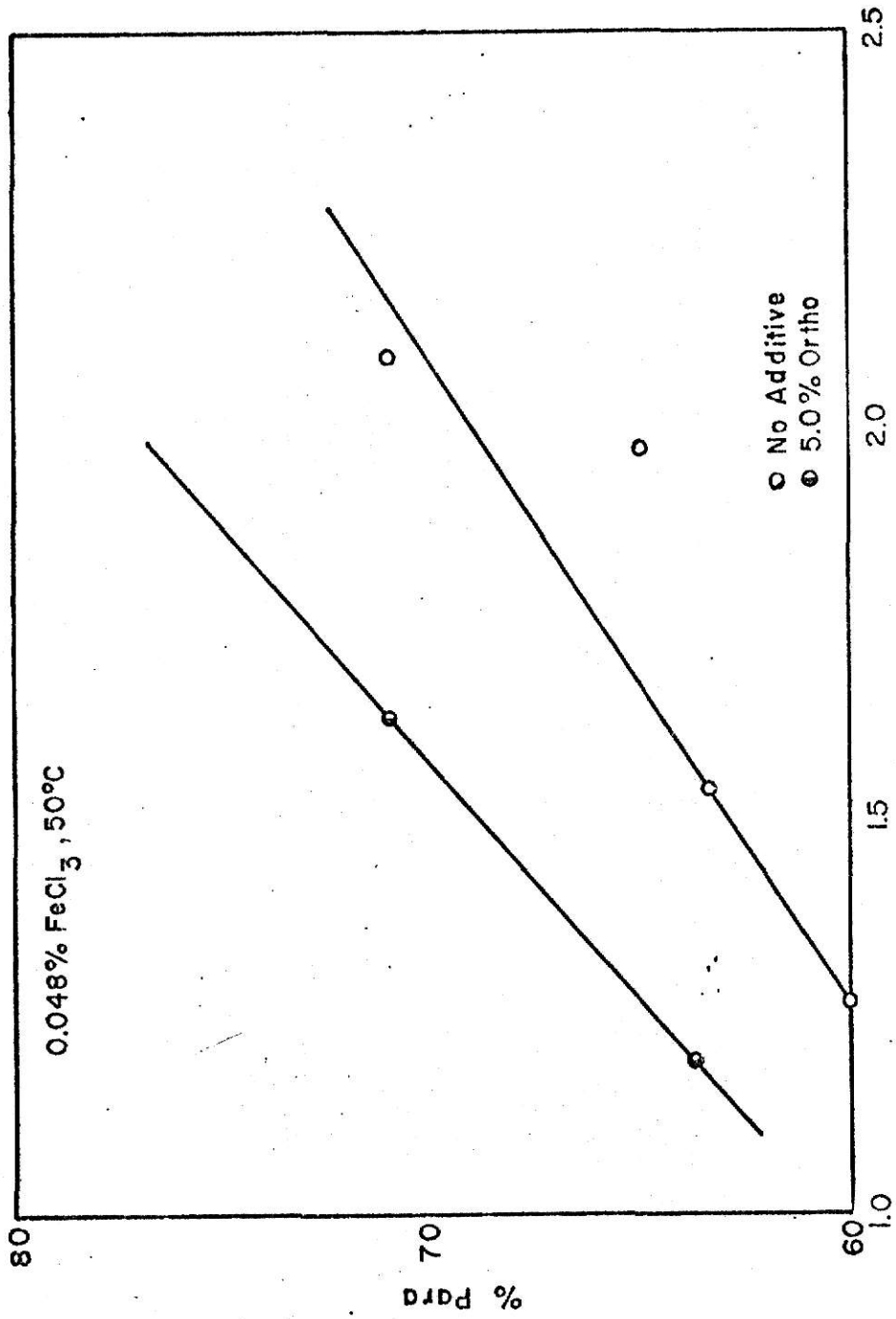


Figure 27. Effect of Incorporating o-Dichlorobenzene in Charge on Distribution of Dichloro Isomers [31].

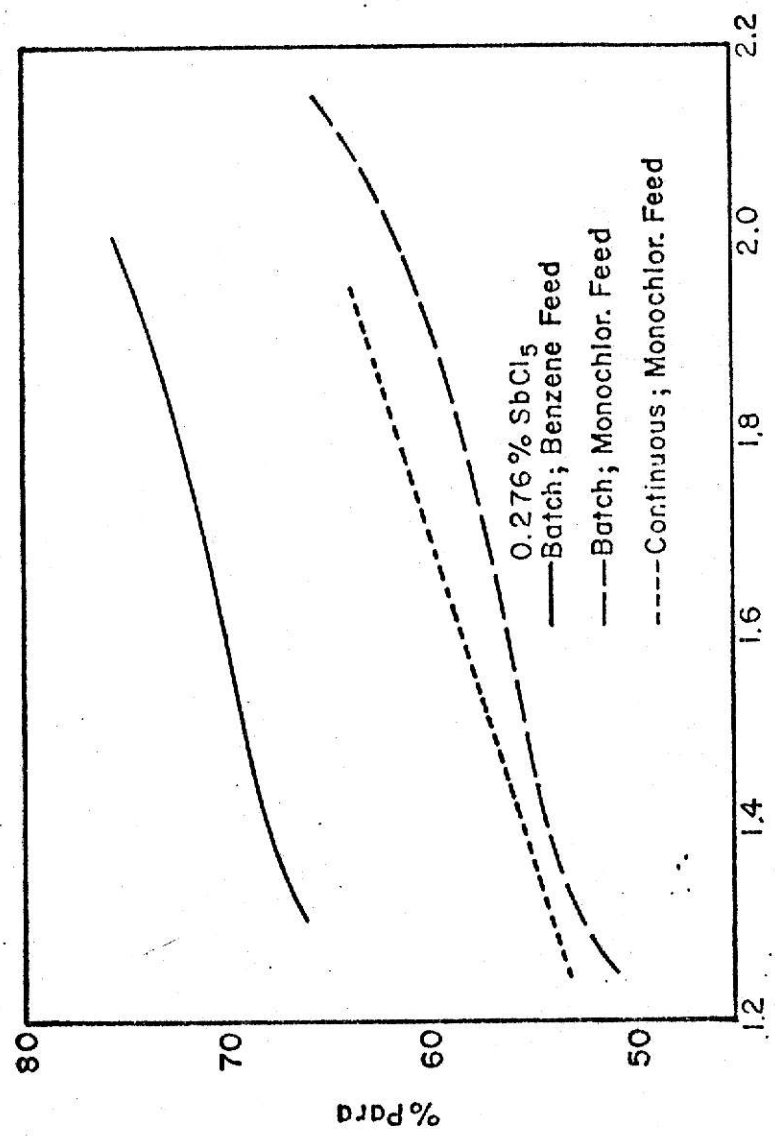


Figure 28. Effect of Feed Composition on Isomer Distribution at 50° C [31].

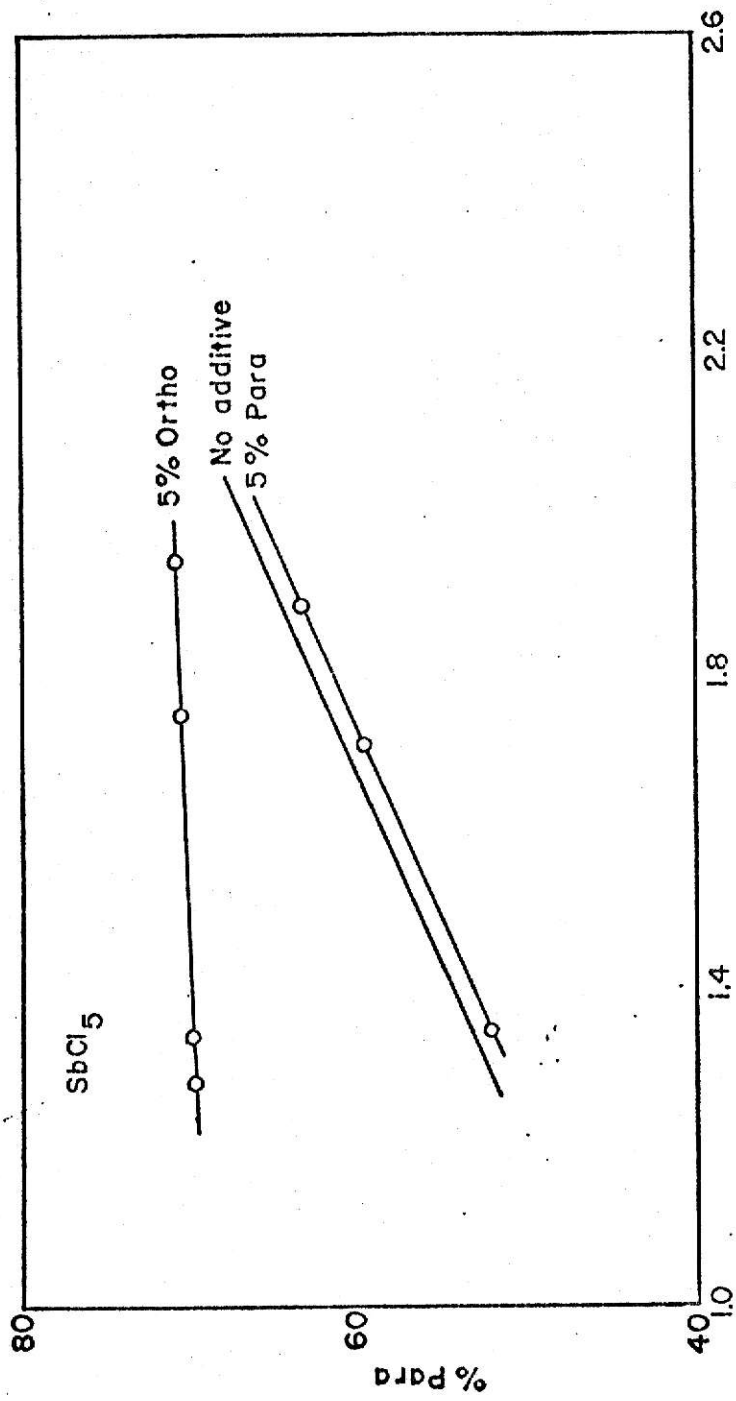


Figure 29. Effect of o- or p-Dichlorobenzene in Feed to Continuous Chlorinator on Isomer Distribution at 50° C. [31].

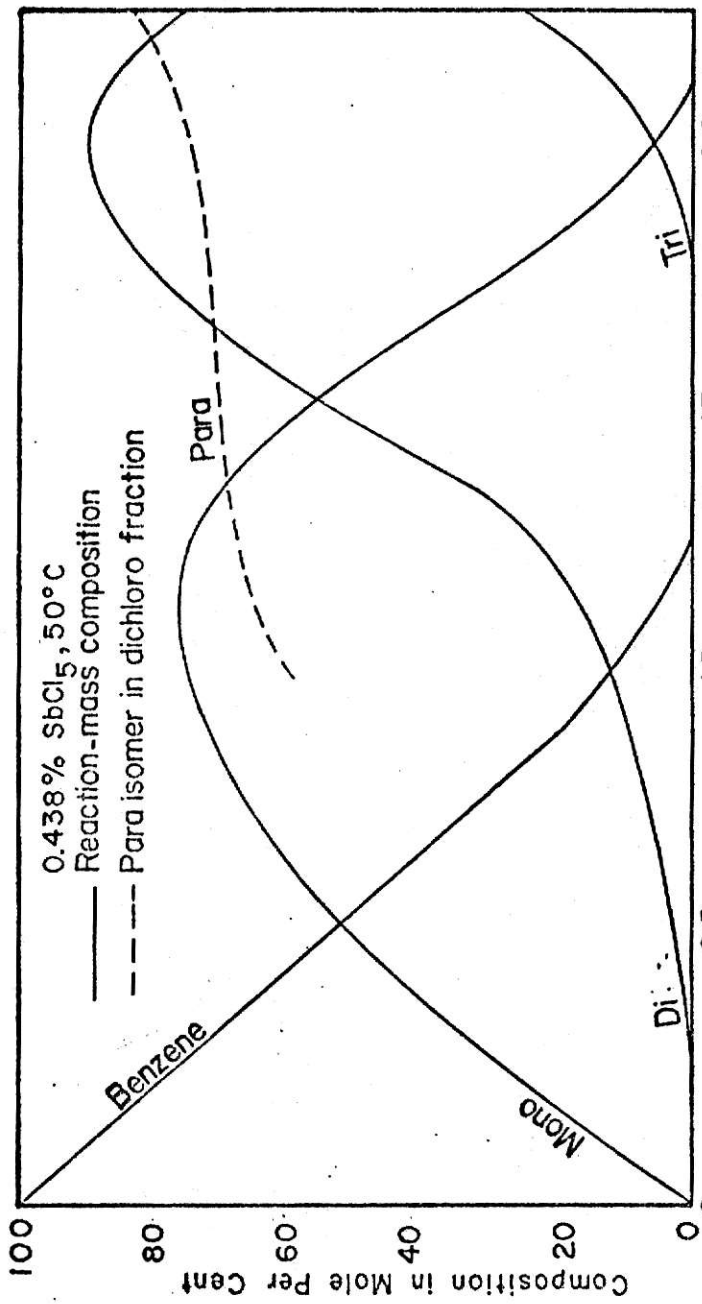


Figure 30. Product Distribution of a Typical Benzene Batch Chlorination at 50° C [31].

Problem 1: Batch and single stage continuous reactor.

For the Chlorination of benzene the following reactions occur:

$$C_6H_6 + Cl_2 \xrightarrow{K_1} C_6H_5Cl + HCl \qquad \Delta H_1 = -31 \text{ Kcal/mole}$$

$$C_6H_5Cl + Cl_2 \xrightarrow{K_2} C_6H_4Cl_2 + HCl \qquad \Delta H_2 = -25 \text{ Kcal/mole}$$

$$C_6H_4Cl + Cl_2 \xrightarrow{K_3} C_6H_3Cl_3 + HCl \qquad \Delta H_3 = -20 \text{ Kcal/mole}$$

and $R = K_1/K_2$, $S = K_2/K_3$

Calculate the mole fraction of the liquid components in the product stream, which are C_6H_6, C_6H_5Cl, $C_6H_4Cl_2$, and $C_6H_3Cl_3$, when a maximum yield of C_6H_5Cl is required for the following cases:

a) batch reactor

b) steady state continuous reactor

where R = 8.5 and S = 33

Problem 2:

For the Chlorination process, the prices of raw materials and products are:

C_6H_6 = \$5.7/gal (density = .873gm/cm^3)

C_6H_5Cl = \$14.15/1 (density = 1.1gm/cm^3)

o - $C_6H_4Cl_2$ = \$8.15/Kg p - $C_6H_4Cl_2$ = \$17.10/Kg

m - $C_6H_4Cl_2$ = \$6.65/25gm

1, 2, 4 $C_6H_3Cl_3$ = \$8.75/Kg

Cl_2 = 22¢/lb

From the mole fraction obtained in the first problem, calculate the profit for:

a) batch reactor containing 100gm mole benzene initially

b) continuous reactor with a molar benzene flow rate of 100gm mole/min (basis 1 min) if the $C_6H_4Cl_2$ is composed of 59% ortho, 40% para and 1% meta and the $C_6H_3Cl_3$ is considered pure 1, 2, 4 $C_6H_3Cl_5$.

Disucss how to increase the yield of p - $C_6H_4Cl_2$ and its industrial use.

Note: The prices were taken from "Fisher 77" catalog.

Problem 3:

The following table shows the relation between the ratio of the rate constants and the temperature for the reactions described in problem one.

t°C	$R = K_1/K_2$	$S = K_2/K_3$
18	9.3	34.8
25	8.4	32.5
35	8.1	31
45	7.8	30.5

Calculate the temperature which maximizes the dichlorobenzene yield in a batch reactor.

Many problems concerning heat transfer area, cooling water, and operating cost for the reactor and the distillation column can also be easily formulated.

E) Safety Considerations

Most processes of commercial value have some safety hazards - high temperature or pressure, toxic or flammable material, or mechanical dangers. Generally in the educational environment, attempts are made to eliminate, as far as possible, all safety problems. To some extent this was the case in the present design, too. However, for a moderately complex process such as the one proposed, some hazards are inevitable and, perhaps, even a benefit. Part of the educational value can be the dealing with the safety aspects - if they are not too severe. It is felt that this process will provide experience with moderate temperatures and pressures, as well as handling materials which are somewhat toxic. The toxic materials involved can be physically sensed long before they become dangerous and, as a result, they are not considered extremely dangerous. The following table shows the potential hazards for the different chemical compounds used in proposed chlorination of benzene process.

Table 5. Hazard Chart for the Proposed Process [19 and 20]

Compound	(1)* TLV (ppm)	(2)* NFPA 704M System			Flash point °C	Ignition temper. °C	Flam. Limits %	(3)* Extingui. Agents
		Health	Fire	React.				
C_6H_6	C 25 S	2	3	0	-17	562	1.4 - 8	2,3
Cl_2	C 1	3	0	1				
C_6H_5Cl	75	2	3	0	29	638	1.3 - 7.1	
o-$C_6H_4Cl_2$	C 50	2	2	0	66	648	2.2 - 9.2	1, 2, 3
p-$C_6H_4Cl_2$	75	2	2	0	66			1, 2, 3
$FeCl_3$ 60%		1						
C_6Cl_6		1	1		242			1, 3
HCl	C 5	3	0	0				
1,2,4,5-$C_6H_2Cl_4$			1	0	155			1, 3
1,2,4-$C_6H_3Cl_3$		2	1	0	99			1, 2, 3

*See next page for explanation of codes.

Note (1) Threshold Limit Value (TLV) refers to air-borne concentrations of substances and represent conditions under which it is believe that nearly all workers may be exposed, day after day, without adverse effect. Prefix C denotes ceiling limit which means that the concentration must not exceed the ceiling limit and suffix S denotes skin, which means that appropriate measures must be taken for prevention of cutaneous absorption.

Note (2) The hazard signals listed were established by the National Fire Protection Association as set forth in their publication, "Identification System for Fire Hazards of Materials" 704-M, 1966 which identifies hazards as follows:

Health

4 - can cause death or major injury despite medical treatment

3 - can cause serious injury despite medical treatment

2 - can cause injury, require prompt treatment

1 - can cause irritation if not treated

0 - no hazards

Fire

4 - very flammable gases or very volatile flammable liquids

3 - can be ignited at all normal temperatures

2 - ignites if moderately heated

1 - ignites after considerable preheating

Reactivity

4 - readily detonates or explodes

3 - can detonate or explode but requires strong initiating force or heating under confinement

2 - normally unstable but will not detonate

1 - normally stable, unstable at high temperature and pressure. Reacts with water

0 - normally stable. Not reactive with water.

Note (3)

Extinguishing agents:

1 - water

2 - foam

3 - carbon dioxide or dry chemical

4 - agents for gas fire

5 - approved dry compound for metal fires

Table 6 gives some safety information which must be followed in case of handling and spilling of the chemical compounds in question.

Table 6 DISPOSAL PROCEDURE [19]

Compound	Spills	Disposal of Bulk Quantities
C_6H_6	eliminate all sources of ignition and flammables A liquid: absorb on paper. Evaporate on an iron pan in a hood. Burn the paper.	1) A gas: Pipe the gas into the incinerator. Or lower into a pit and allow it to burn away. 2) A liquid: Atomize into an incinerator. Combustion may be improved by mixing with a more flammable solvent
Cl_2	Gas leak: If the gas valve is leaking because it cannot be closed, the gas can be bubbled through a reducer (sodium sulfite) and excess sodium bicarbonate solution. Be sure to include a trap in the line to prevent the solution being sucked back into the cylinder. If this cannot be done, the cylinder should be placed in or adjacent to a fume hood and left to bleed off. If the leak is in the valve assembly, a plastic bag can be fastened over the head of the cylinder which can then be taken outside or to a fume hood	Add to a large volume of concentrated solution of reducer (hypo, a bisulfite or a ferrous salt and acidify with 3M-H_2SO_4). When reduction is complete add soda ash or dilute hydrochloric acid to neutralize the solution. Wash into drain with large excess of water.
$C_6H_5Cl_2$ 1,2,4,5 $C_6H_2Cl_4$ 1,2,4 $C_6H_3Cl_3$	Eliminate all sources of ignition. Absorb on paper tower or with vermiculite. Place on an iron, glass or plastic disk in a hood. Allow to evaporate. Burn the paper or vermiculite. Wash site with soap solution.	Dissolve in a flammable solvent. Spray into the fire box of an incinerator equipped with afterburner and scrubber (alkali)
$C_6H_4Cl_2$	1) On skin: wash with strong soap solution immediately. Rinse well. 2) Small spills on tables or floor: absorb liquid spills on paper towels or vermiculite; sweep solid spills onto paper. Put on an iron pan in the fume hood and allow to evaporate. Burn the paper or vermiculite in the absence of other flammables. Wash the site thoroughly with strong soap solution. 3) Large spills: Absorb or mix with vermiculite, sodium bicarbonate or sand. Package this in a paper carton and burn it in an open pit. Use fuel such as crumpled paper and wood splinters. Wash site thoroughly with strong soap solution.	The waste may be mixed with a flammable solvent (alcohol, benzene, etc.) and sprayed into the fire chamber of an incinerator with afterburners and scrubber
HCl	Cover the contaminated surface with sodium bicarbonate or a soda ash-slaked lime mixture (50-50). Mix and add water if necessary to form a slurry. Scoop up slurry and wash down the drain with excess water. Wash site with soda solution.	Add slowly to a large volume of agitated solution of soda ash and slaked lime. Add neutralized solution to excess running water. As an added precaution, the sink can be lined with protective mating and filled with coarse chipped marble.

Since benzene, monochlorobenzene, and dichlorobenzene are flammable liquids which can be ignited at normal temperature, all heat sources should be separated from the various storage tanks. The distillation column or reboiler could also cause a fire hazard if any leakage occurs. Fires can be handled with a CO_2 or dry chemical fire extinguisher which should be located in close proximity to the equipment.

Chlorine and hydrogen chloride are more toxic than benzene or the chlorinated benzene compounds; they can cause serious health hazard due to their lower threshold limit value. As a result, any leakage must be detected as soon as possible. Generally, ammonium hydroxide can be used as a detecting compound because of its fast reaction with chlorine, hydrogen chloride, and hydrochloric acid to produce white fumes of ammonium chloride. Both chlorine and hydrogen chloride are extremely pugnant, which is an aid to safety in their handling.

Explosion hazards do not exist due to chemical reaction, but the chlorine cylinder could explode if it is not handled properly. Mechanical and electrical hazards exist due to the use of pumps, motors, and electric power for the various controllers, amplifiers, and heaters. The moderate pressure - 2 to 6 atmospheres in the reactor and feed streams will cause minor pressure hazards in operating the process, but they are not considered dangerous.

For safe operation, the experiment should be installed in a fume hood which has an explosion proof door. A CO_2 or dry chemical fire extinguisher must be available for immediate use in case of fires, and the pipelines have to be inspected to detect any leakage of chlorine or hydrogen chloride. In case of spills or leakage in one of the storage tanks, the

instructions for disposal procedure given in the last table must be followed carefully. Check valves were provided in the manual control operation to eliminate any backflow of chlorine or hydrogen chloride. The chlorine cylinder should be secured to a wall or other firm support, or chained in place, or placed in a cylinder stand (bench-clamp-type or floor-stand-type cylinder support) to prevent it from falling over and breaking the regulator.

V. EQUIPMENT SPECIFICATIONS AND COST ESTIMATION

A) Equipment Specifications

In this section, the equipment and accessories that will be installed, based on the chlorination of benzene flowsheet (Figure 8) and the control of the process, are described in detail (Table 7 and 8). All fittings, connections, measuring instruments, and valves are included. The specifications and cost of each item was taken from representative manufacturer's catalogs. Detailed drawings for the reactor, absorber, ditillation column, and distillation unit are shown in Figures 31, 32, 33, and 34 respectively. Sometimes more than one type of valve, controller, equipment, or accessory is installed on the same stream. This is due to the fact that some streams will be controlled manually, or automatically, or by computer, depending on the educational objectives.

Table 7 Summary of Flowsheet Operating Conditions

STREAM # OR MAJOR EQUIPMENT (see Fig. 8)	DESCRIPTION			CONDITIONS			
	Phase*	MOLE FRACTION	DESCRIPTION	P(bars)	T(°K)	gm/sec	cm^3/sec
1) B			benzene feed tank		298		
2) Stream 1	L	1.0	benzene feed	5.0	298	0.742	
3) Stream 2	S	1.0	catalyst ($FeCl_3$)		298		
4) A			chlorine cylinder				
5) Stream 3	G	1.0	chlorine gas feed	5.0	298		34-38
6) Stream 4	L	0.97-0.99	recycled stream	5.0	298	1.6-2.5	
7) Stream 5	L	1.0	cooling water for reactor		291-301	12.5-13	
8) C			jacketed reactor	1-5	298-328		
9) Stream 6	L,G,V		reactor product	1-4	298-328	2.6-3.6	
10) E			flash tank	1.0	298-328		
11) Stream 7	G	1.0	hydrogen chloride gas	1.0	298-328		123-133
12) Stream 8	L	1.0	water for absorption	1.0	298	0.5-0.56	

*S = Solid
L = Liquid
V = Vapor
G = Gas

Table 7 (cont'd)

13) Stream 9	L		dilute hydrochloric acid		298	0.67-0.74	
14) Stream 26	G		chlorine and hydrogen chloride	1.0	298-328		
15) G			chlorine and hydrogen chloride absorber	1.0	298		
16) Stream 10	L	0.82-0.87	C_6H_6, C_6H_5Cl, HCl, Cl_2	1.0	298-328	2.5-3.4	
17) D			reactor product tank		298-328		
18) F			electric heater				
19) Stream 12	L	0.82-0.87	C_6H_6, C_6H_5Cl, HCl, Cl_2	1.0	357-359	2.5-3.4	
20) I			four-plate distillation column	1.0			
21) J			glass reboiler				
22) K			reflux splitter with solenoid value				
23) Stream 14	L,V	1.0	steam for reboiler	1-4	373-420	0.37-1.0	
24) H			glass condenser				
25) Stream 24	G	1.0	non-condensable gases (HCl and Cl_2)	1.0	353-354		

Table 7 (cont'd)

26) Stream 18	L	1.0	cooling water for condenser	1.0	293-303	18-48	
27) Stream 15	L	0.19-0.41	bottom product from reboiler	1.0	375-388	0.93-1.1	
28) Stream 25	L	0.19-0.41	bottom product	1.0	298	0.93-1.1	
29) N			bottom product cooler				
30) Stream 23	L	1.0	cooling water for cooler N	1.0	293-313	1.3-1.7	
31) O and P			bottom product and distillate storage tanks				
32) Stream 21	L	0.97-0.99	distillate product	1.0	353-354	1.6-2.5	
33) M			reflux storage tank				
34) Stream 22	L	1.0	cooling water for cooler L	1.0	293-303	3.8-5.9	
35) L			distillate cooler				

TABLE 8. EQUIPMENT SPECIFICATIONS

S.#.OR M E[1]	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE[2]	COST
1) B		5 gallons vertical fiber glass tank with cover (1/4" side hole and 1/2" cover hole)	U. S. Plastics	b	$16.40
	bulkhead female connector	400-71-4, 1/4" to 1/4"	Crawford Fitting Co.	b	9.00
	crank action hand pump	solvent pump #9116K 11	McMaster-Carr Supply Co.	b	47.00
2) Stream 1		304 S.S. tube, 1/4" O.D. and 1/8" O.D. (welded)	Metal Goods Corporation	b	
	male connector	400-1-4, 1/4" to 1/4"	Crawford Fitting Co.	b	9.00
	metering pump	210-10R, Ryton, 2 X 1/4" Female, 5 to 350cm^3/min, 160 psi	March Manufacturing Co., Inc.	b	154.00
	male connector	200-1-4, 1/4" to 1/8"	Crawford Fitting Co.	b	9.00
	needle valve	1315G2Y,1/8" Gyrolok	Hoke Inc.	m	20.00
	2 male connectors	200-1-4, 1/8" to 1/4"	Crawford Fitting Co.	m	18.00
	rotameter	size 1/4", cat. #28, 10A3000	Fisher	m	150.00
	male branch tee	200-3-4 TTM, 2 X 1/8", 1/4"	Crawford Fitting Co.	b	9.00
	gauge pressure	series 1020, 1/4" female, 0-100 psi	Dresser Industries (Ashcroft)	b	65.00
	Electric Tel-O-Set controller	input ± 10DC volt, output 4-20 maDC, three modes	Honeywell	a	228.00
	I/P transoluccr & valve operator	input 4-20 maDC, output 3-15 psig	Honeywell	a	186.00
	2 male connectors	200-1-4, 1/8" to 1/4"	Crawford Fitting Co.	a	18.00
	air operated needle valve	1/4" female, 316 S.S., 3-15 lb pneumatic (standard air to close valve), Model 78S	Badger Meter Inc.	a	142.50
	2 female connectors	400-7-6, 1/4" to 3/8" (tube-flowmeter-tube)	Crawford Fitting Co.	c	18.00
	2 reducing unions	400-6-2, 1/8" to 1/4" (tube-tube)	Crawford Fitting Co.	c	18.00
	turbine flowmeter	Model 10C1510A1XRXXXXX, 3/8" male	Fisher and Porter	c	540.00
	transducer	Model 55GE3238BRF, output 4-20ma (475 ohm max.)	Fisher and Porter	c	275.00
	indicator	Model 55ME1200 Model 602, 4-20 ma input	Fisher and Porter	c	80.00
	resistor	250 ohm			0.25

1 stream # or Major Equipment CODE (SEE FIGURE 8, PAGE 22)

2 m = manual control
a = automatic control
c = computer control
b = basic equipment

Table 8 (cont'd)

S.#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
3) Stream 2		ferric chloride catalyst			
4) A		size IV, 150 lb	The Matheson Co., Inc.	b	$33.00
	corrosion resistant regulator	B15B-(CGA), 1/4" NPT male	The Matheson Co., Inc.	b	123.00
	tee purge assembly	4750-660	The Matheson Co., Inc.	b	42.00
	check valve	401X	The Matheson Co., Inc.	b	7.00
5) Stream 3		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	female connector	200-7-4, 1/4" to 1/8" (regulator-tube)	Crawford Fitting Co.	b	9.00
	2 male connectors	200-1-4, 1/8" to 1/4" (tube-rotameter-tube)	Crawford Fitting Co.	m	18.00
	rotameter	size 1/4", cat. #28, 10A3000	Fisher	m	150.00
	female connector	810-7-4, 1/4" to 1/2" (regulator-tube)	Crawford Fitting Co.	c	9.00
	male connector	810-1-8, 1/2" to 1/2" (tube-turbine meter)	Crawford Fitting Co.	c	9.00
	male connector	400-1-8, 1/2" to 1/4" (turbine meter-tube)	Crawford Fitting Co.	c	9.00
	tube	304 S.S. tube, 1/4" O.D. and 1/2" O.D. (Welded)	Metal Goods Corporation	c	
	reducing union	400-6-2, 1/4" to 1/8"	Crawford Fitting Co.	c	9.00
	turbine meter	Model 4902, 1/2" female	Emerson Electric Co.	c	659.00
	transducer indicator	Model 4360, output 5V or 10V DC	Emerson Electric Co.	c	425.00
6) Stream 4		304 S.S. tube, 1/4" O.D. and 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	3 male connectors	200-1-2, 1/8" to 1/8" (stream4-solenoid valve)	Crawford Fitting Co.	b	27.00
	3 way solenoid valve	catalog #8300C55, normally open, 3 X 1/8" female	Asco	b	115.00
	reducing union	400-6-2, 1/8" to 1/4"	Crawford Fitting Co.	b	9.00
	union tee	400-3, 1/4" (for sampling port)	Crawford Fitting Co.	b	9.00
	cap	400-C, 1/4" (for sampling port)	Crawford Fitting Co.	b	9.00
	female run tee	400-3-4 TTF, 1/4", 1/4", 1/4" female	Crawford Fitting Co.	b	9.00
	thermocouple	J116G-304-SST 1/4"-5"-0"S	Thermo Electric	b	27.00
	male connector	400-1-4, 1/4" to 1/4" (tube-rotameter)	Crawford Fitting Co.	m	9.00
	rotameter	size 1/4", cat. #34, 10A3000	Fisher	m	150.00

Table 8 (cont'd)

S.#, OR M E	ACCESORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	male connector	200-1-4, 1/4" to 1/8" (rotameter-tube)	Crawford Fitting Co.	m	9.00
	2 female connectors	400-7-6, 1/4" to 3/8" (tube-flowmeter-tube)	Crawford Fitting Co.	c	18.00
	3 way valve	7165G25, 1/8" Gyrolok	Hoke Inc.	b	20.00
	reducing union	400-6-2, 1/4" to 1/8" (tube-tube)	Crawford Fitting Co.	c	9.00
	turbine flowmeter	Model 10C1510A1XRXXXXX, 3/8" male	Fisher and Porter	c	540.00
	transducer	Model 55GE3238BRF, output 4-20ma (475 ohm max.)	Fisher and Porter	c	275.00
	indicator	Model 55ME1200 Model 602, input 4-20ma	Fisher and Porter	c	80.00
	resistor	250 ohm		c	0.25
	gauge pressure	series 1020, 1/4" female, 0-100 psi	Dresser Industries (Ashcroft)	b	65.00
	male branch tee	200-3-4TTM, 2 X 1/8", 1/4"	Crawford Fitting Co.	b	9.00
	amplifier for thermocouple	610J, gain=1470	Analog Devices, Inc.	c	39.00
7) Stream 5		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	2 male connectors	200-1-4, 1/8" to 1/4" (tube-valve-tube)	Crawford Fitting Co.	b	18.00
	air operator needle valve	1/4"female, bronze, 3-15 lb pneumatic (standard air to close valve), Model 78S	Badger Meter Inc.	b	142.50
	union tee	200-3, 3 X 1/8"	Crawford Fitting Co.	b	9.00
8) C		a) 304 S.S. tube, 3" O.D. (Welded), 2 1/2" height b) 304 S.S. tube, 4" O.D. (Welded), 2 1/2" height	Metal Goods Corporation	b	
	reactor base	304 S.S., 5" D., 1/8" thickness	Metal Goods Corporation	b	
	magnet support	304 S.S. tube, 1 3/8" O.D., 1/2" height with 1/8" side holes	Metal Goods Corporation	b	
	flange	304 S.S., 2.87" I.D., 5" O.D., 1/8" thickness, 6 X 1/4" holes	Metal Goods Corporation	b	
	cover	304 S.S., 5"D.,1/8"thickness,4 X 1/8"holes, 6 X 1/4" holes, 2 X 1/4" and 1/8" threaded holes	Metal Goods Corporation	b	
	6 bolts and nuts	1/4" S.S., 1" bolt length	Metal Goods Corporation	b	
	4 bulkhead unions	200-61, 1/8"	Crawford Fitting Co.	b	36.00
	male connector	200-1-2, 1/8" to 1/8" (product)	Crawford Fitting Co.	b	9.00
	thermocouple	J116G-304-SST 1/4"-5"-0"S	Thermo Electric	b	27.00
	amplifier	610J, gain =1055	Analog Devices, Inc.	c	39.00

Table 8 (cont'd)

S.E. OR M.E.	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	magnetic stirrer	Fisher code: 14-511-200	Fisher	b	$64.00
	magnet	1" length, Teflon coating		b	1.30
	male connector	400-1-4, 1/4" to 1/4" (reactor-sampling port)	Crawford Fitting Co.	b	9.00
	port connector	401-PC, 1/4" to 3/8"	Crawford Fitting Co.	b	9.00
	cap	600-C, 3/8"	Crawford Fitting Co.	b	9.00
9) Stream 6		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	back pressure regulator	S.S. with teflon seat, 0-150 psi, 1/4" female inlet and outlet	Tescom Corp. (Fluid System Div.)	b	200.00
	2 male connectors	200-1-4, 1/8" to 1/4" (tube-regulator-tube)	Crawford Fitting Co.	b	18.00
	male branch tee	200-3-4TTM, 2 X 1/8", 1/4"	Crawford Fitting Co.	m	9.00
	gauge pressure	series 1020, 1/4" female, 0-100 psi	Dresser Industries (Ashcroft)	m	65.00
	2 male connectors	200-1-4, 1/8" to 1/4" (tube-transducer-tube)	Crawford Fitting Co.	c	18.00
	pressure transducer	P7D, 0-100 psig, 1/8" female	Celesco Transducer Products,Inc	c	251.00
	transducer indicator	Model CD25A, output + 5 DC volt	Celesco Transducer Products,Inc	c	462.00
10) E		conical glass tee, 2" X 1", code 72-1261	Corning Glass Work	b	30.50
	2 flanges (top and bottom)	2 size 2" complete kit, code 72-0338 and 4 gaskets code 72-9256	Corning Glass Work	b	22.40
	2 metal sheets	2 metal sheets 2" D., 1/8" thickness, 304 S.S., each with 1/8" threaded hole at center	Metal Goods Corporation	b	
	flange (side arm)	size 1" complete kit, code 72-0138 and 2 gaskets code 72-9254	Corning Glass Work	b	9.20
	metal sheet	metal sheet 1" D., 1/8" thickness, 304 S.S., with 1/8" threaded hole at center	Metal Goods Corporation	b	
	3 male connectors	200-1-2, 1/8" to 1/8"	Crawford Fitting Co.	b	27.00
	liquid level control	lab monitor II, Part #50021, 115V, with semi-flat clip #50041	Pope Scientific Corp.	b	160.00
11) Stream 7		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	Check valve (ball)	6133G2S, 1/8" Gyrolok	Hoke Inc.	b	20.00
	union tee	200-3, 1/8"	Crawford Fitting Co.	b	9.00
12) Stream 8		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	2 male connectors	200-1-2, 1/8" to 1/8" (tube-valve-tube)	Crawford Fitting Co.	b	18.00

Table 8 (cont'd)

S.#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	regulating valve	3232F2B, 1/8" female	Hoke Inc.	b	$ 9.00
13) Stream 9		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
	union tee	200-3, 1/8"	Crawford Fitting Co.	b	9.00
14) Stream 26		304 S.S. tube, 1/8" O.D. (Welded)	Metal Goods Corporation	b	
15) G		2" pyrex conical pipe, I.D. X L. = 2" X 18", Code 72-7195	Corning Glass Work	b	23.40
	2 bulkhead unions	200-61, 1/8"	Crawford Fitting Co.	b	18.00
	2 flanges (top and bottom)	2 size 2" complete kit, code 72-0338 and 4 gasket code 72-9256	Corning Glass Work	b	22.40
	top metal sheet	304 S.S., thickness = 1/8", D. = 2 5/8" with 1/8" hole at center	Metal Goods Corporation	b	
	bottom metal sheet	304 S.S., thickness = 1/8", D. = 2 5/8" with 2 X 1/8" holes one at center	Metal Goods Corporation	b	
	bottom catalyst suport	304 S.S., thickness = 1/8", D.=1 7/8" with 3/8"distributed holes & half ball of 1/2"D.,1/8"thick, welded at center	Metal Goods Corporation	b	
	bottom leg support	4 X 1/8" D. rod, 304 S.S., L = 1.5"	Metal Goods Coporation	b	
	nozzle	1/8" G1 (full cone spray)	Fulljet Co.	b	6.50
	2 male connectors	200-1-2, 1/8" to 1/8"	Crawford Fitting Co.	b	18.00
	packing	1/4" multi-turn helices, code 86-0058, .175 ft^3	Corning Glass Work	b	98.00
16) Stream 10		304 S.S. tube, 1/8" O.D. and 1/4" O.D. (Welded)	Metal Goods Corporation	b	
	2 male connectors	400-1-6, 1/4" to 3/8" (tube-valve-tube)	Crawford Fitting Co.	b	18.00
	solenoid valve	Teflon seat, 8210B33, 3/8" female	Asco	b	65.00
	2 check valves	1) 6133G4S, 1/4" Gyrolok 2) 6133G2S, 1/8" Gyrolok	Hoke Inc.	b	40.00
	male connector	400-1-2, 1/4" to 1/8"	Crawford Fitting Co.	b	9.00
	female run tee	200-3TFT, 1/8"	Crawford Fitting Co.	b	9.00
	2 reducing unions	200-6-1, 1/8" to 1/16" (tube-refractometer-tube)	Crawford Fitting Co.	b	18.00
	Diffe. conti. refractometer	series 400, output 100mV, 1/16" inlet and outlet	Waters Associates Inc.	b	2800.00
	resistance	5 ohm		b	0.25
	recorder	Electrick Tel-O-Set recorder, input 4-20 Ma, output + 10 DCV	Honeywell	b	516.50
	grounded resistance (3 resistors)	to decrease voltage to 5V		c	0.75

Table 8 (con'd)

S.f, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	male connector	200-1-4, 1/8" to 1/4" (tube-pump)	Crawford Fitting Co.	b	$9.00
	male connector	400-1-4, 1/4" to 1/4" (pump-tube)	Crawford Fitting Co.	b	9.00
	centrifugal pump	D6, 1/4" female	Eastern Industries, Inc.	b	259.00
	male connector	400-1-4, 1/4" to 1/4" (tube-rotameter)	Crawford Fitting Co.	m	9.00
	rotameter	size 1/4", cat. #35, 10A3000	Fisher	m	150.00
	male connector	200-1-4, 1/4" to 1/8" (rotameter-tube)	Crawford Fitting Co.	m	9.00
	2 female connectors	400-7-6, 1/4" to 3/8" (tube-flowmeter-tube)	Crawford Fitting Co.	c	18.00
	turbine flowmeter	Model 10C1510A1XRXXXX, 3/8" male	Fisher and Porter	c	540.00
	transducer	Model 55GE3238BRF, output 4-20ma (475 ohm max.)	Fisher and Porter	c	275.00
	indicator	Model 55ME1200 Model 602, input 4-20 ma	Fisher and Porter	c	80.00
	resistor	250 ohm		c	0.25
	female connector	200-7-4, 1/4" to 1/8" (flowmeter-tube)	Crawford Fitting Co.	c	9.00
	union tee	200-3, 1/8" (for sampling)	Crawford Fitting Co.	b	9.00
	cap	200-C, 1/8" (for sampling)	Crawford Fitting Co.	b	9.00
	3 way valve	7165G2S, 1/8" Gyrolok	Hoke Inc.	b	20.00
	needle valve	1315G2Y, 1/8" Gyrolok	Hoke Inc.	b	20.00
	Electric Tel-O-Set controller	input ± 10 DC volt, output 4-20 maDC, three modes	Honeywell	a	228.00
	1/P transducer and valve operator	input 4-20 maDC, output 3-15 psig	Honeywell	a	186.00
17) D		5 gallons vertical fiber glass with cover, 2 X 1/8" side hole near top and bottom	U. S. Plastics	b	16.40
	2 bulkhead female connectors	200-71-2, 1/8" to 1/8" (tank-tube)	Crawford Fitting Co.	b	18.00
18) Stream 11 (F)	immersion heater	glass shield, O.D. X L = 17 X 457 mm, cat. #11-463-18B, L = 13 cm, 500 W	Fisher Scientific 77	b	31.62
	temperature regulator	code 11-463-45	Fisher Scientific 77	b	23.00
	jacket	304 S.S. tube, 1 1/2" O.D., L = 8" with 2 threaded holes near each end: 1/4" and 1/8" D.	Metal Goods Corporation	b	
	2 flanges	304 S.S., I.D. = 1 1/2", O.D. = 3", 1/8" thick with 4 X 1/4" holes	Metal Goods Corporation	b	
	2 metal sheets (cap)	304 S.S., 3" O.D., one with 4 X 1/4" holes and the other with 4 X 1/4" holes and 17 mm hole at the center, 1/8"thick	Metal Goods Corporation	b	

Table 8 (cont'd)

S.#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	2 male connectors	a) 200-1-2, 1/8" to 1/8" (stream 10 - jacket) b) 400-1-4, 1/4" to 1/4" (stream 12 - jacket)	Crawford Fitting Co.	b	$18.00
	8 bolts and nuts	1/4" D., Lenth of bolts = 1.5", S.S.	Metal Goods Corporation	b	
19) Stream 12		304 S.S. tube, 1/8" O.D. and 1/4" O.D. (Welded)	Metal Goods Corporation	b	
	female run tee	400-3-4TTF, 1/4", 1/4", 1/4" female	Crawford Fitting Co.	b	9.00
	thermocouple	J116G-304-SST 1/4"-5"-0"S	Thermo Electric	b	27.00
	amplifier for thermocouple	AD520J, gain = 820	Analog Devices, Inc.	c	18.00
	reducing union	400-6-2, 1/4" to 1/8" (tube-tube)	Crawford Fitting Co.	b	9.00
	3 union tees	200-3, 1/8"	Crawford Fitting Co.	b	27.00
	4 ball valves	7115G2S, 1/8" O.D. Gyrolok	Hoke Inc.	b	80.00
	male branch tee	200-3-4TTM, 2 X 1/8", 1/4"	Crawford Fitting Co.	b	9.00
	gauge pressure	series 1020, 1/4" female, 0-60 psi	Dresser Industries (Ashcroft)	b	65.00
20) I		conical pyrex glass	Corning Glass Work	b	50.00
	4 flanges for side outlet	4 size 1" complete kit, code 72-0138 and 8 gaskets code 72-9254	Corning Glass Work	b	36.80
	4 metal sheets for side output	304 S.S., 1" D. with 2 threaded holes:1/4"&1/8",1/8"thick	Metal Goods Corporation	b	
	4 sieve trays	2" D., 9" tray spacing	Chem-Pro Equip. Corp.	b	352.00
	4 male connectors	200-1-2, 1/8" to 1/8" (stream 12 - column)	Crawford Fitting Co.	b	36.00
	4 thermocouples	J116G-304-SST 1/4"-5"-0"S	Thermo Electric	b	108.00
	4 amplifiers for thermocouples	AD520J, gain = 890, 875, 840, and 760	Analog Devices, Inc.	c	72.00
	6 flanges: a) column-tee b) tee-6" pipe c) tee - 18" pipe d) 18" pipe-reducer tee e) reducer tee - 6" pipe f) column-splitter	6 size 2"complete kit,style 1, code 72-0338 and 6 gaskets code 72-9256	Corning Glass Work	b	67.20
	tee	2" X 2" pyrex conical tee, code 72-8250	Corning Glass Work	b	30.50
	3 glass pipes	pyrex conical pipe, 2" D. a) L = 6", code 72-1570 b) L=6", code 72-1570 c) L=18", code 72-7195	Corning Glass Work	b	61.78
	reducer tee	2" X 1" X 2" pyrex conical tee, code 72-4748	Corning Glass Work	b	39.70
	flange(2" pipe-concentric reducer)	size 2" complete kit, code 72-0338 and 2 gaskets code 72-9256	Corning Glass Work	b	12.85

Table 8 (cont'd)

S.#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	metal tube (pipe-ell 90° reducer)	304 S.S., 2 1/4" O.D. (welded), L=1" with 1/4" threaded hole in the middle	Metal Goods Corporation	b	
	concentric reducer	2" X 1" conical concentric reducer, pyrex glass code 72-0060	Corning Glass Work	b	$20.70
	flange (concentric reducer 90°-ell)	size 1" complete kit, code 72-0138 and gasket code 72-9254	Corning Glass Work	b	8.00
	90° ell mitered	1" pyrex glass, code 72-8320	Corning Glass Work	b	14.85
	flange (2" pipe - 90° ell reducer)	size 2" complete kit, code 72-0388 and 2 gaskets code 72-9256	Corning Glass Work	b	12.85
	metal tube (pipe-concentric reducer)	304 S.S., 1 1/14" O.D. (welded), L=2 3/4" with 1/4" threaded hole 1/2" from edge	Metal Goods Corporation	b	
	2 male connectors	400-1-4, 1/4" to 1/4", teflon for glass pipe	Crawford Fitting Co.	b	18.00
	pyrex glass pipe	1/4" O.D., L=24"		b	0.20
	flange (reducer tee-stream 15)	size 1" complete kit, code 72-0138 and 2 gaskets code 72-9254	Corning Glass Work	b	9.20
	metal sheet (reducer tee - steam 15)	304 S.S., 1" D., 1/8" thick with 1/4" threaded hole at center	Metal Goods Corporation	b	
	male connector	200-1-2, 1/8" to 1/8" (reducer-stream 15)	Crawford Fitting Co.	b	9.00
	ell 90° reducer	PBR 4/2, code 86-1004	Corning Glass Work	b	70.00
	liquid level controller (on 1/4 glass pipe)	lab. monitor II, Part #50021, 115V	Pope Scientific Incorporated	b	157.50
21) J		HEB4, 4", 3 X 1" side tube, code 86-0010	Corning Glass Work	b	353.00
	flange (ell 90° reducer - reboiler)	size 4" complete kit, code 72-0538 and gasket code 72-9808	Corning Glass Work	b	36.70
	flange for thermocouple	size 1" complete kit, code 72-0138 and 2 gaskets code 72-9254	Corning Glass Work	b	9.20
	metal sheet for thermocouple -	304 S.S., 1" D., 1/8" thick with 1/4" threaded hole at center	Metal Goods Corporation	b	
	thermocouple	J116G-304-SST 1/4"-5"-0"S	Thermo Electric	b	27.00
	amplifier for thermocouple	AD250J, gain = 650	Analog Devices, Inc.	c	18.00
	2 flanges for inlet and outlet steam	2 size 1" complete kit, code 72-0138 and 4 gaskets code 72-9254	Corning Glass Work	b	18.40
	2 metal sheets for inlet and outlet steam	2 304 S.S., 1" D, 1/8" thick with 1/2" threaded hole at the center	Metal Goods Corporation	b	
	2 male connectors	810-1-8, 1/2" to 1/2" (inlet and outlet steam)	Crawford Fitting Co.	b	18.00
	flange (reboiler-90°ell)	size 1" complete kit code 72-0138 and gasket code 72-9254	Corning Glass Work	b	8.00
22) K		size 2-28, 2"connection	Chem-Flow Corporation	b	491.00
	temperature recorder and controller	Model RS-TRC	Chem-Pro Equip. Corp.	b	1850.00

Table 8 (cont'd)

S,#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	I/P transducer & valve operator	input 4-20 ma DC, output 3-15 psig	Honeywell	b	$228.00
	amplifier	AD 250 J, gain 890	Analog Devices, Inc.	b	18.00
	resistance	250 ohm		b	0.25
	flange (splitter-condenser)	size 2" complete kit, code 72-0338 and gasket code 72-9256	Corning Glass Work	b	11.20
	flange for stream 21	size 2" complete kit, code 72-0338 and 2 gaskets code 72-9256	Corning Glass Work	b	12.85
	metal sheet for stream 21	304 S.S., 2" D., 1/8" thick with 1/4" threaded hole at center	Metal Goods Corporation	b	
	male connector	400-1-4, 1/4" to 1/4", for stream 21	Crawford Fitting Co.	b	9.00
23) Stream 14		304 S.S. tube, 1/2" O.D. (welded)	Metal Goods Corporation	b	
	6 male connectors	810-1-8, 1/2" to 1/2"	Crawford Fitting Co.	b	54.00
	pressure regulator	#960, 1/2" female, 20-100 psi	Crane Company	b	250.00
	male branch tee	810-3-8 TIM, 1/2" X 1/2" X 1/2"	Crawford Fitting Co.	b	9.00
	gauge pressure	series 1020, 1/2" female, 0-60 psi	Dresser Industries (Ashcroft)	b	65.00
	strainer	#4417K21, screwed connection, size 1/2" female	McMaster-Carr Supply Co.	b	4.21
	steam trap	#4897N21, 1/2" female	McMaster-Carr Supply Co.	b	32.51
24) H		HE2, 2" connection, code 86-0002	Corning Glass Work	b	254.00
	flange (condenser-vent)	size 2" complete kit, code 72-0338 and 2 gaskets code 72-9256	Corning Glass Work	b	12.85
	metal sheet for vent	304 S.S., 2" D., 1/8" thick with 1/8" threaded hole at center	Metal Goods Corporation	b	
	male connector	200-1-2, 1/8" to 1/8" (condenser-stream 24)	Crawford Fitting Co.	b	9.00
25) Stream 24		304 S.S., tube, 1/8" O.D. (welded)	Metal Goods Corporation	b	
	check valve	6133G2S, 1/8" Gyrolok	Hoke Inc.	b	20.00
26) Stream 18		a) 5/8" I.D., rubber hose b) 304 S.S. tube, 1/4" O.D. and 1/2" O.D. (welded)	Metal Goods Corporation	b	2.00
	insert	1215-10, 3/4", 5/8"	Crawford Fitting Co.	b	9.00
	2 reducing unions	a) 1210-6-8, 3/4" to 1/2" b) 810-6-4, 1/2" to 1/4"	Crawford Fitting Co.	b	18.00
	throttling valve	3212G4B, 1/4" Gyrolok	Hoke Inc.	b	20.00
27) Stream 15		a) 304 S.S. tube, 1/4" O.D. and 1/8" O.D. (welded) b) coils: coil diameter = 1", 1/8" O.D., 13 turns, L=42", 1/4" spacing	Metal Goods Corporation	b	

Table 8 (cont'd)

S, #, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	male connector	400-1-6, 1/4" to 3/8" (tube-valve)	Crawford Fitting Co.	b	$9.00
	solenoid valve	8210B33, teflon seat, 3/8" female	Asco	b	65.00
	male adapter	401-A-6, 3/8" to 1/4" (valve-reducer)	Crawford Fitting Co.	b	9.00
	reducing union	400-6-2, 1/4" to 1/8"	Crawford Fitting Co.	b	9.00
28) Stream 25		304 S.S. tube, 1/4" O.D. and 1/8" O.D. (welded)	Metal Goods Corporation	b	
	reducing union	400-6-2, 1/8" to 1/4"	Crawford Fitting Co.	b	9.00
	union tee	400-3, 1/4" (for sampling)	Crawford Fitting Co.	b	9.00
	cap	400-C, 1/4" (for sampling)	Crawford Fitting Co.	b	9.00
	female run tee	400-3-4TTF, 1/4", 1/4", 1/4"	Crawford Fittting Co.	b	9.00
	thermocouple	J116G-304-SST 1/4" - 5" - 0"S	Thermo Electric	b	27.00
	amplifier for thermocouple	610J, gain = 1470	Analog Devices, Inc.	c	18.00
	2 male connectors	a) 400-1-4, 1/4" to 1/4" (tube-rotameter) b) 200-1-4, 1/4" to 1/8" (rotameter-tube)	Crawford Fitting Co.	m	18.00
	rotameter	size 1/4", cat. #28, 10A3000	Fisher	m	150.00
	2 female connectors	400-7-6, 1/4" to 1/8" (tube-flowmeter-tube)	Crawford Fitting Co.	c	18.00
	reducing union	400-6-2, 1/4" to 1/8" (tube-tube)	Crawford Fitting Co.	c	9.00
	turbine flowmeter	Model 10C1510A1XRXXXXX, 3/8" male	Fisher and Porter	c	540.00
	transducer	Model 55GE3238BRF, output 4-20 ma	Fisher and Porter	c	275.00
	indicator	Model 55ME1200 Model 602, input 4-20 ma	Fisher and Porter	c	80.00
	resistor	250 ohm		c	0.25
	needle valve	1315G2Y, 1/8" Gyrolok	Hoke Inc.	b	20.00
29) N		yellow brass, hard drawn round tubing, 1 1/2" O.D., 1/8" wall thickness, L=8" with 2 X 1/8" threaded hole, 3/4" from each edge	Metal Goods Corporation	b	
	2 flanges	yellow brass, 1 1/2" I.D., 3" O.D., 1/4" thick with 4 X 1/4" hole at 1 1/8" from center	Metal Goods Corporation	b	
	8 bolts and nuts	1/4" diameter, length of bolt = 1 1/2", S.S.	Metal Goods Corporation	b	
	2 male connectors	200-1-2, 1/8" to 1/8" (stream 23-jacket)	Crawford Fitting Co.	b	18.00

Table 8 (cont'd)

S,#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	2 bulkhead unions	200-61, 1/8" to 1/8" (stream 15 and 25-caps)	Crawford Fitting Co.	b	$18.00
30) Stream 23		brass 1/8" O.D., L=20"	Metal Goods Corporation	b	
	regulating valve	3192G2B, 1/8" Gyrolok	Hoke Inc.	b	20.00
31) O and P		5 gallons vertical fiber glass tank, with cover (2 X 1/8" side holes near top and bottom)	U.S. Plastics		32.80
	4 bulkhead unions	200-61, 1/8" to 1/8" (stream 25-tank, stream 4-tank)	Crawford Fitting Co.	b	36.00
32) Stream 21		304 S.S. tube, 1/4" O.D. and 1/8" O.D. (welded), coil: L=125", coil diameter=1", 38 turns, 1/8" spacing, 1/8" O.D. tube	Metal Goods Corporation	b	
	female run tee	400-3-4TTF, 1/4", 1/4", 1/4"	Crawford Fitting Co.	b	9.00
	thermocouple	J116G-304-SST 1/4" - 5" - 0"S	Thermo Electric	b	27.00
	amplifier for thermocouple	AD520J, gain= 890	Analog Devices, Inc.	c	18.00
	male connector	400-1-4, 1/4" to 1/4" (stream 21-pump)	Crawford Fitting Co.	6	9.00
	metering pump	210-10R, 5-350 cm^3/min, Ryton, 1/4" female	March Manufacturing Co., Inc.	b	154.00
	male connector	200-1-4, 1/4" to 1/8" (pump-stream 21)	Crawford Fitting Co.	b	9.00
33) M		2" D., pyrex conical pipe, L-6", code 72-1570	Corning Glass Work	b	19.19
	bottom flange	size 2" complete kit, code 72-0338, 2 gaskets code 72-9256	Corning Glass Work	b	12.85
	bottom metal sheet	304 S.S., 1/8" thick, 2 5/8" D. with 1/4" threaded hole at center	Metal Goods Corporation	b	
	top flange	size 2" complete kit, code 72-0338, 2 gaskets code 72-9256	Corning Glass Work	b	12.85
	top metal sheet	304 S.S., 1/8" thick, 2 5/8" D. with 2 threaded holes 1/8" and 1/4", 1/2" from center	Metal Goods Corporation	b	
	liquid level control	lab. monitor II, Part #50021, 115 Volt with semi-flat clip #50041	Pope Scientific Corporation	b	160.00
34) Stream 22		brass 1/8" O.D., L=20"	Metal Goods Corporation	b	
	regulating valve	3192G2B, 1/8" Gyrolok	Hoke Inc.	b	20.00
35) L		yellow brass, hard drawn round tubing, 1 1/2" O.D., 1/8" wall thickness, L-12", with 2 X 1/8" threaded holes, 3/4" from each edge	Metal Goods Corporation	b	

Table 8 (cont'd)

S,#, OR M E	ACCESSORIES	EQUIPMENT DESCRIPTION	MANUFACTURER	TYPE	COST
	2 flanges	yellow brass, 1 1/2" I.D., 3" O.D., 1/4" thick with 4 X 1/4" holes at 1 1/8" from center	Metal Goods Corporation	b	
	8 bolts and nuts	1/4" diameter, length of bolt = 1 1/2", S.S.	Metal Goods Corporation	b	
	2 caps	yellow brass, 3" D., each with 4 X 1/4" holes at 1 1/8" from center and 1/8" hole at center, 1/4" thick	Metal Goods Corporation	b	
	2 male connectors	200-1-2, 1/8" to 1/8" (stream 22-jacket)	Crawford Fitting Co.	b	$18.00
	2 bulkhead unions	200-61, 1/8" to 1/8" (stream 21 and 4-caps)	Crawford Fitting Co.	b	18.00
36) Recorder		speedomax W (multi-point recorder), 24 points with flexelect B	Leeds and Northup	b	1500.00

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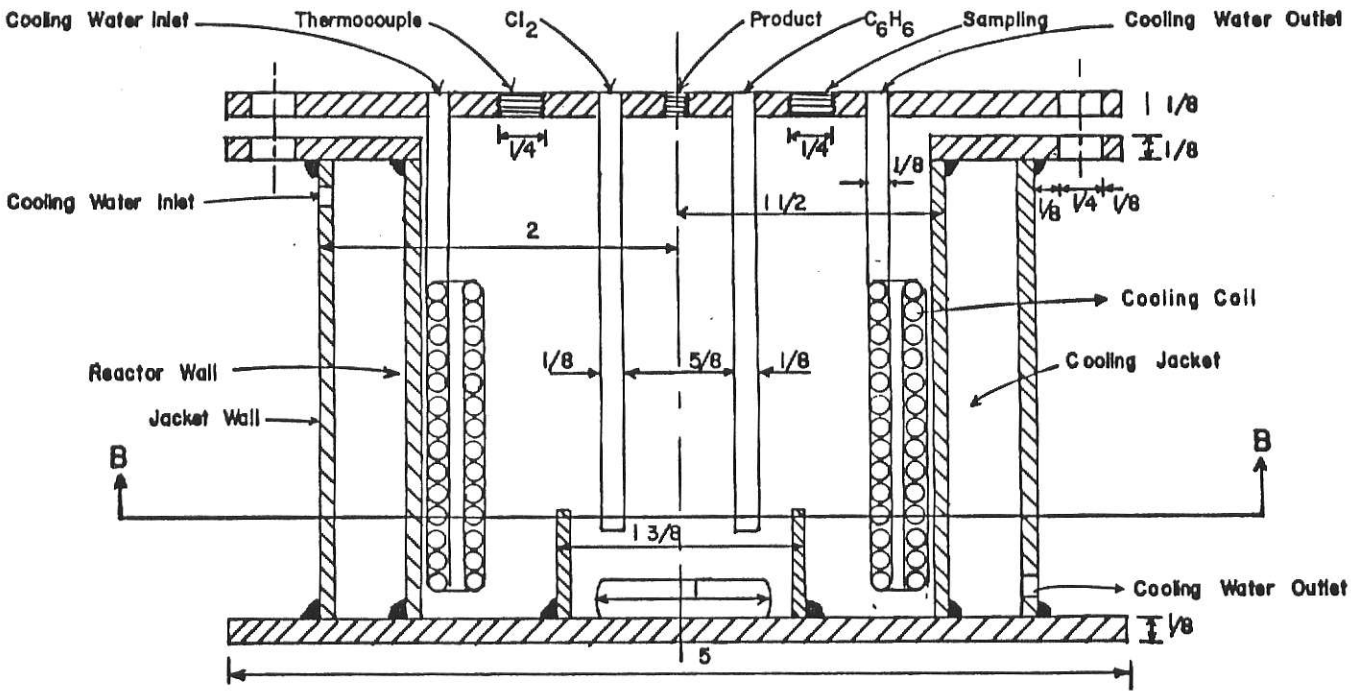
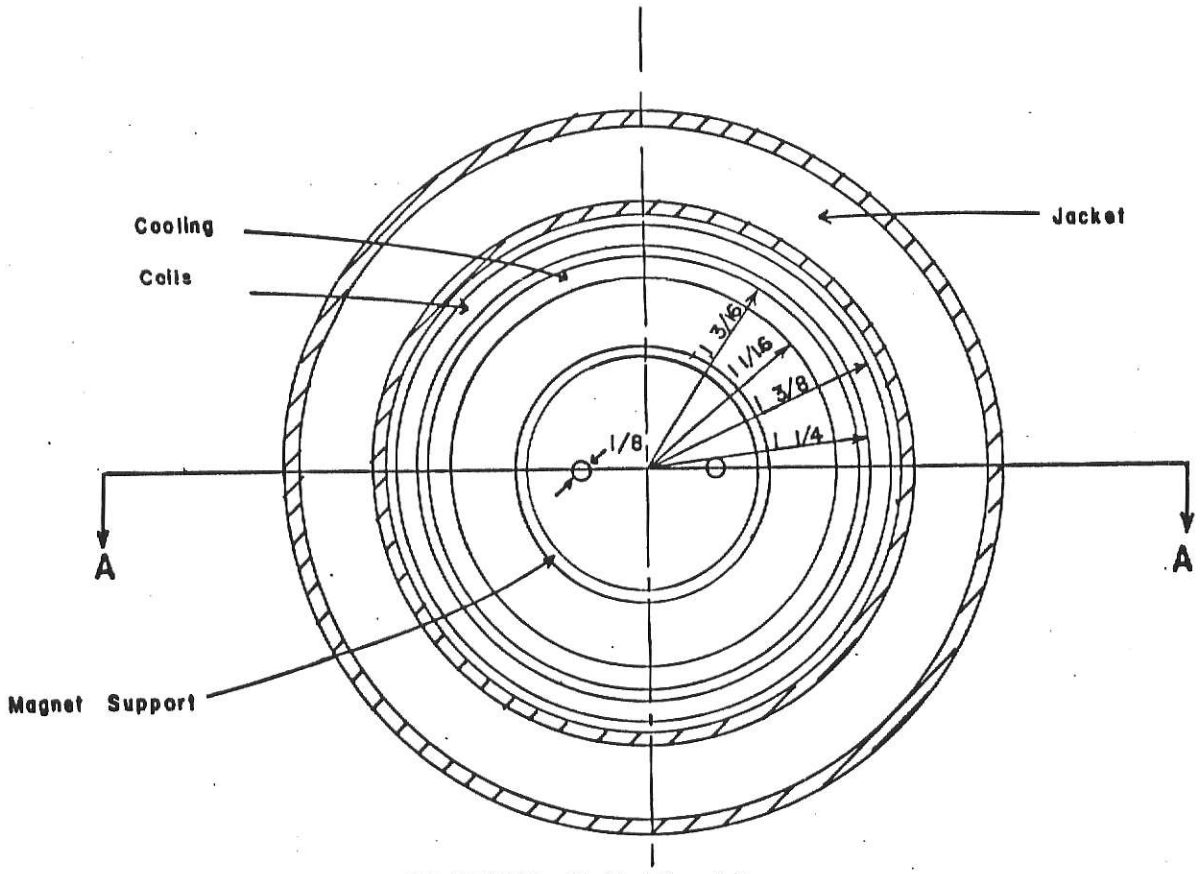


SECTION A-A Side View

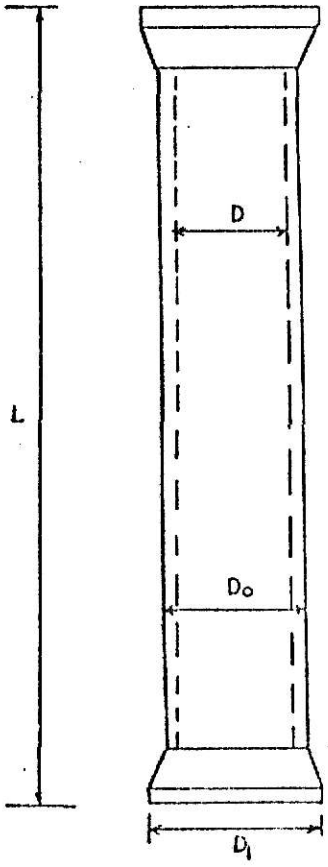


SECTION B-B Top View

Figure 31. Reactor Assembly

(All Dimensions in Inches)

Figure 32.
Absorber Assembly



COLUMN

$D = 2''$ $D_o = 2\text{-}11/32''$

$D_1 = 2\text{-}5/8''$ $L = 18''$

Cone Angle = 12^o

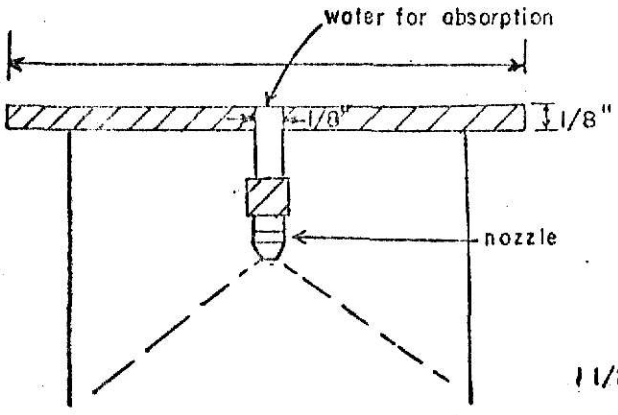
Corning: Conical glass pipe

code 72-7195

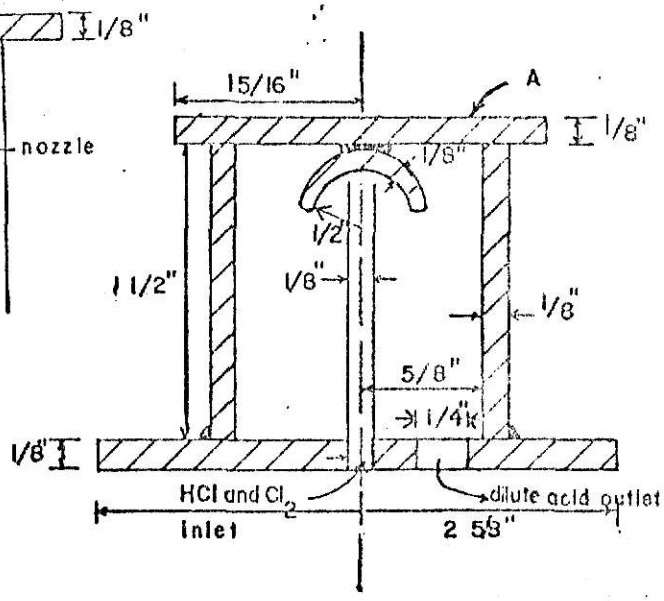
Plate A is a perforated plate

(1/16" hole at random distribution)

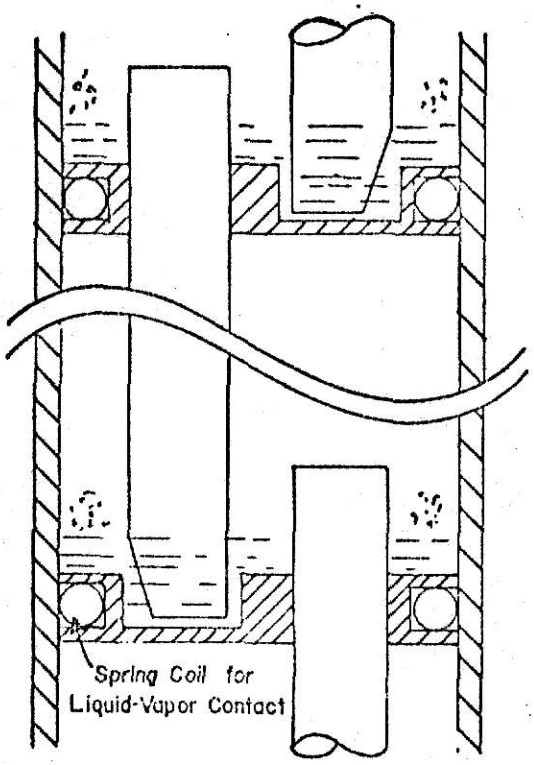
TOP FLANGE, SS316



BOTTOM FLANGE, SS 316



The distillation column, shown in Figure 33, will consist of four cartridge mini-trays - special sieve-type used in 2" column. The cartridge assembly fits easily into standard glass pipe or tubing. Because of the extremely limited space in the column, the spring is designed with a special spacing and height so that it acts as the liquid-vapor contact area of the tray. Vapor bubbles up through the spring coils and efficiently contacts the liquid above. The overflow weirs, downcomers, and throughbolts are placed in the center of the tray. Spring seals are normally teflon-covered for maximum corrosion resistance and tight sealing. Materials are normally stainless steel. Tests show that these trays give the same performance as regular sieve trays.



Mini-Trays Assembly
From CHEM-PRO CORP.

Column Specification

D = 2" D_o = 2 11/32"

D_1 = 2 5/8" D_2 = 1"

D_3 = 1 5/16" L = 36"

Cone Angle = 12°

From CORNING

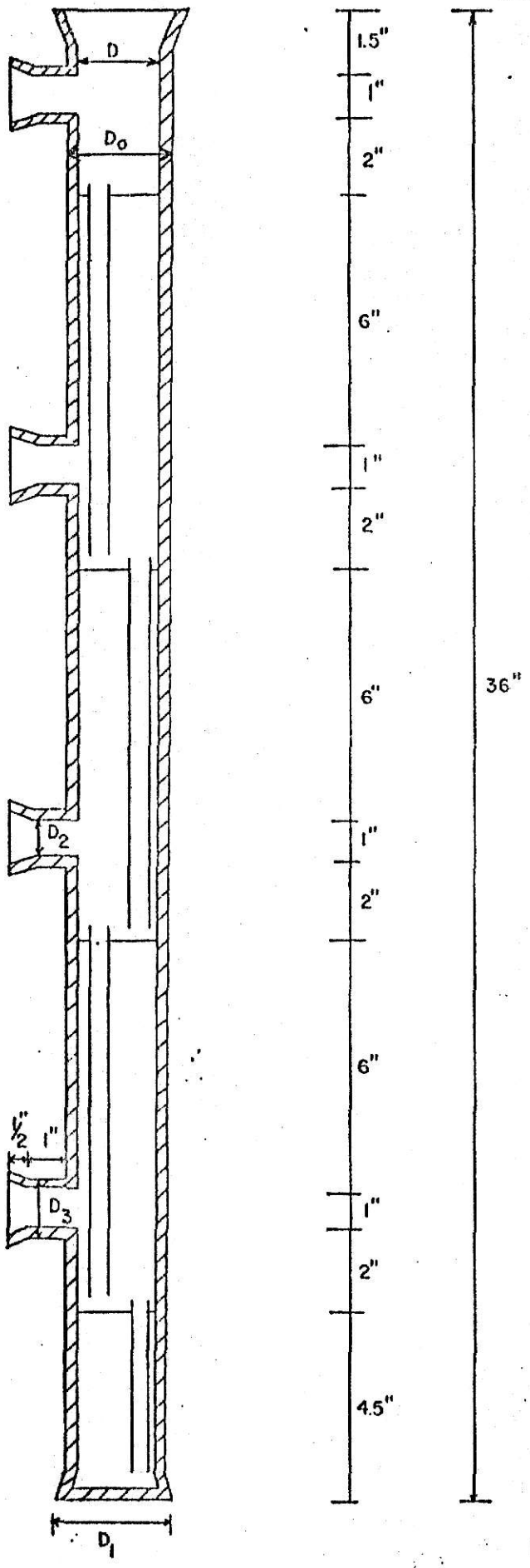


Figure 33.

Distillation Column Assembly

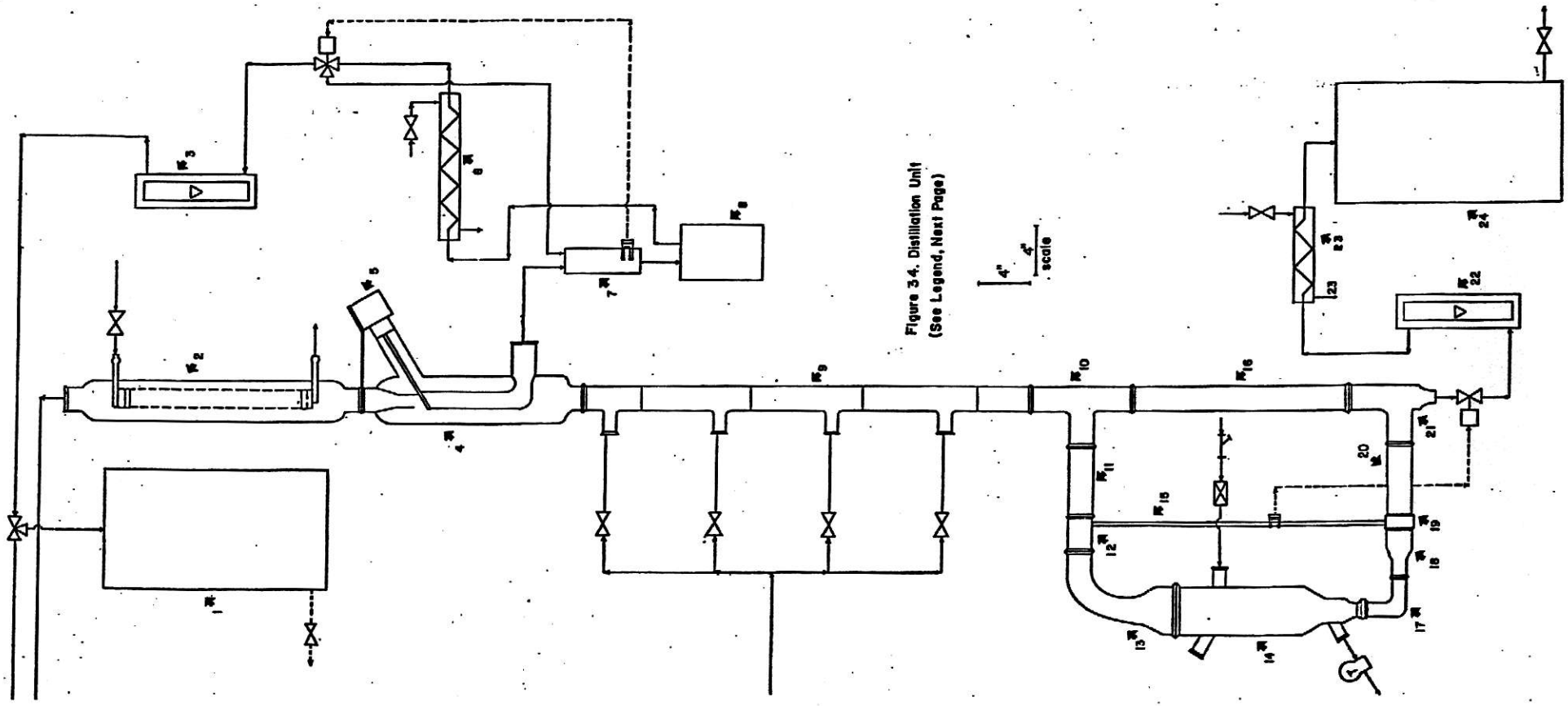


Figure 34. Distillation Unit
(See Legend, Next Page)

LEGEND FOR FIGURE 34

1 Distillate Storage Tank

2 Condenser

3 Rotameter

4 Reflux Splitter

5 Solenoid Valve For Reflux Splitter

6 Distillate Cooler

7 Reflux Storage Tank

8 Metering Pump

9 4-Plate Distillation Column

10 Glass Tee 2" x 2"

11 Glass Pipe L X D_i = 6" x 2"

12 Metal Tube Connecting Parts 11 And 13

13 Ell 90° Reducer 4" x 2"

14 Reboiler

15 ¼" O.D. Pyrex Glass Pipe

16 Glass Pipe L x D_i = 18" x 2"

17 90° Ell Mitered 1" x 1"

18 Concentric Reducer 1" x 2"

19 Metal Tube Connecting Parts 18 And 20

20 Glass Pipe L x D_i = 6" x 2"

21 Reducer Tee 2" x 1" x 2"

22 Rotameter

23 Bottom Product Cooler

24 Bottom Product Tank

B) Cost Estimation

The equipment cost for manual operation includes all basic equipment and accessories along with all manual valves and measuring instruments which are listed in Table 8 under type 'b' and 'm'. For tube fittings, an average price of $9.00 per piece was assumed based on the prices from Crawford Fitting Company catalog (Swagelok). The average price for manual valves was taken to be $20.00 as per - Imperial Eastman Corporation catalog. The cost of glassware, which includes the distillation unit shown in Figure 34 (page 147) was obtained by adding the price of each part as listed in the 1976 Corning Glass Works catalog, plus a 10% price increase. The price of items such as pipes, tubes, sheets, rods, bolts, and nuts was estimated to be $600. The cost for manual operation was obtained by adding the price of all items listed as type 'b' and 'm'; the total cost was $15,000.

The additional equipment and accessories needed for the automatic control investigations, which are listed as type 'a' in the last table, include the automatic controllers, transducers, valve operators, and pneumatic valves. Their estimated cost was $1,000.

Type 'c' equipment are transducers and conditioners to produce $\pm$ 5 D.C. volt signals required as input for the PDP 11/10 for data logging and/or control. This includes amplifiers, indicators, pressure transducers, and turbine meters. The additional cost for computer control was estimated to be $6,000.

The estimated cost for manual control is higher than the cost for automatic or computer control because it includes the cost of the basic equipment (distillation column, reactor, and piping) in addition to the cost of that

required for manual operation. Therefore the total cost for the proposed experimental equipment will be $22,000. This cost does not include recording or data logging equipment.

For an estimate of the cost for each run, a five-hour laboratory period was used as a basis. The cost of utilities (electricity, steam, and cooling water) were not included in the estimated cost. The cost of raw materials for a five-hour run would be:

1) benzene: 4 gallons at $70/55 gallons = $5.00

2) chlorine: 22 lb at $33/150 lb = $5.00

3) ferric chloride catalyst: its price is $3.10/lb and its cost will not be considered due to the small amount used for each run.

The total cost for a five-hour run will be about ten dollars.

VI CONCLUSION

As chemical engineering practice and education have progressed and become more and more complicated, the need for more sophisticated laboratory experiments becomes evident. This is especially true in the area of process control. The proposed experiment using the chlorination of benzene seems to be suited for use as a small, moderately complex experiment for undergraduate chemical engineering students.

The design has indicated that this experiment can be constructed for a very reasonable sum of about $22,000. In addition to the classical kinetics and distillation experiments, it will provide operating experience in several aspects of process control - multiple process control, feed forward and backward control, cascade control, and direct digital control, as well as providing a rather intersting reaction for study.

Although the proposed process is complex enough to provide challenging control problems for study, it should not be beyond the average chemical engineering department's ability to construct, maintain, and operate. Individual departments may wish to develop control schemes and add equipment to this basic process as their interests dictate.

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APPENDICES

Abbreviation used in APPENDIX A, B, and C

A molar heat of vaporization (cal/g mole)

B.P. boiling point (°c)

c°_{p} specific heat of gas (cal/mole/°K)

c_{p_l} specific heat of liquid (cal/gm/°K)

DB density of liquid benzene (gm/cm^3)

DC density of liquid monochlorobenzene (gm/cm^3)

G constant

$H^{\circ} - H^{\circ}_{298}$ enthalpy (Kcal/mole)

J constant

k_1 rate constant for benzene-chlorine reaction (liter/mole/sec)

k_2 rate constant for monochlorobenzene - chlorine reaction (liter/mole/sec)

$K = k_1/k_2$

K constant

K_p equilibrium constant

M.P. melting point (°c)

M.W. molecular weight

P_v vapor pressure (mm Hg)

S° entropy (cal/mole/°K)

t temperature (°c)

T temperature (°K)

X_B benzene mole fraction in liquid phase

Y_B benzene mole fraction in gaseous phase

Z	compressibility factor at boiling point
ΔG°_{f}	Gibbs free energy of formation (Kcal/mole)
ΔH_{c}	heat of combustion at 25°c (Kcal/mole)
ΔH°_{f}	heat of formation (Kcal/mole)
ΔH_{m}	heat of fusion (cal/g)
ΔH_{v}	heat of vaporization (cal/g)
n_{d}	refractive index
ν	kinematic viscosity (centistoke)
μ	absolute viscosity (micropoise or millipoise)
σ	surface tension (dyne/cm)

APPENDIX A

Data For Benzene And Chlorinated Benzene Compounds

Table 9, Molecular Weight, Melting Point and Boiling Point of Compounds of Interest [11 and 16]

Compound	M.W.	M.P. (°c)	B.P. (°c)
Benzene	78.11	5.5	80.10
Monochlorobenzene	112.56	-45.48	131.70
1, 2 - Dichlorobenzene	147.01	-17.00	180.46
1, 3 - Dichlorobenzene	147.01	-24.76	173.08
1, 4 - Dichlorobenzene	147.01	53.10	174.21
1, 2, 3 - Trichlorobenzene	181.46	52.50	218.50
1, 2, 4 - Trichlorobenzene	181.46	16.95	213.48
1, 3, 5 - Trichlorobenzene	181.46	63.50	208.50
1, 2, 3, 4 - Trichlorobenzene	215.90	46.50	254.00
1, 2, 3, 5 - Tetrachlorobenzene	215.90	54.50	246.00
1, 2, 4, 5 - Tetrachlorobenzene	215.90	139.00	243.00
Pentachlorobenzene	250.35	85.50	276.00
Hexachlorobenzene	284.80	229.50	309.00
Chlorine gas	70.91	-100.98	-34.05
Hydrogen chloride gas	36.47	-114.19	-85.03

Table 10. Critical Properties [11]

Compound	Critical density (g/ml)	Critical volume (ml/g)	Critical temp. (°c)	Critical pressure (mm Hg)
Benzene	0.3	3.33	289.45	36936
Monochlorobenzene	0.3654	2.737	359.2	33926
1, 2 - Dichlorobenzene	0.408	2.449	424.1	30800
1, 3 - Dichlorobenzene	0.410	2.44	410.8	29112
1, 4 - Dichlorobenzene	0.395	2.53	411.6	29300
1, 2, 4 - Trichlorobenzene	0.471	2.12	461.8	29900
Chlorine gas	0.573	1.745	146.0	71060
Hydrogen chloride gas	0.4214	2.35	51.4	61978

Table 11. Density [11, 16, and 27]

Compound	17°c	20°c	22°c	25°c	30°c	60°c
Benzene		0.87901		0.87370	0.86837	
Monochlorobenzene		1.10578		1.10037	1.09477	
1, 2 - Dichlorobenzene		1.3057		1.30015	1.2945	
1, 3 - Dichlorobenzene		1.28844		1.2828	1.27712	
1, 4 - Dichlorobenzene						1.24166
1, 2, 4 - Trichlorobenzene		1.4542		1.44829	1.44237	
1, 2, 3 - Trichlorobenzene		1.5562				
1, 2, 4, 5 - Tetrachlorobenzene			1.858			
Pentachlorobenzene	1.834					
Hexachlorobenzene			2.044			

Table 12. Refractive Index [11, 16, and 27]

Compounds	Refractive index				
	10°c	20°c	25°c	30°c	60°c
Benzene		1.50112	1.49792	1.49468	
Monochlorobenzene		1.52406	1.52138	1.51837	
1, 2 - Dichlorobenzene		1.55154	1.5492	1.5465	
1, 3 - Dichlorobenzene		1.54586	1.54337	1.54076	
1, 4 - Dichlorobenzene					1.52586
1, 2, 4 - Trichlorobenzene		1.57168	1.56933	1.55765	
1, 2, 3 - Trichlorobenzene		1.5809			
1, 2, 4, 5 - Tetrachlorobenzene	1.734				

Table 13. Kinematic Viscosity (centistokes) [11]

Benzene		Monochlorobenzene		1,2-Dichlorobenzene		1,2,4-Trichlorobenzene	
t(°c)	ν	t(°c)	ν	t(°c)	ν	t(°c)	ν
20	0.7427	20	0.7232	20	1.0656	20	1.4225
30	0.6592	40	0.5837	40	0.8288	40	1.0252
50	0.5156	60	0.4858	60	0.6636	60	0.7915
70	0.4148	80	0.4139	80	0.5729	80	0.6402

Table 14.Absolute Viscosity of Benzene and Monochlorobene [20]

Benzene vapor		Benzene liquid		Monochlorobenzene liquid	
t(°c)	μ(micropoise)	t(°c)	μ(millipoise)	t(°c)	μ(millipoise)
14.2	73.8	0	9	0	10.53
100	91.8	10	7.57	9.7	9.17
212.5	123	20	6.47	20.1	8
		30	5.61	25.1	7.51
		40	4.92	30.2	7.04
		60	3.89	40.2	6.29
		70	3.5	49.9	5.7
				60	5.13
				80.4	4.28
				119.6	3.07

Table 15. Surface Tension [11]

Compound	Surface tension (dyne/cm) 20°c	30°c	40°c	60°c
Benzene	28.88	27.49	26.14	
Monochlorobenzene	33.19	31.98	30.77	
1, 2 - Dichlorobenzene	37.18	36.02	34.92	
1, 3 - Dichlorobenzene	36.84	35.56	34.32	
1, 4 - Dichlorobenzene				31.33
1, 2, 4 - Trichlorobenzene	39.10	37.98	36.86	

Vapor pressure

$$\log_{10} P_v = -0.2185\ A/T + K$$

where P_v is the vapor pressure (mmHg) and T is the temperature (degree Kelvin) of benzene and chlorinated benzene compounds [30]

Table 16. Vapor Pressure

Compound	A (cal/gm mole)	K (constant)	temperature range (°c)
Benzene	10254.3	9.556	-58 to -30
	8146.5	7.833714	-36.7 to 290.3
Monochlorobenzene	10098.0	8.5	-35.0 to -15
	9067.3	7.717535	-13 to 349.8
1, 2 - Dichlorobenzene	10943.0	8.185275	20.0 to 179
1, 3 - Dichlorobenzene	10446.8	8.017555	12.1 to 173
1, 4 - Dichlorobenzene	17260.5	12.48	30 to 50
1, 2, 3 - Trichlorobenzene	11349.5	7.916468	40 to 218.5
1, 2, 4 - Trichlorobenzene	11425.1	8.030523	38.4 to 213
1, 3, 5 - Trichlorobenzene	11211	7.977218	63.8 to 208.4
1,2,3,4-Tetrachlorobenzene	12872.5	8.251056	68.5 to 254
1,2,3,5-Tetrachlorobenzene	11982.1	7.925176	58.2 to 246
1,2,4,5-Tetrachlorobenzene	12828.8	8.282213	146 to 245
Pentachlorobenzene	15124.2	8.907497	98.6 to 276
Hexachlorobenzene	15199.1	8.550497	114.4 to 309.4

Table 17. Vapor Pressure of Chlorine and Hydrogen Chloride [11]

compound	temperature range (°c)	G (constant)	K (constant)	J (constant)
HCl	-127 to -60	7.06145	710.584	255
Cl_2	-60 to critical temperature	7.91458	1146.89	315.916
		6.86773	821.107	240

For hydrogen chloride and chlorine, the Antoine equation is used

$$\log_{10} P_v = G - K\ (t + J)$$

where P_v is the vapor pressure (mmHg) and t is the temperature (°c)

Table 18. Heat of Fusion, Vaporization, and Combustion, Compressibility Factor and Specific Heat of Liquid [11]

Compound	ΔH_m (cal/g)	ΔH_v (cal/g)		ΔH_c (cal/g)	Z	liquid specific heat	
		25°c	B.P.			T(°K)	c_{P_l}/cal/g/°K
Benzene	30.09	103.57	94.14	757.52	.9596	300	.4178
						320	.4315
Monochlorobenzene	20.4	90.31	74.39		.9604	283	.298
						293.2	.3186
1, 2 - Dichlorobenzene	21.7	81.61	63.88	671.8	.9423	293	.275
						313	.298
1, 3 - Dichlorobenzene	20.55	78.96	62.79		.9510	273	.269
1, 4 - Dichlorobenzene	30.434	79.49	63.04		.9481	326	.297
1, 2, 4 - Trichlorobenzene	21.53	71.12	57.43		.9476		
Chlorine	21.59	57.14	68.8		.9652		
Hydrogen chloride	13.05		103.12		.9447		

Table 19. Chemical Thermodynamics Table (Ideal Gas State) [26]

Compound	TK	cal/(mole°K) c°p	S°	Kcal/mole H°-H° 298	ΔH° f	ΔG° f	log K p
Benzene	298	19.52	64.34	0.00	19.82	30.99	-22.714
	300	19.65	64.47	0.04	19.79	31.06	-22.623
	400	26.74	71.11	2.37	18.56	35.01	-19.126
	500	32.80	77.75	5.36	17.54	39.24	-17.152
Monochlorobenzene	298	23.43	74.92	0.00	12.39	23.70	-17.368
	300	23.57	75.07	0.05	12.37	23.76	-17.31
	400	30.62	82.84	2.77	11.46	27.71	-15.139
	500	36.49	90.33	6.13	10.74	31.86	-13.925
1, 2 - Dichloro-benzene	298	27.12	81.61	0.00	7.16	19.76	-14.485
	300	27.26	81.78	0.06	7.15	19.84	-14.452
	400	34.12	90.60	3.14	6.53	24.17	-13.207
	500	39.69	98.83	6.84	6.07	28.64	-12.518
1, 3 - Dichloro-benzene	298	27.2	82.09	0.00	6.32	18.78	-13.765
	300	27.34	82.26	0.06	6.31	18.85	-13.735
	400	34.18	91.10	3.14	5.69	23.14	-12.642
	500	39.74	99.34	6.85	5.24	27.56	-12.045
Hexachlorobenzene	298	41.90	105.45	0.00	-8.10	10.56	- 7.740
	300	42.03	105.71	0.08	-8.09	10.67	- 7.776
	400	48.08	118.67	4.60	-7.54	16.85	- 9.207
	500	52.52	129.90	9.64	-6.97	22.89	-10.003

From the "Bureau of Standard" [5], the value of k (rate constant) in liter/mole/sec, for the benzene-chlorine reaction to produce monochlorobenzene is given by the following table

Table 20. Rate Constant for Monochlorobenzene Production

t(°c)	catalyst used	k (liter/mole/sec)
24	--	1.48×10^{-6}
34.2	--	3.9×10^{-6}
24	HCl	6.7×10^{-6}

where the reaction is

$$C_6H_6 \text{ (.5 mole)} + Cl_2 \text{ (.05 mole)} \xrightarrow[\text{solvent}]{(CH_3COOH\ 99\%,\ 1\%\ H_2O)} C_6H_5Cl + HCl$$

and the rate of reaction - $K\, C_{C_6H_6}\, C_{Cl_2}$

From the kinetic study of F. Bourion [3], the effect of temperature on the ration of the rate constant is given by table 21

Table 21. Effect of Temperature on Rate Constant

t°c	K
18	.107
25	.118
35	.123

where $K = k_2/k_1$ and is defined by the following reactions

$$C_6H_6 + Cl_2 \xrightarrow[k_1]{Fe} C_6H_5Cl + HCl$$

$$C_6H_5Cl + Cl_2 \xrightarrow[k_2]{Fe} C_6H_4Cl_2 + HCl$$

APPENDIX B

Data For Binary System (benzene-monochlorobenzene)

Table 22. Density (gm/cubic centimeter) of Benzene-Monochlorobenzene System [28].

benzene mole %	0°C	50°C	benzene mole %	70°C
100	-	.8458	100	.8246
72.14	.9214	.8713	71.54	.8954
80.12	.9485	.8963	43.36	.9466
59.93	.9986	.9441	12.17	1.0275
39.80	1.0435	.9907	0	1.0521
29.52	1.0663	1.0125		
0	1.1272	1.0737		

Table 23. Refractive Index of Benzene-Monochlorobenze System [28].

20°C		25°C	
benzene mole %	η_D	benzene mole %	η_D
100	1.5006	100	1.4970
75.21	1.5059	82.07	1.5022
59.40	1.5089	63.18	1.5072
34.43	1.5149	43.27	1.5108
22.94	1.5178	22.24	1.5173
0	1.5242	0	1.5227

Table 24. Viscosity in Micropoise of C_6H_6-C_6H_5Cl System [28].

Pure benzene		77 benzene mole%		48.8 benzene mole%		29.3 benzene mole%		Pure monochlorobenzene	
t(°C)	μ	t(°C)	μ	t(°C)	μ	t(°C)	μ	t(°C)	μ
19.2	6963	20.4	7110	19.9	7588	19.7	7862	19.5	8501
19.96	6851	40.1	5469	40.2	5930	40.1	6187	30.4	7430
30.8	5989	60.0	4432	61.6	4825	60.3	5074	39.6	6695
40.0	5391			73.7	4414	74.1	4521	49.3	6069
49.7	4803							60.2	5515
60.1	4408							69.1	5092

Table 25. Surface Tension (dyne/cm) of Benzene-Monochlorobenzene System [28].

Pure benzene		52.88 benzene mole %		Pure monochlorobenzene	
t(°C)	σ(dyne/cm)	t(°C)	σ(dyne/cm)	t(°C)	σ(dyne/cm)
50.2	25.09	50.1	27.12	30.0	32.46
60.2	23.82	60.1	26.25	40.0	31.28
69.9	22.55	70.0	25.00	50.1	29.99
79.7	21.27	80.1	23.73	60.2	28.79
90.1	29.87	90.2	22.51	70.2	27.63
100.0	18.62	100.0	21.30	80.1	26.45
110.4	17.42	110.0	20.10	90.1	25.30
120.4	16.25	120.2	18.97	100.0	24.18
130.2	15.09	130.0	17.78	110.0	23.07
140.1	13.93	140.1	16.63	120.1	21.92
150.3	12.76	149.9	15.53	130.1	20.70
159.7	11.70	160.0	14.47	140.0	19.63
169.7	10.56			150.0	18.57
				160.1	17.52

benzene mole %	σ(dyne/cm)
10°C	
100	29.210
71.19	30.13
46.94	31.00
30.06	31.70
0	33.325
40°C	
0	25.361
72.67	26.16
44.54	27.27
30.18	27.99
100	29.695

Heat of mixing

1) at 67.76 mole % MCB = -0.101 cal/gram of mixture

2) at 46.7 mole % MCB = -3.6 cal/mole mixture

APPENDIX C

Data For Subroutines

Table 26. Density of Liquid Benzene and Monochlorobenzene at 298°K for Subroutine DMVSPB [28].

Monochlorobenzene mole fraction	Density (gm/cm^3)	Monochlorobenzene mole fraction	Density (gm/cm^3)
0.0	0.87288	0.39808	0.97115
0.04095	0.88351	0.44497	0.98187
0.06985	0.89103	0.56517	1.00925
0.11537	0.90263	0.68606	1.03578
0.14715	0.91013	0.80654	1.06148
0.16443	0.91481	0.87587	1.07593
0.25771	0.93763	0.94889	1.09083
0.34176	0.95781	1.0	1.10113

Table 27. Heat of Vaporization and Liquid Specific Heat for Subroutine HBCVST and VAVST [13].

temperature (°K)	C_{P_l} (cal/gm/°K)		ΔH_v (cal/gm)	
	Benzene	Monochlorobenzene	Benzene	Monochlorobenzene
294.11	0.405	0.31		
305.2	0.415	0.32		
321.88	0.43	0.335		
338.55	0.45	0.345		
353.1			94.667	
355.22	0.47	0.36	94.445	77.778
371.88	0.485	0.375	92.222	75.0
388.55	0.5	0.39	88.889	72.222
405.2	0.52	0.4	85.556	70.0

Table 28. Density of Pure Liquid Benzene (DB) and Monochlorobenzene (DC) for Subroutine DBVST [27].

T(°K)	DB(gm/cm^3)	DC(gm/cm^3)	T(°K)	DB(gm/cm^3)	DC(gm/cm^3
273	0.0006	1.12786	353	0.8145	1.0419
283	.8895	1.1171	363	.8041	1.0305
293	.879	1.1062	373	.7927	1.0189
303	.8685	1.0954	383	.7809	1.0079
313	.8576	1.0846	393	.7692	.9960
323	.8466	1.0742	403	.7568	.9836
333	.8357	1.0636	413	.7440	.9723
343	.8248	1.0526			

Table 29. Isobaric Vapor-Liquid Equilibrium for Benzene-Monochlorobenzene System at One Atmosphere for Subroutine LIXY [10]

t(°c)	x_b	y_b
131.7	0.0	0.0
126.4	0.053	0.174
121.8	0.104	0.311
115.1	0.192	0.480
108.2	0.295	0.628
102.7	0.399	0.731
97.1	0.514	0.816
93.9	0.591	0.860
90.3	0.684	0.904
89.5	0.703	0.912
86.7	0.786	0.942
86.1	0.804	0.952
83.5	0.884	0.971
80.1	1.0	1.0

DESIGN OF AN UNDERGRADUATE CHEMICAL ENGINEERING EXPERIMENT

(Chlorination of Benzene)

by

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B. S., Cairo University, 1971

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ABSTRACT

There seems to be a need for a more elaborate and complex experiment, for the undergraduate chemical engineering laboratories, which contains more than the traditional one major operation. After reviewing several chemical processes, the chlorination of benzene was chosen because it provides numerous investigations in kinetics, distillation, and process control and dynamics.

In the proposed experiment, chlorine would react with benzene in a jacketed reactor with internal cooling coils. The operating conditions of the approximately 200 cubic centimeter catalytic reactor would be:

1) temperature: 25-55°C
2) pressure: 1-5 atmosphere
3) catalyst: ferric chloride
4) benzene conversion: 10-20%

A flash tank is planned for separation of the gaseous and liquid reactor products. The liquid product, consisting of benzene and chlorinated benzene compounds, would be distilled and the distillate (mostly benzene) would be recycled to the reactor.

The steady state calculations and the operating conditions of each stream were obtained by using an iterative trial and error method, on a "PDP 11/10" mini-computer.

The design allows for manual or automatic control operation of the reactor or distillation column, individually or as a unit. A number of possible laboratory experiments are described. Allowance for direct-digital data acquisition and/or control has been included.

The total cost of the proposed experiment, excluding recording and computer equipment, would be $22,000.