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# AN ELECTRONIC ANALOG COMPUTER FOR SOLVING THE FLASH VAPORIZATION EQUILIBRIUM EQUATION

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## SUMMARY

It is the purpose of this paper to describe an electrical computer which has been constructed to solve the equations for vapor-liquid equilibrium in multi-component systems. The instrument consists of seven component-computing units each with proper indicating means and power supplies. Each unit is a resistance network with a voltage matching servomechanism, and each provides an output voltage proportional to the mol-fractions for vapor and liquid phases. These voltages are summed and matched with a reference voltage to provide the solutions. Any reasonable number of such units may be put together to make a computer. The theory and operation of the computer is discussed. A number of applications and examples of computer results are given. The computer yields the over-all vapor or liquid fraction to a probable error of 0.002. An interpolation method is described which reduces the probable error to 0.0002.

## INTRODUCTION

The process known as Flash Vaporization may be described as follows: A mixture of known composition of relatively volatile components is allowed to come to thermodynamic equilibrium at some given temperature and pressure by any path whatsoever. In general, a vapor and a liquid phase will be present at equilbrium. The problem is to determine the fractions of the mixture in the vapor and liquid phases, and to determine the mol fractions of the various components in each phase. The relations that exist between these various quantities at equilibrium are well known and will be given later. These equations are difficult to solve, yielding only to trial-and-error methods.

The virtues of the analog computer are its speed and the automatic character of its calculations. The device is operated by turning a crank which varies the value of v, the total vapor fraction. This actuates a number of servomechanisms which perform automatically all computations.

This computer facilitates the solution of such problems as (to mention a few): Analysis of separator operation, studies of changes in composition of reservoir fluids with pressure decline, and analysis of natural gasoline plant operation. Examples of some of these problems are given in detail later.

## STATEMENT OF THE PROBLEM

The essential equations are

$$x_m = \frac{z_m}{1 + (K_m - 1)v} \quad . \; . \quad (1)$$

$$y_m = \frac{K_m z_m}{1 + (K_m - 1)v} \quad . \; . \quad (2)$$

$$\sum_{m=1}^{n} x_m = \sum_{m=1}^{n} \frac{z_m}{1 + (K_m - 1)v} = 1 \quad . \; . \; . \; . \; . \; . \; . \quad (3)$$

$$\sum_{m=1}^{n} y_m = \sum_{m=1}^{n} \frac{K_m z_m}{1 + (K_m - 1)v} = 1 \quad . \; . \; . \; . \; . \; . \; . \quad (4)$$

where

$y_m$ = $V_m/V$ = Mol fraction of m-th component in vapor phase.
$x_m$ = $L_m/L$ = Mol fraction of m-th component in liquid phase.
$z_m$ = $F_m/F$ = Mol fraction of m-th component in mixture.
$K_m$ = $y_m/x_m$ = Equilibrium constant for m-th component at the given temperature and pressure.
v = V/F = Mol fraction of vapor in the mixture.
F = Total mols of a mixture of n components.
V = Total mols of vapor in the mixture.
L = Total mols of liquid in the mixture.
$F_m$ = Total mols of m-th component.
$L_m$ = Mols of m-th component in liquid phase.
$V_m$ = Mols of m-th component in vapor phase.

Assuming the total mols of the mixture F and its composition (all the $F_m$) to be known — either from a quantitative analysis or from the amounts put together to make the mixture — the $z_m = F_m/F$ may be regarded as known quantities. From the given temperature and pressure of the mixture the $K_m$ are known (principally from experimental data). The primary problem is then: having given all the $z_m$ and $K_m$ to calculate v and all the fractions $x_m$ and $y_m$. Having calculated these ratios, it is a simple matter to calculate V, L, $V_m$, $L_m$ from their defining equations.

## SOLUTION OF THE PROBLEM

### Basic Computer Unit

The computer consists of n units, each of which provides voltages $xE_o$ and $yE_o$ proportional to x and y as in

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Equations (1-4). Fig. 1 shows the basic computing unit with the connections made for the case where $K<1$. Fig. 2 shows the same basic computing unit with connections made for the case where $K>1$. Certain modifications of this basic circuit are made for special values of K and v which render the basic circuit of Fig. 1 and 2 insensitive. Description of these modifications will be omitted. Provision is made for adding the voltages $x_mE_o$, or $y_mE_o$, for varying each voltage and hence their sum, and by means of a ganged variation of v for balancing the sum $\Sigma x_mE_o$ or $\Sigma y_mE_o$ to equal the line voltage $E_o$. When balance is attained by finding the correct value of v, cancellation of $E_o$ yields Equation (3) or (4). The corresponding value of v which can be read from a dial is then the solution of (3) or (4).

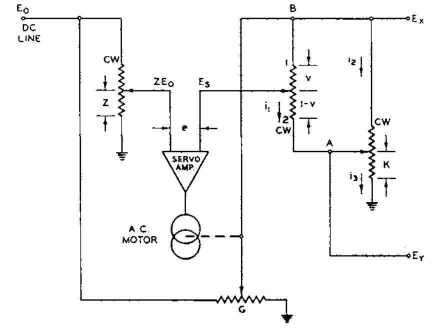

FIG. 1 — BASIC COMPUTER UNIT CIRCUIT FOR K<1 AND MODERATE VALUES OF "v".

## Computing Unit — Case Where K<1

The basic unit for providing the voltage $E_x = xE_o$ (and $E_y = yE_o$) for the case where $K<1$, is shown in Fig. 1. Four potentiometers marked x, v, G, K are connected as shown. The given fractions z and K are set by means of dials (calibrated to 0.1 per cent and which can be estimated by eye to 0.01 per cent). The potentiometer v is set by hand (and ganged with the v potentiometer of all other units so that the same value of the fraction v is simultaneously set on all units). The contact on the G potentiometer is set automatically by means of a servomotor. This motor is driven by an AC amplifier. The amplifier is actuated by the difference in voltages $zE_o$, from the contact on the z potentiometer, and $E_s$, from the contact on the v potentiometer. If $E_s<zE_o$, the motor moves the G contact to a position of higher voltage and raises the potential $E_s$. If $E_s>zE_o$, the motor moves the G contact to pick off a lower potential and reduces the $E_s$ potential. In either case, the motor quickly positions the G contact so that

$$E_s = zE_o \quad . \; . \; . \quad (5)$$

an equation which we are now justified in using with the circuit equations below.

The following circuit equations, where R is the (large) resistance of the v potentiometer and r is the (small) resistance of the K potentiometer, are obvious:

$$Ri_1 = B - A \quad . \; . \; . \quad (6)$$

$$(1-K)ri_2 = B - A \quad . \; . \; . \quad (7)$$

$$Kri_3 = A \quad . \; . \; . \; . \quad (8)$$

$$i_1 + i_2 = i_3 \quad . \; . \; . \; . \quad (9)$$

$$E_s = vA + (1-v)B \quad . \; . \; . \; . \; . \; . \quad (10)$$

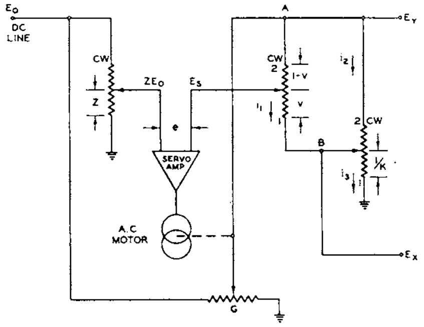

FIG. 2 — BASIC COMPUTER UNIT CIRCUIT FOR K>1 AND MODERATE VALUES OF "v".

Eliminating $i_1$, $i_2$, $i_3$, and $E_s$ from the Equations (5-10), and solving for B and A, we have

$$B = \frac{zE_o[1 + K(1-K)\rho]}{[1 + (K-1)v] + K(1-K)\rho} \quad . \; . \; . \; . \; . \quad (11)$$

$$A = \frac{zE_o[K + K(1-K)\rho]}{[1 + (K-1)v] + K(1-K)\rho} \quad . \; . \; . \; . \; . \quad (12)$$

where

$$\rho = r/R \quad . \; . \; . \; . \; . \; . \; . \quad (13)$$

This ratio of the resistance, r, of the potentiometer, K, to the resistance, R, of the potentiometer, v, will be taken so small that the parts of (11) and (12) containing $\rho$ can be reglected. Hence, to a sufficient approximation $B = E_x$ and $A = E_y$, where

$$E_x = \frac{zE_o}{1 + (K-1)v} \quad . \; . \quad (14)$$

$$E_y = \frac{KzE_o}{1 + (K-1)v} \quad . \; . \quad (15)$$

## Computing Unit — Where K>1

The basic unit for a $K>1$ is the same unit as for $K<1$, but the setting of potentiometer, K is as shown in Fig. 2, and the connections to the potentiometer, v are reversed. The servomechanism sets potentiometer, G, as before so that Equation (5) is satisfied. The circuit equations differ slightly from Equations (6-10), but follow the pattern above and result in the same Equations (14) and (15).

## Computer Assembly

The basic computing unit will be represented, for convenience, by the block shown in Fig. 3. The units are assembled as shown schematically in Fig. 4. Each output potential $E_x$, or $E_y$, is placed on one end of a high resistance R′. The other ends of these resistances are connected to a common lead whose potential is E, and which is connected to one terminal of a galvanometer M. The current, $i_m$, of the m-th unit through R′ is given by $x_mE_o - E = R'i_m$. The currents, $i_m$, will add; hence, summing the last equation from 1 to n, we have

$$E_o \sum_{m=1}^{n} x_m - nE = R' \sum_{m=1}^{n} i_m \quad . \; . \; . \; . \; . \quad (16)$$

A potential $E_o/n$ is placed on the other terminal of the galvanometer. The ganged contacts on the v potentiometers are adjusted by hand until the galvanometer M reads zero. When this condition is attained $\sum_{m=1}^{n} i_m = 0$ and the last equation reduces to $E_o \sum_{m=1}^{n} x_m = nE$. But $nE = E_o$, and cancelling these equal factors, we have $\sum_{m=1}^{n} x_m = 1$ and

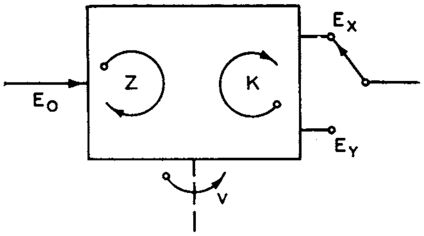

FIG. 3 — BASIC COMPUTING UNIT.

the v, so obtained, is the required solution of Equation (3).*

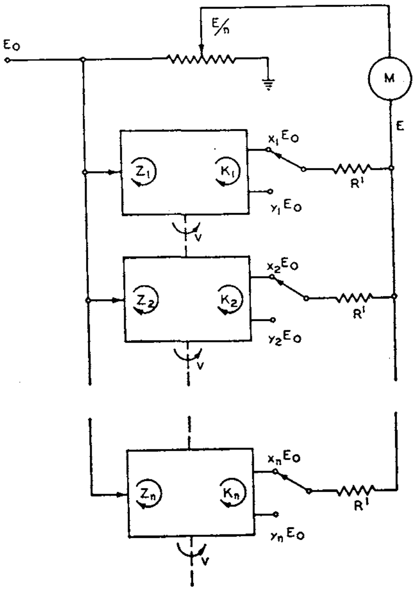

FIG. 4 — SCHEMATIC ASSEMBLY OF COMPUTER.

If the adding resistances R' be switched to the other output terminals $yE_o$ of the computing units, and if v be adjusted so that M reads zero, then v is the solution of the equation $\sum_{m=1}^{n} y_m = 1$, namely, the solution of the equivalent Equation (4). The two values of v should agree.

For conciseness, the complete wiring diagrams of this computer are omitted. For the same reason, we omit details concerning the sensitive units, the servomechanism details, the manual of operation, and design data.

The computer is packaged for convenience of operation and maintenance. The general arrangement is shown by the photographs (Figs. 5-7).

## APPLICATIONS AND EXAMPLES

A few applications of this computer should be of interest.

### Determination of Optimum Separator Operating Conditions

Just what is considered optimum may vary considerably. For instance, it may be desirable to obtain a maximum of stock tank liquid from a given crude; or, it may be desirable to maintain the gas composition uniform when a gas line is being fed from several separators. Since the crude composition, the temperature and pressure of the stock tank, and separator temperature are beyond control there remains only the separator pressure which may be varied to yield the desired product out of the separator. A series of flash calculations may, therefore, be made at different pressures intermediate between reservoir pressure and stock tank pressure. A second calculation gives the stock tank liquid and vapor compositions. That operating pressure is then selected which satisfies the requirements of the problem in question.

### Evaluation of Reserves

Evaluation of reserves involves a study of changes in composition of the reservoir fluids during the life of a field. If the flash vaporization process is adopted as a simplifying assumption for small pressure increments, then this computer can be used as an aid in making such a study. Two general cases arise in this connection: (1) gas-condensate reservoirs, and (2) oil fields with gas-saturated crude. In either case, if the initial compositions of the phases present are known, and a reliable set of K constants is available, then the effect of pressure decline on composion may be calculated and an evaluation of recoverable fluids made. That is, the amount of condensation of heavy components with pressure decline can be calculated in the first case, or the loss of solution gas with pressure decline can be calculated in the second case.

### Natural Gasoline Plant Calculations

At every stage where the pressure and/or temperature of the product is changed in natural gasoline plant operation, and natural gas processing, the flash vaporization process is involved, at least as a simplifying assumption, if not in fact. In cases where complete

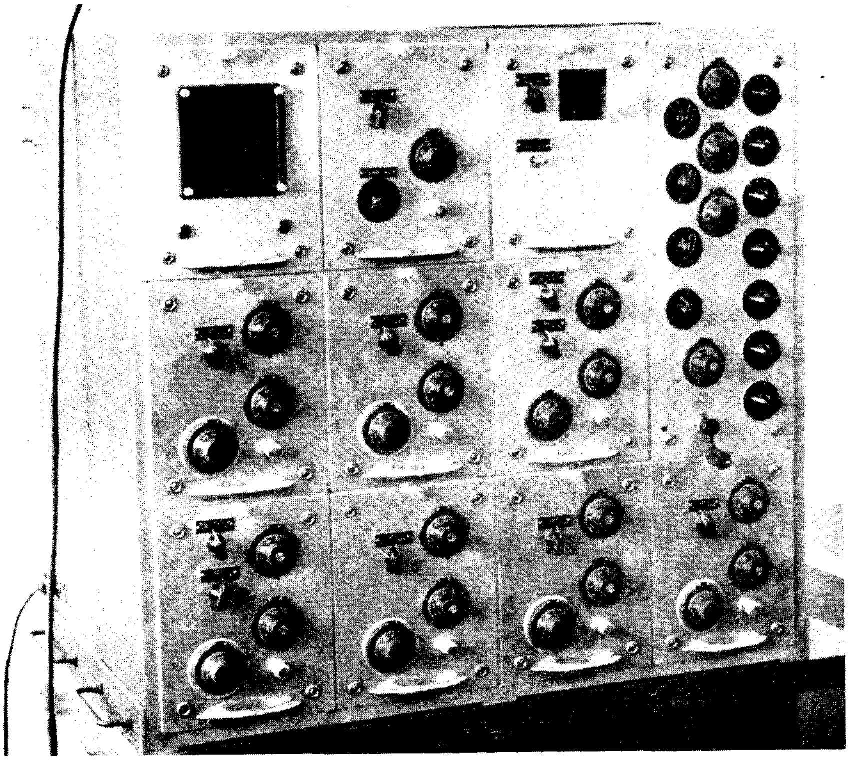

FIG. 5 — VAPOR LIQUID EQUILIBRIUM COMPUTER FRONT VIEW.

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* The current, $i_m$, drawn from the $X_mE_o$ terminal of Fig. 1 is drawn from the G potentiometer and does not disturb in any way the rest of the circuit. If the current, $i_m$, is drawn from the $Y_mE_o$ terminal, this current must pass through a portion of the K-potentiometer and consequently $i_2$ in Fig. 1 will be disturbed. This effect is negligible, however, since the adding resistance R' is very large (500,000 ohms) compared with the 500 ohm K-potentiometer. This disturbing effect is further reduced by the fact that the voltage at the opposite end of R' is limited to $E_o/n$. This reduces the voltage drop across R' and hence the current through it.

Similar considerations lead to the conclusion that this disturbing effect is also negligible when the connections shown in Fig. 2 are used.

equilibrium between liquid and vapor does not exist, conditions do differ from the ideal, but the fundamental calculations must be made before the deviations can be determined. The computer may be used to make these fundamental calculations.

## Estimation of K Values

In the case of each of these applications only the straight forward operation of the computer is involved. However, other interesting variations are possible. One in particular was employed in this laboratory during the course of some PVT work. A quantity of reservoir fluid was equilibrated in a PVA cell. A portion of the vapor phase was bled off and analyzed. This process was repeated at constant temperature in a series of equal pressure steps. It was desirable to know the distribution of the components in the vapor and liquid states at each of the pressure points involved. The known quantities were initial composition of sample, weight per cent of total sample of vapor bled off, and composition of the vapor bled off. This process is a differential vaporization process, but if the pressure increments are small, flash vaporization calculations may be made as a first approximation. Such calculations will yield the desired information provided a reliable set of K-constants is available. In this particular case, the values of the K-constants for the heaviest components were in doubt, although the values for the lighter components were fairly well established. Before the desired information could be derived from the data, it was necessary, therefore, first to establish the values of the K-constants for the heaviest component. This is readily accomplished through the use of this computer.

The initial composition of the sample was set up on the Z-dials. The K-values at the temperature and pressure in question were set up on the K-dials using an approximate value for the seventh component ($C_7$). The computer was balanced to determine v and the vapor fraction of $C_7$ noted and compared with the experimental value obtained from the analysis of that portion of the vapor phase bled off. Since only an approximate value of $K_7$ was used, the computed $C_7$ vapor fraction differed from the experimental value. By resetting the $K_7$ dial and readjusting the v-dial for balance, a $K_7$ was found which would cause the computed $C_7$ vapor fraction to equal the experimental value. This process was repeated at each new pressure making allowance for the weight fraction of the sample bled off as a vapor. In this way a satisfactory set of $K_7$ values was obtained and the vapor-liquid distribution of each component at each pressure was obtained. The same results could have been obtained by cut-and-try methods, but probably would not have been attempted because of the time required to make such tedious calculations.

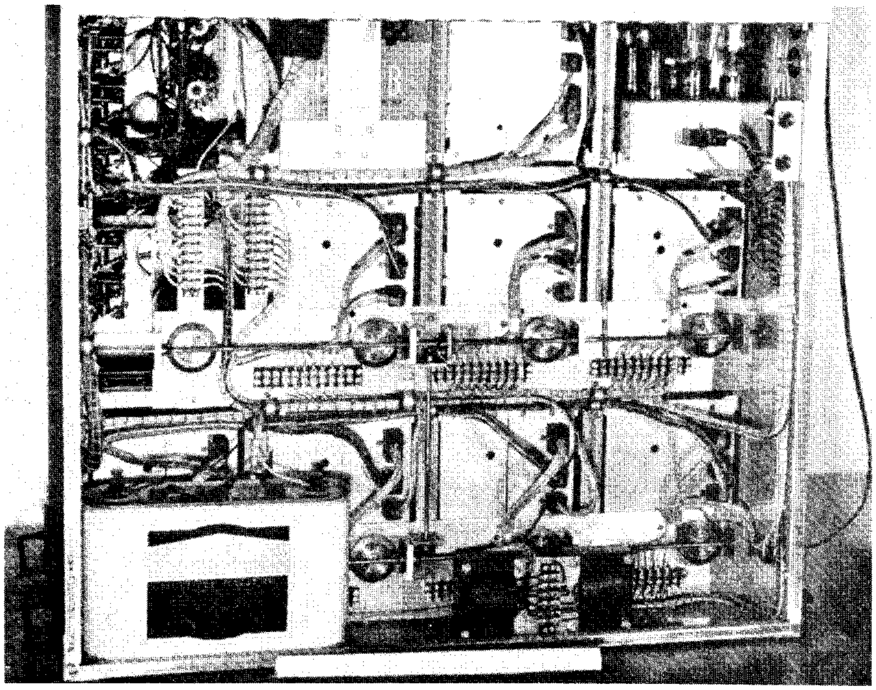

FIG. 6 — COMPUTER WITH BACK PANEL REMOVED.

## Examples

As an example of the more usual type of problem solved with this computer, the results of a typical run are shown in Table I, together with a comparison between results obtained by the trial-and-error method and those obtained with the computer. The time required to make a complete calculation, including determining v and reading all liquid $x_m$ and vapor $y_m$ fractions is about ten minutes.

## Error Studies

An evaluation of the accuracy of this computer has been made using data of the same type as that shown in Tables I and II. The results are shown in Fig. 8 and Table III. Fig. 8 is a frequency distribution curve of differences between computer and trial-and-error values of liquid and vapor fractions. Table III lists certain factors characterizing the frequency distribution of errors for this computer.

It will be noted that the standard deviation from the mean is $\sigma = .0015$. Accordingly, 68.3 per cent of the errors may be expected to fall in the range $+.0002 \pm .0015$. This range is indicated on the frequency curve in Fig. 8.

A similar comparison of the computer values of v with those obtained by the trial-and-error method for 20 examples indicates that the probable error is $\pm 0.0020$.

Percentage errors have not been used in these studies, since the magnitude of the errors appears to be more or less uniform throughout the scale ranges. This would result in large percentage errors at small scale readings and small percentage errors at large scale readings. It was felt, therefore, that percentage errors would not give a true measure of the accuracy to be expected of this computer.

## Second Approximation

The value of v as computed by this instrument may be considered a first approximation. The figures, just given, on the accuracy will then be a measure of the closeness of this approximation. If greater accuracy is desired, the computer may also be used to give a second approximation. This is accomplished by means of an interpolation formula and two additional readings on the instrument. This formula is

$$\epsilon_o = F \frac{v_2 - v_1}{|G_1| + |G_2|} \beta$$

in which

$v_1$ is a v-dial setting less than that required for balance ($v_1 < v_o$)

$v_2$ is a v-dial setting greater than that required for balance ($v_2 > v_o$)

$G_1$ is the galvanometer deflection in scale divisions corresponding to $v_1$

$G_2$ is the galvanometer deflection in scale divisions corresponding to $v_2$

F is a proportionality constant found to be 336.5

$$\beta = 1 - \sum_{m=1}^{n} \frac{z_m}{1 + (K_m - 1) v_o}$$

$\epsilon_o$ is the correction to be applied to $v_o$ to give the second approximation, $\bar{v}$, to the correct value of v, thus

$$\bar{v} = v_o + \epsilon_o$$

In the example given in Table I the quantities in the interpolation formula were found to be

$v_1 = .480$ $G_1 = +2$ $v_o = .4837$
$v_2 = .490$ $G_2 = -3$ $F = 336.5$
$\beta = .001755$

$$\epsilon_o = 336.5 \frac{.01 \times .001755}{5}$$

$$= \frac{336.5 \times 1.755 \times 10^{-5}}{5}$$

$$= 12 \times 10^{-4} = +.0012$$

$$\bar{v} = .4837 + .0012 = .4849$$

This value compares favorably with the trial-and-error value of .4850.

Eight similar examples were calculated as outlined above and gave results with an average probable error of 0.0002.

The additional time required to make the second approximation is largely that required to calculate $\beta$, which is a straight-forward operation, and the time required depends on one's skill with a desk calculator. The time required to make the two pairs of readings of $V_1$, $G_1$ and $V_2$, $G_2$ is negligible.

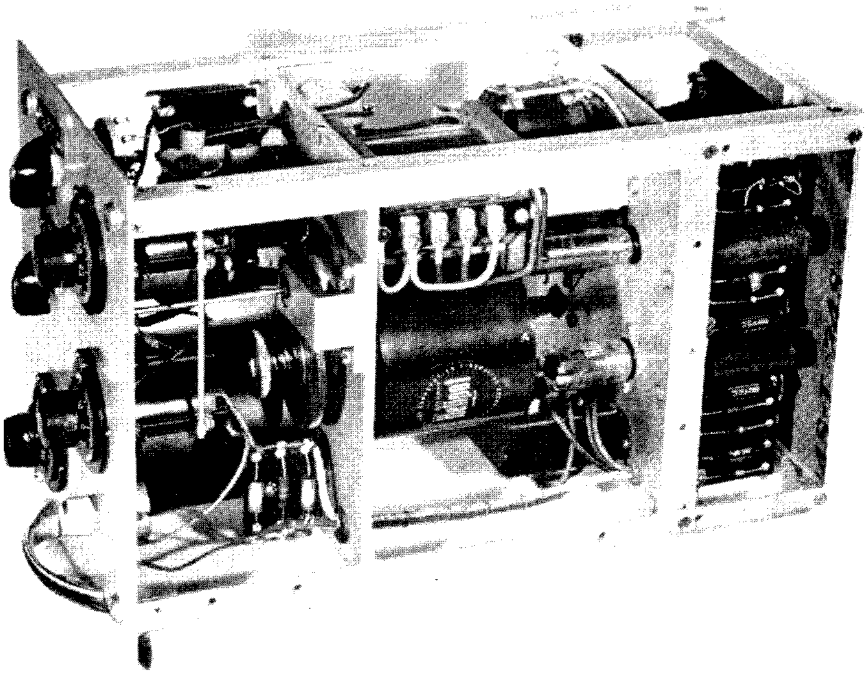

FIG. 7 — SINGLE COMPUTING UNIT.

### Table I

### Sample Problem with Comparison of Results

| Component Number | $z_m$ | $K_m$ | Computer Values $x_m$ | Computer Values $y_m$ | Trial-and-Error Values $x_m$ | Trial-and-Error Values $y_m$ | Differences $\Delta x_m$ | Differences $\Delta y_m$ |
|---|---|---|---|---|---|---|---|---|
| $C_1$ | .2085 | 173.0 | .0040 | .4285 | .0025 | .4277 | +.0015 | +.0008 |
| $C_2$ | .1185 | 21.0 | .0123 | .2328 | .0111 | .2327 | +.0012 | +.0001 |
| $C_3$ | .1069 | 5.35 | .0350 | .1834 | .0344 | .1840 | +.0006 | −.0006 |
| $C_4$ | .0776 | 1.67 | .0585 | .0970 | .0586 | .0979 | −.0001 | −.0009 |
| $C_5$ | .0590 | 0.46 | .0800 | .0372 | .0799 | .0368 | +.0001 | +.0004 |
| $C_6$ | .0485 | 0.162 | .0805 | .0142 | .0817 | .0132 | −.0012 | +.0010 |
| $C_7$ | .3810 | 0.0105 | .7300 | .0090 | .7318 | .0077 | −.0018 | +.0013 |
| Totals | 1.0000 | | 1.0003 | 1.0031 | 1.0000 | 1.0000 | | |

v (Computer value) = 0.4837 v (Trial-and-error value) = 0.4850

Table II shows another example. In this case one of the K's is large (247) and the v is small (0.0060), a case which calls for the use of one of the sensitive units not described in this paper.

### Table II

### Sample Problem Using One of the Sensitive Units

| Component Number | $z_m$ | $K_m$ | Computer Values $x_m$ | Computer Values $y_m$ | Trial-and-Error Values $x_m$ | Trial-and-Error Values $y_m$ | Differences $\Delta x_m$ | Differences $\Delta y_m$ |
|---|---|---|---|---|---|---|---|---|
| $C_1$ | .0025 | 247 | .0013 | .2474 | .0010 | .2470 | +.0003 | +.0004 |
| $C_2$ | .0111 | 30 | .0096 | .2840 | .0095 | .2809 | +.0001 | +.0031 |
| $C_3$ | .0344 | 7.6 | .0332 | .2460 | .0331 | .2500 | +.0001 | −.0040 |
| $C_4$ | .0586 | 2.4 | .0575 | .1372 | .0581 | .1394 | −.0006 | −.0022 |
| $C_5$ | .0799 | .66 | .0797 | .0525 | .0800 | .0528 | −.0003 | −.0003 |
| $C_6$ | .0817 | .23 | .0815 | .0196 | .0821 | .0189 | −.0006 | +.0007 |
| $C_7$ | .7318 | .01 | .7355 | .0122 | .7362 | .0110 | −.0007 | +.0012 |
| Totals | 1.0000 | | .9983 | .9997 | 1.0000 | 1.0000 | | |

v (Computer value) = .0054 v (Trial-and-error value) = .0060

Table III

Factors Characterizing the Frequency Distribution Curve of Errors

Arithmetic Mean Error ($\overline{X}$) = + .0002
Quadratic Mean Error (RMS) = ± .0015
Median Value = + .0004
Mode = + .0005
Standard Deviation ($\sigma$) from the Mean ($\overline{X}$) = ± .0015
(Approximately the RMS)

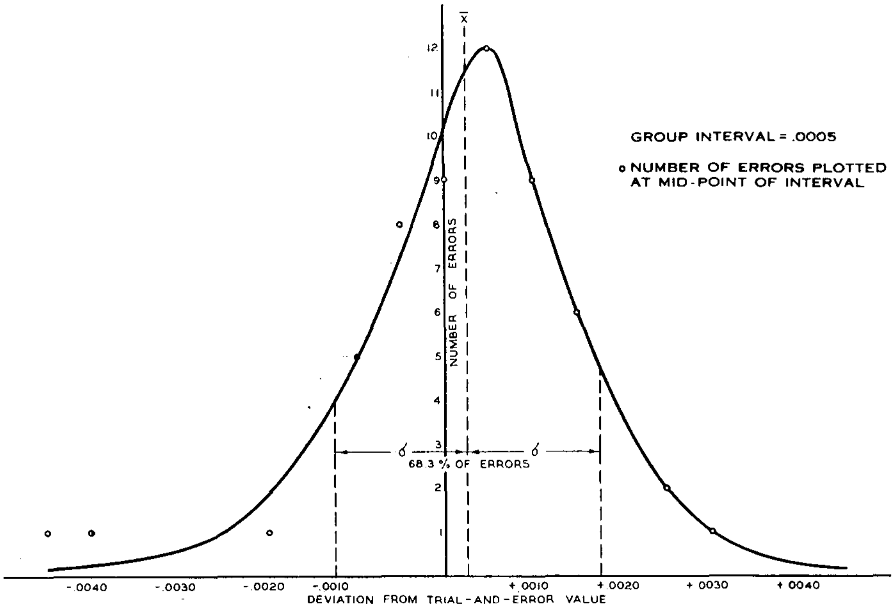

FIG. 8 — FREQUENCY DISTRIBUTION CURVE OF ERRORS IN $X_m$ AND $Y_m$.

## Use of the Sensitive Units

Special values of K and V which render the basic circuit insensitive are:

(a) $K \rightarrow 0$ and $V \rightarrow 1$
(b) K very large ($1/K \rightarrow 0$) and $V \rightarrow 0$

Condition (a) exists when one or more components are relatively involatile but are present only in small quantities. In such a case the denominators in Equations (14) and (15) approach zero and the units become insensitive. This occurs for values of $K < .01$ and of $V > .99$.

Condition (b) exists when one or more components are very volatile but are present in only small quantities. This is the case for the second example given. Because of the difference in connections shown in Figs. 1 and 2 the relative positions of the K and V potentiometers are the same as for condition (a) and the sensitive unit must be used. This occurs for values of $K > 100$ and of $V < .01$.

## CONCLUSION

An electronic analog computer has been described which provides a solution to the vapor-liquid equilibrium problem. The computed value of v has a probable error of 0.0020 in the first approximation and 0.0002 in the second approximation. The operation is simple and rapid. In thus speeding up the solution, the way is opened for the application of the method to problems which would not otherwise be undertaken because of the amount of time required to obtain a solution. ★ ★ ★