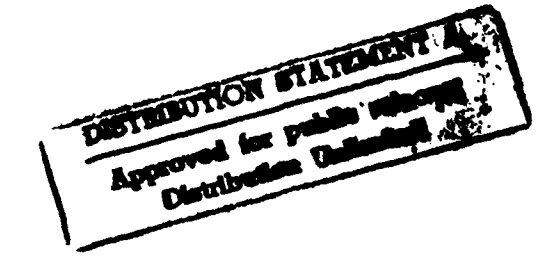

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18 December 1961

A SOLUTION OF THE SYSTEM OF NONLINEAR ALGEBRAIC BALANCE EQUATIONS OF GAS-MIXTURE BY "UNIVAC-60" DIGITAL COMPUTING MACHINE

by N. Parezanovic and J. Petric

- Yugoslavia -

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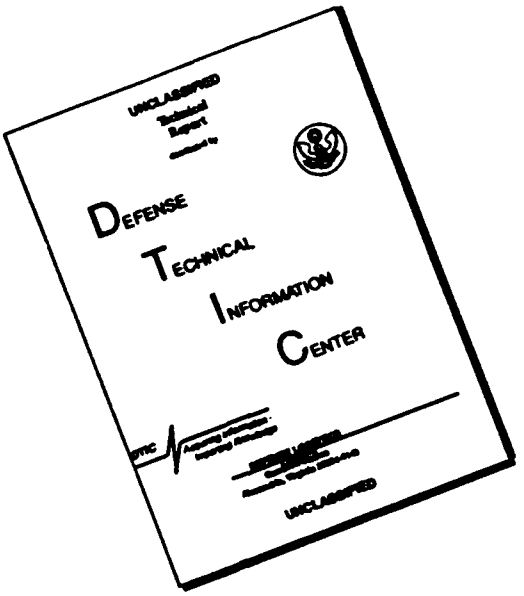

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A Solution of the System of Nonlinear Algebraic Balance Equations of Gas-Mixture by "Univac-60" Digital Computing Machine(*

- Yugoslavia -

[Following is the translation of an article by N. Parezanovic and J. Petric in Vasiona, No 4, 1960, Belgrade; pp 120-123.]

Summary of the Whole Article

Solution of the problem of finding the balance of a gaseous mixture is rather frequently encountered both by chemical engineers and chemists dealing with rocket propellant research. This problem is defined by a nonlinear system of algebraic equations the computation of which is a lengthy and tiresome numerical job. The numerical solution of such a problem by desk computing machine requires several days of work for each separate solution and is, of course, subject to human errors made by the calculator himself. It, therefore, became apparent that the use of digital computing machine was indispensable. So far, this problem has been tackled by high memory capacity computing machines, but since many of the engineers dealing with it cannot have such machines made readily available, the author believes that they should be given a method of solving the problem by employing the optimum efficiency of low-capacity digital computing machines. A complete solution is given here for all components of the solution, this being the most complicated part of the problem. No numerical difficulties should be experienced by using the calculated components for plotting the (i, s) T-diagrams.

(Concluding Part) *

The cards were organized in such a way that it was not necessary to transfer information from one card to the other, nor was it necessary to order the cards. This means that once the cards are ready and the machine starts computing, the process continues until the whole work is finished. Three to four corrections were done for every solution; the program was, however, constructed in

* [This is a concluding part of the article. The preceeding part(s) appeared in an issue(s) of Vasiona which is not available at this time.]

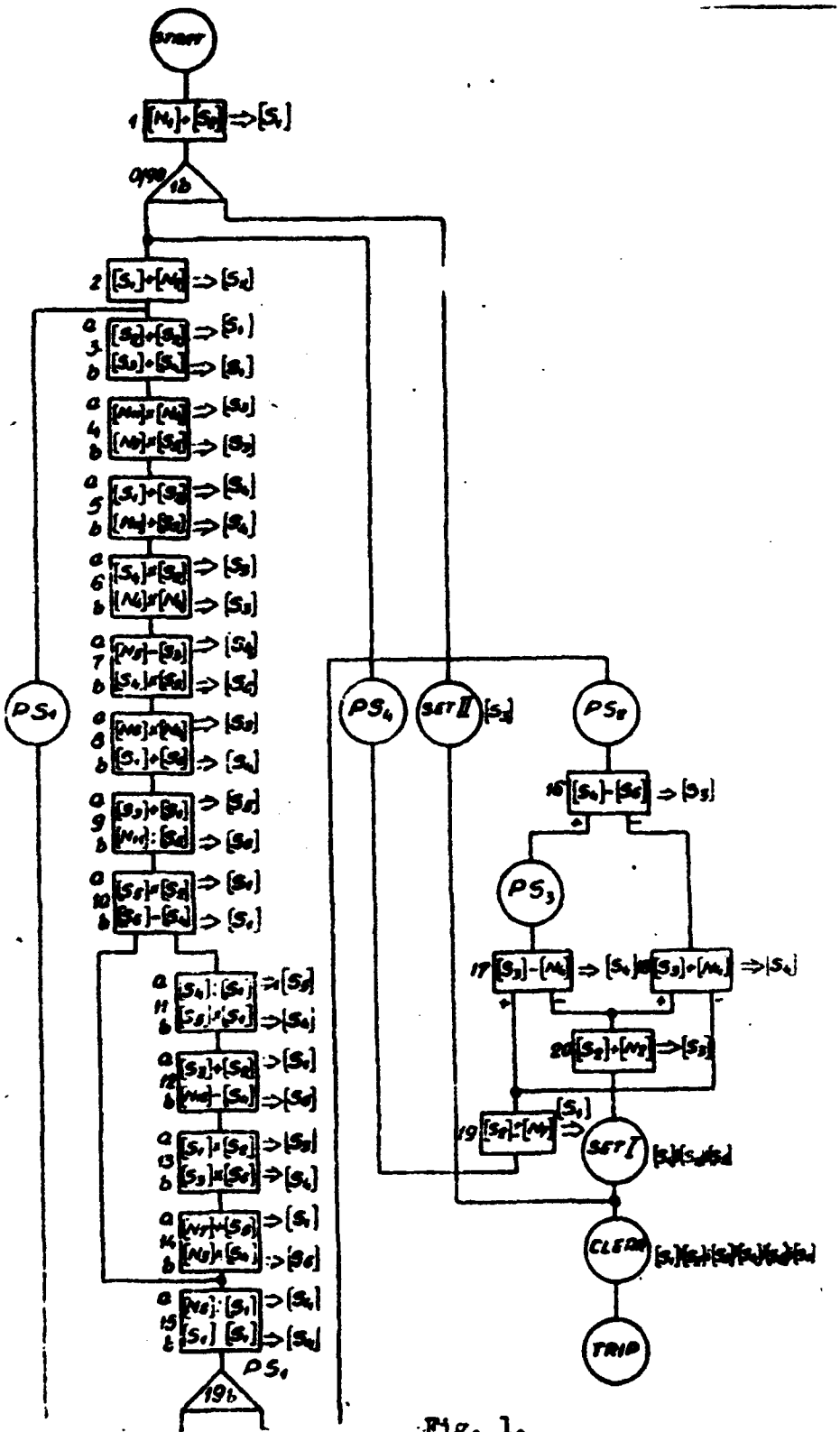
START
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
SET II
SET I
CLEAR
TRIP

Fig. 1.

such a way that it permitted an arbitrary number of corrections. If one performs k corrections to achieve one solution, one has to take k + 1 cards. Note that only the first card should carry (0/90) and the assumed values $X^{\sharp}$ and δ.

The problem of equilibrium in the gaseous mixture is of such a nature that one has to find components of the composition of a similar group of problems where a_i's are fixed constants while K_i's are variable parameters. Let us take n to represent the number of similar problems and k to denote the number of corrections leading to the solution of each problem, then the total number of cards used for the solution of the similar group is n x (k + 1). Only the first card among those used has punched the assumed $x^{\sharp}$ value. Since in one similar group there exist n similar problems whose cards are ordered following decreasing or increasing values of K_i, it seems convenient to use the corrected value for $x^{\sharp}$ from the previous problem as the assumed value for the next problem of the same group. This means that the computed value for $x^{\sharp}$, i.e. x, obtained in the first correction serves as the assumed value for the next correction.

Assuming the value $x^{\sharp}$ instead of x, one introduces one of the big simplifications into the solution of this problem. In this way, the solution is obtained much faster, the setting-up of the program is much simpler, and the use of the memory is much more economical. One can conclude from the large number of problems solved using the UNIVAC-60 that each solution requires one minute of time.

Fig. 1 shows the flow diagram for program I. One should mention that during the calculation of the first correction of $x^{\sharp}$ one does not erase the storages S_2 and S_3 which permits, as mentioned earlier, that the computed value for $x^{\sharp}$ from the previous problem can be used as the assumed value for the next problem belonging to the same similar group of problems. When computing the second, third, etc., correction one should erase the storages S_2 and S_3.

The program selector PS_1 permits a selection of data in program steps 3-15 and together with PS_2 and PS_4 makes the iterative process of $x^{\sharp}$ correction possible, while the PS_3 determines if one has to increase or decrease the $x^{\sharp}$ values during the correction. On Fig. 2 are indicated the connections between various selectors used in program I.

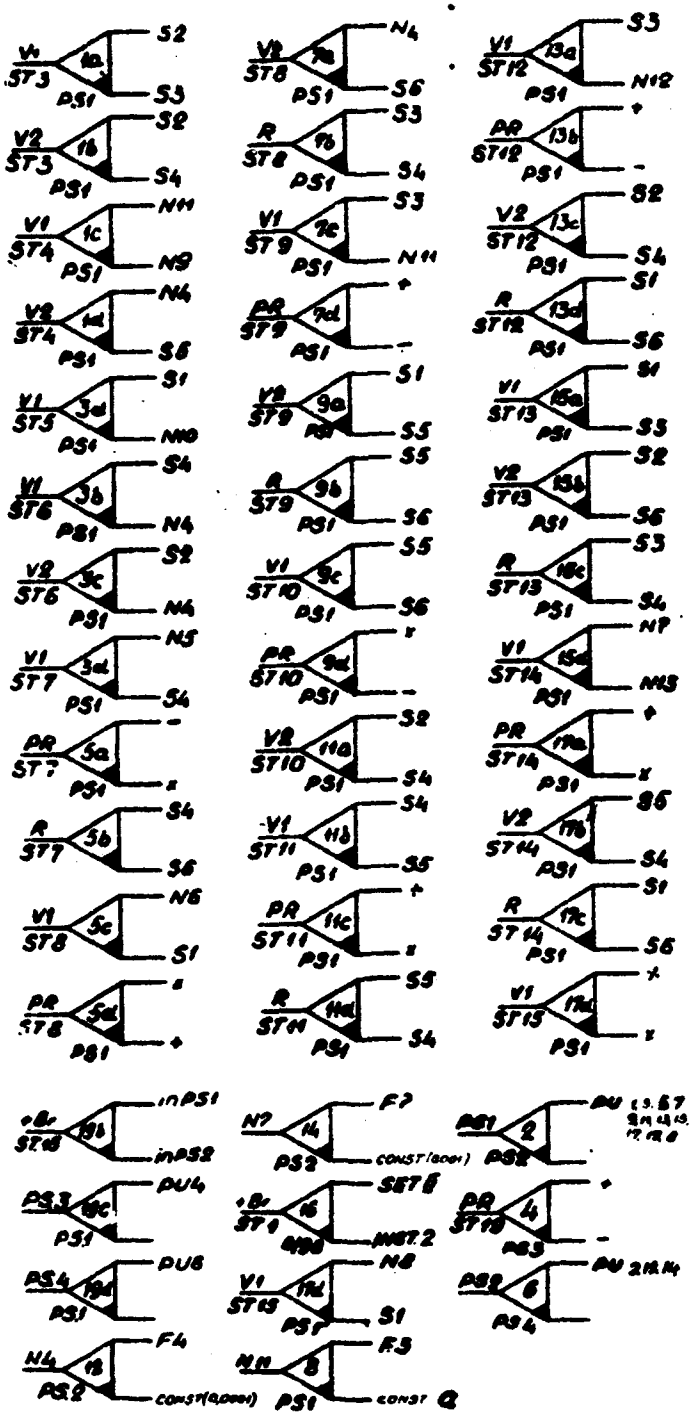

Fig. 2.

Elements and storages used for program I contain the following values.

$[N_1] \Rightarrow X^{\frac{1}{2}}$ assumed

$[N_2] \Rightarrow 0$

$[N_3] \Rightarrow \frac{K^2_3}{2}$

$[N_4] \Rightarrow \left(\frac{\sigma}{p}\right)^{\frac{1}{2}}$ (i.e.) $F = 10^{-4}$

$[N_5] \Rightarrow a_1$

$[N_6] \Rightarrow K_{10}$

$[N_7] \Rightarrow K_1$. i.e., 10^{-3}

$[N_8] \Rightarrow a_3$

$[N_9] \Rightarrow 2\,K_6$

$[N_{10}] \Rightarrow K_7$

$[N_{11}] \Rightarrow K_9$. i.e., a

$[N_{12}] \Rightarrow a_4$ (1)

$[S_1] \Rightarrow Z$

$[S_2] \Rightarrow X^{\frac{1}{2}}$ calculated

$[S_3] \Rightarrow X^{\frac{1}{2}}$ calculated

$[S_5] \Rightarrow y$

Values taken off the cards are

$$X^{\frac{1}{2}} \text{ass.. } K_1, \frac{K^2_3}{2}, 2K_6, K_7, K_9, K_{10}; \left(\frac{\sigma}{p}\right)^{\frac{1}{2}} \qquad (2)$$

while the values from the program plates are

$$a_1;\ a_3;\ a_4;\ a;\ o;\ 0.001 \text{ and } 0.001 \qquad (3)$$

The flow diagram for program II is presented in Fig. 3. The first step in this program should allow the switching of selector 2 if there is (0/90). If this step is missing, it could happen that the selectors do not change to the "selector" position

and the program could proceed in the wrong way. The result of the 13th program step operation is always negative and is utilized for punching the (1/90). The program will be executed beyond this step

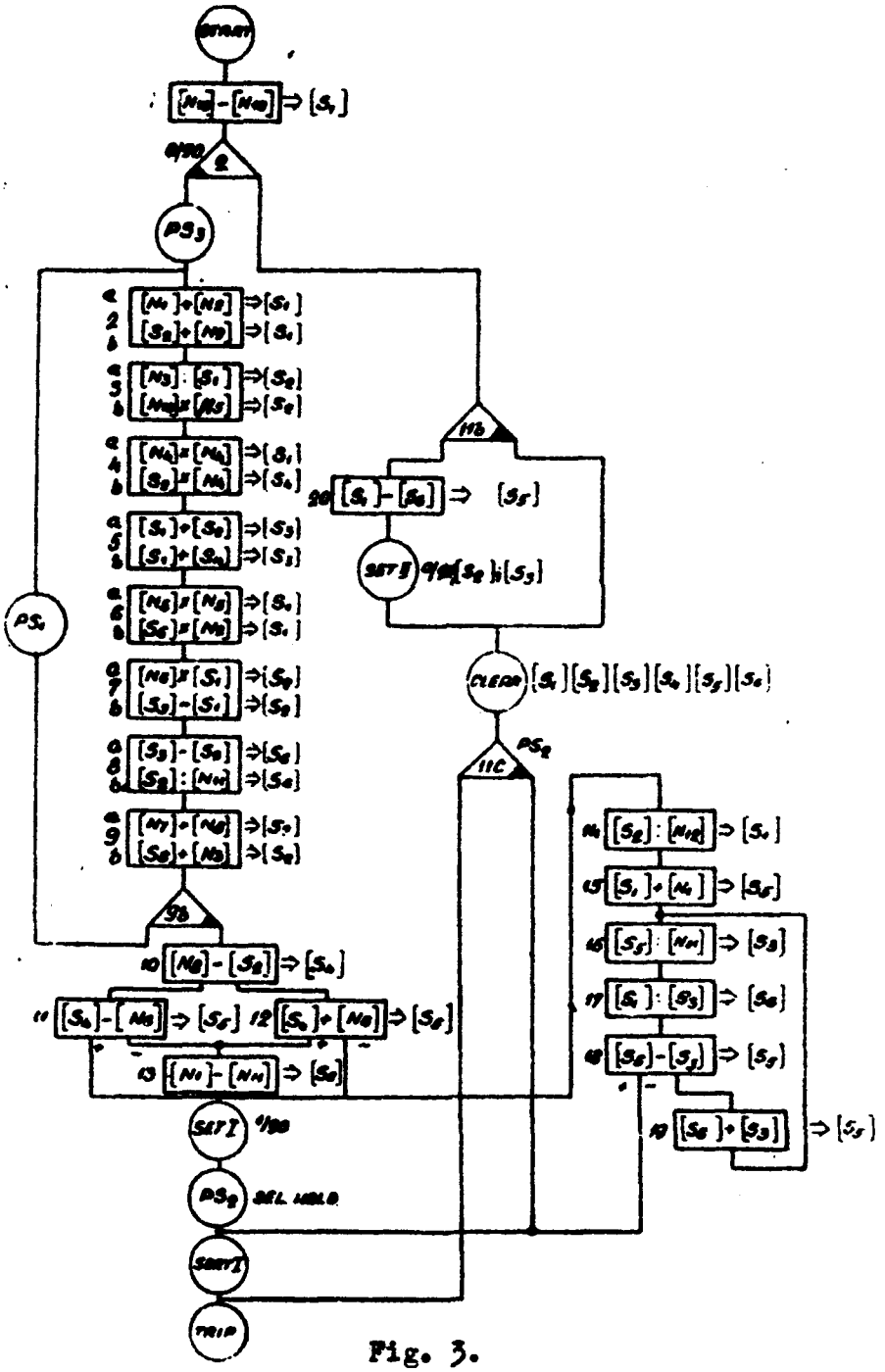

Fig. 3.

only if the value for δ obtained satisfies the required accuracy. Otherwise, the machine computes $(\delta/p)^2$ and the card is sorted out. For the following cards, from the group of cards for a single solution, the program passes or does not pass through the 20th program step depending on the fact was the (1/90) punched on the previous card, i.e., does the solution satisfy the required accuracy or not. If the previous solution requires further correction, the following card is punched with $(\delta/p)^2$ calc., δ calc., and $(^{o}_{90})$

since the result of the arithmetic operation in the 20th program step is always negative. The connection with SEL. HOLD is broken when PS3 enters the operation. Fig. 4 shows the connection of the selector 11a and 4 which are used to maintain selectors 11b and 11c on the selector side after the TRIP command.

Fig. 4.

Elements and storages used in program II contain the following values

$[N_1] \Longrightarrow K_3$ (i.e.) 1

$[N_2] \Longrightarrow y$

$[N_3] \Longrightarrow a_3$

$[N_4] \Longrightarrow X^{\frac{1}{2}}$ calculated

$\left[N_5\right] \Longrightarrow \left(\frac{\sigma}{p}\right)^{\frac{1}{2}}$

$[N_6] \Longrightarrow K_7$ (i.e. $|\sigma p - \sigma_i| = 0.004$

$[N_7] \Longrightarrow a_1$

$[N_8] \Longrightarrow \sigma$, (i.e. a

$[N_9] \Longrightarrow a_4$

$[N_{10}] \Longrightarrow K_9$

$[N_{11}] \Longrightarrow 2$

$[N_{12}] \Longrightarrow p$

$[S_2] \Longrightarrow \sigma$

$\left[S_3\right] \Longrightarrow \left(\frac{\sigma}{p}\right)^{\frac{1}{2}}$ (4)

This program uses elements $x^{\frac{1}{2}}$, Y, K_1, K_7, K_9, δ calc., and $(\delta/p)^{\frac{1}{2}}$ from the card, and a_1, a_3, a_4, a, p, 2, 1, and 0.004 from the program plates.

Fig. 5 indicates the connections between individual selectors used in the program II.

The flow diagram for program II is shown on Fig. 6. This program is utilized after the solutions are found for x, y, and z from all problems. These solutions are punched on cards with the (1/90) label and after each such card one should insert two empty cards which will be punched with the x_i (i = 1, 2,...., 10) solutions. During the first passage will be calculated and punched the values for x_3, x_4, x_5, x_6, and x_8, while the second passage will yield x_1, x_2, x_7, x_9, x_{10}. The program for finding these ten components is constructed after Equations (17-26). Elements and storages used contain the following values:

$$
\begin{aligned}
&[N_1] \Longrightarrow \left(\frac{\sigma}{\rho}\right)^{\frac{1}{2}} && [N_{10}] \Longrightarrow a_2\\
&[N_2] \Longrightarrow 2K_8 && [N_{11}] \Longrightarrow 2\\
&[N_3] \Longrightarrow y && [N_{12}] \Longrightarrow a_4\\
&[N_4] \Longrightarrow Z && [S_1] \Longrightarrow X_8, \text{ (i.e.) } X_9\\
&[N_5] \Longrightarrow K_{10} && [S_2] \Longrightarrow X_5, \text{ (i.e.) } X_{10} \qquad (5)\\
&[N_6] \Longrightarrow K_7 && [S_3] \Longrightarrow X_6, \text{ (i.e.) } X_7\\
&[N_7] \Longrightarrow K_9 && [S_4] \Longrightarrow X_3, \text{ (i.e.) } X_1\\
&[N_8] \Longrightarrow X^{\frac{1}{2}} && [S_5] \Longrightarrow X_4, \text{ (i.e.) } X_8\\
&[N_9] \Longrightarrow K_1
\end{aligned}
$$

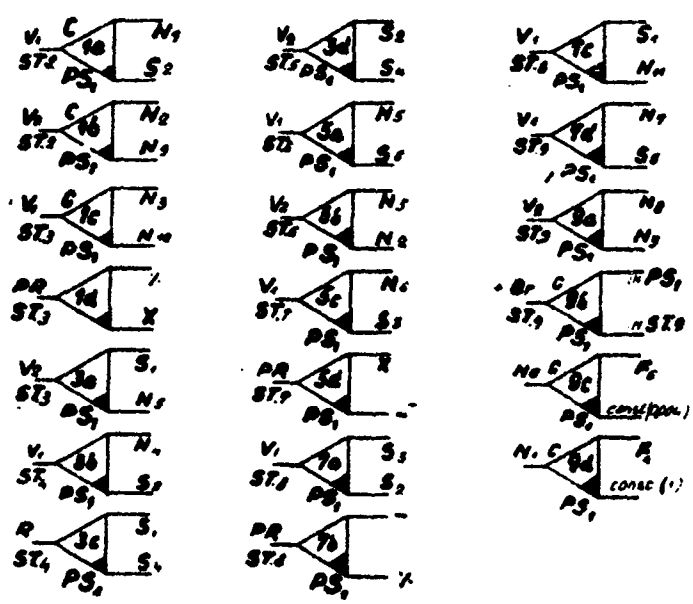

Fig. 5.

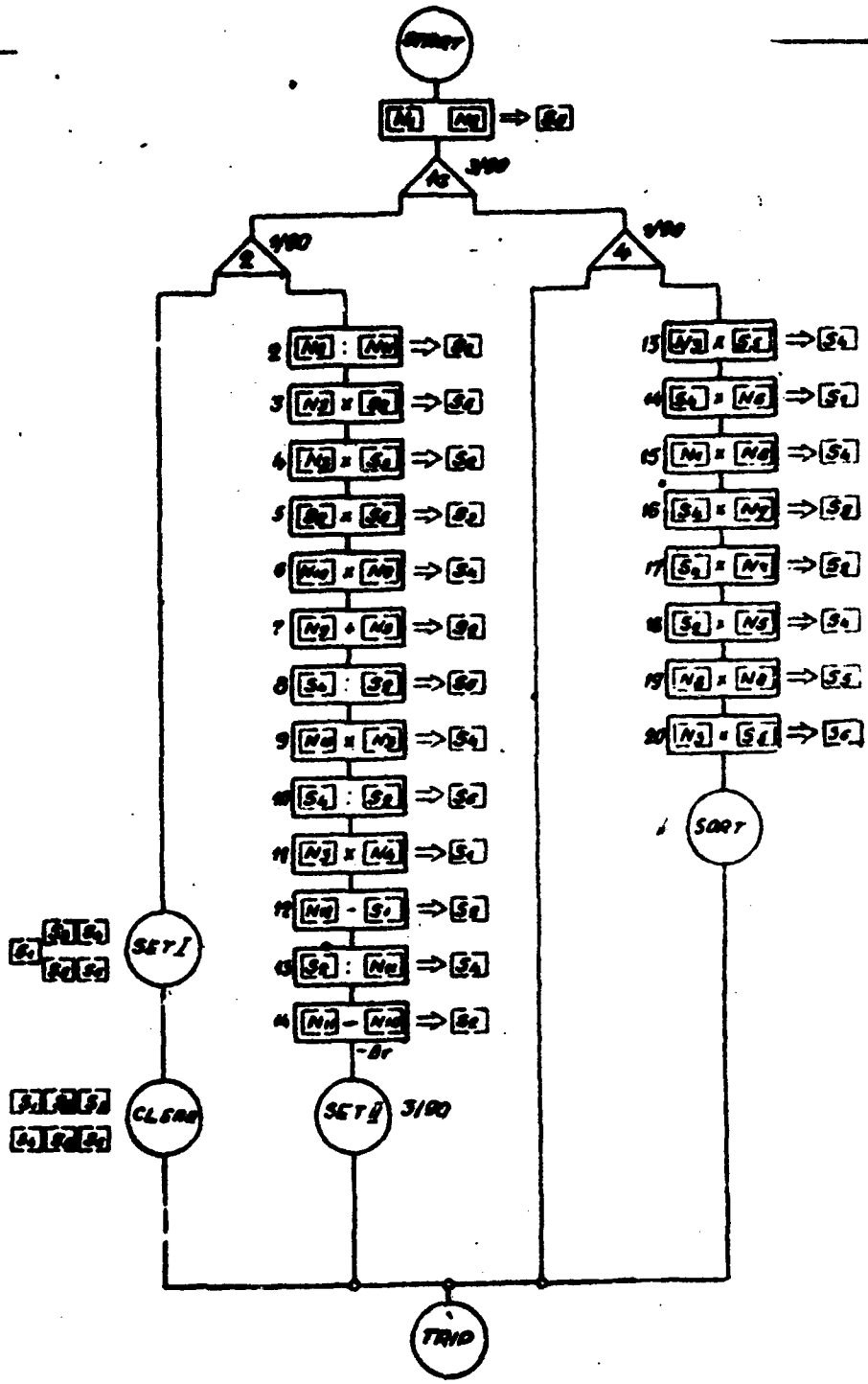

Fig. 6

From the cards are utilized the values of $x^{\frac{1}{2}}$, y, z, K_1, $2K_6$, K_7, K_9, K_{10}, and $(d/p)^2$, while the plates supplied a_3, a_1, and 2.

Fig. 7 indicates the connection between individual selectors used in the program III.

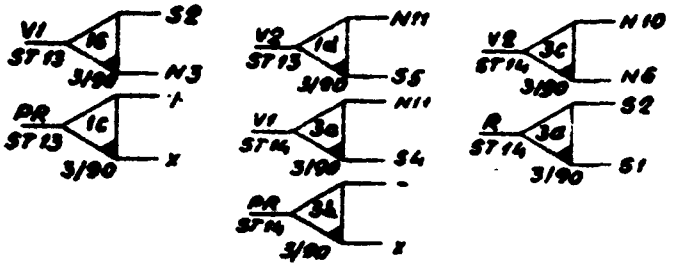

Fig. 7.

VI - Conclusion

This article presents the possibility of solving the problem of equilibrium in a gaseous mixture using digital computers with small capacities of memories. The working equations are given in a convenient form which allows a substantial saving of program steps independently from the type of digital computer used for the solution of this problem. The assumption of $x^{\frac{1}{2}}$ instead of x was of great help during the solution of working equation. After finding all the components of the composition of the gaseous mixture one can consider as solved the bulk of the numerical calculation required for the practical application of this problem. Further numerical work does not present any difficulty.

2376

- END -