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A SOLUTION OF THE SYSTEM OF BALANCE EOUATIONS OF GASEOUS COMBUSTION PRODUCTS BY „UNIVAC-60" DIGITAL COMPUTING MACHINE

I — SUMMARY

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 non-linear 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 machines 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 to them, the authors believe that there 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.

II — INTRODUCTION

The problem at issue has been dealt with by quite a number of authors, all of whom proceeded from the well known system of nonlinear algebraic equations used to define the balance of a gaseous mixture. Some variations may be noted in the mathematical treatment of this problem by different authors, such variations being the result of different approaches to the problem as well as different methods used for this purpose [1—3]. The so-called method of trial-and-error has been used most frequently and it has also been used in this paper. Up till now, the problem involved has been solved by employing either the desk computing machines or the high me-

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mory digital computing machines, both of which types of computing machines, most certainly, having their disadvantages. The digital computing machines of higher memory capacity are not readily available to a majority of experts engaged with this kind of problem.

However, it is of considerable interest to show that the smaller digital computing machines, operating at their optimum efficiency, can be used most successfully by engineers who study the matter.

For successful solution of the system of non-linear algebraic balance equations for a gaseous mixture by means of the UNIVAC-60 computing machine, it is necessary to draw particular attention to the optimum efficiency of the memorycapacity feature of the machine as well as the transformation of the working equations. The former of these requirements is allowed for by the proper employment of selectors, while the latter is fulfilled by writing the working equations in a more suitable form, which is very useful in establishing operating programmes.

This paper brings forth a complete solution for all components of the system, this being the most complicated numerical part of the whole job. Further employment of the results obtained for practical purposes, such as plotting the (i, s) T-diagrams, does not create any numerical difficulties and therefore will not be dealt with by this paper. It has been felt that it will be superfluous to discuss the thermodynamical and chemical aspects of the problem, particularly because these questions have already been treated by numerous other authors.

Logical schedules have been used in establishing the working programme for the machine. This method of approaching the setting up of the programme enables an easy and quick establishment of the basic idea of the programme. In these schedules details which may hinder complete anticipation of the problem are omitted. The logical schedule has been drawn up for the entire problem and does not apply to any particular machine. Since, however, such a programme could not have taken up by a single pair of programme discs of the UNIVAC-60 computing machine, it has been broken down into three parts. It was particularly important to include in the first pair of discs the iteration method of working out the unknown quantities from the working equations. The next part of the programme is working out the sum in view of the anticipated value of this sum. The number of corrections depends on the accuracy required and usually is not higher than 4. The third and last part of the programme is in fact the working out of all the ten components of a given system.

The current schedules of the entire programme are given for UNIVAC-60 with complete arrangement instructions for storage and selectors.

III — MATHEMATICAL BASIS OF THE PROBLEM

For the mathematical treatment of this problem, a start will be made from the well known equations (1 through 10) without going into their origin, which may be found in many reference books and papers by a number of authors who have so far dealt with the problem of stability of a gaseous mixture. These equations take the following form:

$$\frac{n_{H_2O}\, n_{CO}}{n_{H_2} n_{CO_2}} = K_1 \ (1), \quad \frac{n_{NO}\, n_{H_2}}{n_{N_2}^{1/2}\, n_{H_2O}} = K_3\left(\frac{\sigma}{p}\right)^{1/2} (2), \quad \frac{n_{H_2}^2\, n_{O_2}}{n_{H_2O}^2} = K_6\left(\frac{\sigma}{p}\right) (3),$$

$$\frac{n_{H_2} \cdot n_O}{n_{H_2O}} = K_7\left(\frac{\sigma}{p}\right) (4), \quad \frac{n_H}{n_{H_2}^{1/2}} = K_9\left(\frac{\sigma}{p}\right)^{1/2} (5), \quad \frac{n_{H_2}^{1/2} \cdot n_{OH}}{n_{H_2O}} = K_{10}\left(\frac{\sigma}{p}\right)^{1/2} (6),$$

$$2n_{H_2} + 2n_{H_2O} + n_{OH} + n_H = H \ (7),$$

$$n_{H_2O} + n_{CO} + 2n_{CO_2} + 2n_{O_2} + n_{NO} + n_{OH} + n_O = O \ (8),$$

$$n_{CO} + n_{CO_2} = C \ (9), \quad 2n_{N_2} + n_{NO} = N \ (10).$$

In these equations, there are variables, constants and parameters as well as the sum

$$\sigma = n_{H_2} + n_{H_2O} + n_{CO} + n_{CO_2} + n_{O_2} + n_{N_2} + n_{OH} + n_{NO} + n_O + n_H.$$

They are listed together with the corresponding mathematical symbols in the following table.

Table 1. — Translation of the chemical notations into mathematical notations

Variables	Constants	Parameters
$n_{H_2} \to x_1$	$H \to a_1$	K_1
$n_{H_2O} \to x_2$	$O \to a_2$	K_3
$n_{CO} \to x_3$	$C \to a_3$	K_6
$n_{CO_2} \to x_4$	$N \to a_4$	K_7
$n_{O_2} \to x_5$	$p \to p$	K_9
$n_{N_2} \to x_6$		parameters dependant upon the temperature
$n_{OH} \to x_7$		
$n_{NO} \to x_8$		
$n_O \to x_9$		
$n_H \to x_{10}$		

By using the symbols from Table 1, the equations (1 through 10) will yield, when the terms x_3, x_4, x_5, x_6, x_7, x_9 and x_{10} have been eliminated, the following three equations:

$$x_2 = \frac{a_1 - 2x_1 - K_9(\sigma/p)^{1/2} x_1^{1/2}}{2 + \dfrac{K_{10}(\sigma/p)^{1/2}}{x_1^{1/2}}}, \tag{11}$$

$$x_8 = a_2 - a_3 \frac{K_1 x_1 + 2x_2}{K_1 x_1 + x_2} - x_2\left\{1 + \frac{K_{10}(\sigma/p)^{1/2}}{x_1^{1/2}} + \frac{K_7(\sigma/p)}{x_1}\right\} - 2K_6\left(\frac{\sigma}{p}\right)\left(\frac{x_2}{x_1}\right)^2, \tag{12}$$

$$\frac{2x_8^2 x_1^2}{K_3^2(\sigma/p)\, x_2^2} + x_8 - a_4 = 0\,, \tag{13}$$

where x_i ($i = 1,2,\ldots,10$) are the components of $\sigma = \sum_{i=1}^{10} x_i$

Thus, the problem of solving the system of non-linear algebraic equations (1 through 10) has been reduced to solving the equations (11 through 13) instead.

However, the equations (11 through 13) in their present form are not very suitable for programming on the low memory capacity computing machines.

Therefore, they are transformed into a more suitable form, such as

$$y = \frac{a_1 - x^{1/2}[2x^{1/2} + K_9(\sigma/p)^{1/2}]}{x^{1/2}[2x^{1/2} + K_{10}(\sigma/p)^{1/2}]}\,, \tag{14}$$

$$z = \frac{a}{y} - \frac{a_3}{K_1 + y} - x^{1/2}\left[x^{1/2} + K_{10}\left(\frac{\sigma}{p}\right)^{1/2} - \frac{\sigma}{p}(K_7 + 2K_6 y)\right], \tag{15}$$

$$F(y,z) \equiv z^2 - \frac{K_3}{2}\left(\frac{\sigma}{p}\right)(a_4 - yz) = 0\,, \tag{16}$$

where

$$x = x_1\,,\ y = \frac{x_2}{x_1}\,,\ z = \frac{x_8}{\frac{x_2}{x_1}} \qquad \text{and} \qquad a = a_2 - a_3\,.$$

We have called these equations working equations, and they will prove to be more convenient for programme making than their previous form (equations 11 through 13) has ever been. Computing the factors x, y and z from Equations (14 through 16) may be accomplished with sufficient accuracy by applying the so-called trial-and-error method, which consists in the following: one assumes the value for $x^{1/2}$ in Eq. (14) and works out the value for y, while Eq. (15) produces the value for z by introducing into Eq. (15) the assumed values for $x^{1/2}$ and x, and the previously computed value for y. Thus, for the computed values for y and z, with assumed value for $x^{1/2}$, Eq. (16) should be fully satisfied. The values for x, y and z obtained on the basis of assumptions, as shown above, will be the solutions for Equations (14 through 16). If the values for x, y and z be such that using Eq. (16), $|F(y,z)| \leqq 10^{-4}$, the system components will be sufficiently accurate. There are several values for x, y and z which may satisfy the condition of $|F(y,z)| \leqq 10^{-4}$ but the first of them to satisfy this condition will be discharged by the machine as the result of the problem.

Computation of the system components is most conveniently carried out by the following equations:

$$x_1 = x \quad (17), \qquad x_2 = x \cdot y \quad (18),$$

$$x_3 = \frac{a_3 K_1}{K_1 + y} \quad (19), \qquad x_4 = \frac{a_3 y}{K_1 + y} \quad (20),$$

$$x_5 = K_8 \left(\frac{\sigma}{p}\right) y^2 \quad (21), \qquad x_6 = \frac{a_4 - yz}{2} \quad (22),$$

$$x_7 = K_{10} \left(\frac{\sigma}{p}\right)^{1/2} x^{1/2} y \quad (23), \qquad x_8 = y \cdot z \quad (24),$$

$$x_9 = K_7 \left(\frac{\sigma}{p}\right) y \quad (24), \qquad x_{10} = K_9 \left(\frac{\sigma}{p}\right)^{1/2} x^{1/2} \quad (26).$$

If greater accuracy is required for the system components $x_i (i=1,2,...,10)$ the value for $|F(y, z)|$ should be chosen to be as low as possible. To do this, particular attention should be paid to the respective amounts by which $x^{1/2}$ and x are corrected in Equations (14 through 16).

An expression for σ is readily obtainable from Equations (17 through 26) in the following manner:

$$\sigma = \frac{1}{2}\left\{a_1 + a + a_4 - y\left[x + \frac{a_3}{K_1 + y} - K_7\left(\frac{\sigma}{p}\right)\right] + K_9\left(\frac{\sigma}{p}\right)^{1/2} x^{1/2}\right\} + a_3 . \quad (27)$$

This expression for σ is very useful for programmes making, as it does not make it necessary to work out the system components x_i $(i=1,2,..., 10)$ until the required accuracy for σ is obtained.

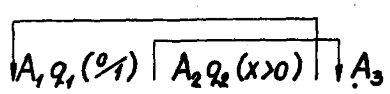
IV — LOGICAL SCHEDULES

The problem of programme making has been tackled by means of logical schedules, since they permit an easy understanding of the problem in its entirety as well as of the method used to solve it.

An effort has been made to reduce the number of symbols in these schedules to a minimum without neglecting the need for making the logical schedules clear. The symbols used in the logical schedules are as follows:

A_i — Arithmetic operation (one or more arithmetic operations).

q_i — Conclusion which may affect the course of the programme. An explanation is given in brackets after the symbol q_i, as to what kind of conclusion is in question. Provided the condition given in the brackets is fulfilled, the programme is continued with the next operation in the same line. If this is not the case, the programme is directed to the operation indicated by the arrow. The condition in the brackets may consist either of a perforated hole in the card or of any result of mathematical operations. For example, in the logical schedule



the condition q_1 is to be understood as meaning that if there is a zero in the first column of the card, the programme should be transferred to the arithmetical operation A_2. If, on the other hand, there is no zero in the first column, the programme goes over to the arithmetical operation A_3. In the same logical schedule, the condition q_2 has the following meaning: if $x > 0$, the programme is passed over to the mathematical operation A_3, and, if however, $x \leq 0$, the operation A_1 is carried out instead.

S — sorting out sequence. A card bearing this symbol is directed to the sorting storage space.

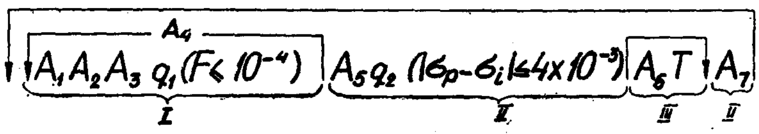
$\downarrow$ — perforation, the object of perforation being given in brackets following the symbol.

C_i — storage cancellation.

T — card discharge and end of programme.

η_i — programe is following the path indicated by the arrow only.

A complete logical schedule for the solution of a system of nonlinear algebraic equations of balance in a gaseous mixture may be written in the following form:



In this schedule, A_1 represents the group of arithmetical operations needed to compute y by means of the first working equation, A_2 represents the arithmetical operation needed to compute z, while A_3 denotes the arithmetical operations of the third working equation.

The conclusion q_1 refers to the degree of accuracy with which a check is made of the condition $|F(y, z)| \leq 10^{-4}$ by means of the third working equation. If $|F(y, z)| \leq 10^{-4}$, σ may be worked out; if not, however, a correction of $x^{1/2}$ is made by the operation A_4 and the procedure just outlined follows anew.

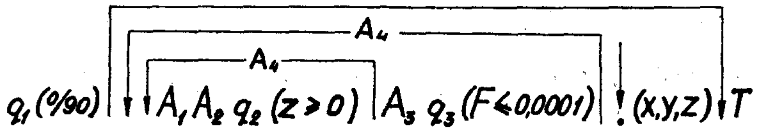
Having completed the computation of σ_i, (A_5), a check is made, by comparing the value of σ_i with the previous σ_p, whether it satisfies the condition or not. If $|\sigma_p - \sigma_i| \leq 4 \times 10^{-8}$ as worked out by the operation (A_5), the computation of all the ten components of the system (A_6) may start, thus completing the programe (T). If the condition is not satisfied, then the term $(\sigma/p)^{1/2}$ (A_7) should be worked out and the procedure is repeated until a satisfactory result is obtained.

For the logical schedule given above, the computation programme could not have been made out on a single pair of UNIVAC-60 programme cards, so it was divided into three parts, I, II and III.

The first pair of the programme cards (I) contain the corrections of the assumed values for $x^{1/2}$ and x, until the condition $|F(y, z)| \leqq 10^{-4}$ is fulfilled. The second pair of the programme cards (II) provides for the computation of σ and its corrections until the prescribed condition is fulfilled. Thus, the entire numerical operation of determination of x, y, z, σ and $|F(y, z)|$ satisfying the required accuracy, is solved on two pairs of programme cards. It should be noted here, that this is the most complicated part in solving this problem. The working out of values for each component of the system should not make any difficulty since the equations for their solutions are very simple. This can be carried out by the third pair of programme cards (III).

Logical Schedule for Programme I

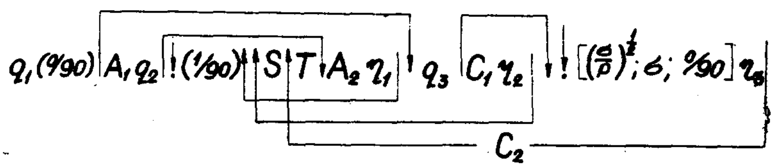
A more complete logical schedule for programme (I) should be given in the form:



where q_1 denotes that the programme is to be continued depending on whether the card contains a zero in the ninetieth column (0/90), or not. For each solution, $k+1$ card are required for k corrections, and only the first card from that set has (0/90). A_1 are the arithmetical operations needed to work out y, A_2 those for z, A_3 for F, and finally A_4 is an arithhemical operation to correct $x^{1/2}$ and x. Since physical conditions impose a restriction that all the values or x_i ($i=1,2,...,10$) be positive, then q_2 is a condition for working out F from the third working equation, provided that $z \geqq 0$ from the second working equation. By means of q_3 a check is made to see whether the values for $x^{1/2}$ and x, computed by means of the assumed values for y and z, do satisfy the condition that F from the third working equation is such that $|F(y, z)| \leqq 10^{-4}$.

Logical Schedule for Programme II

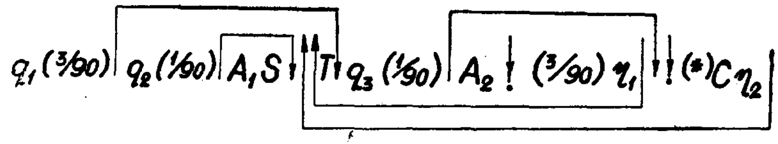
This schedule may be written as follows:



where q_2 denotes a check whether σ is satisfactory or not. If it is, a perforation is made of sign 1 in the ninetieth column (1/90). If it is not, the calculation of $(\sigma/p)^{1/2}$ is taken out. It is important to note that the card which satisfies both F and σ receives the (1/90) performation, thus providing for the final selection of the (1/90) card, only bearing solutions satisfying the condition. The symbol q_3 means that the programme is to be taken out depending on whether the previous card received the (1/90) perforation or not. If the card contains (1/90), the storages are cancelled and the programme is completed. If it does not, perforations of $(\sigma/p)^{1/2}$, σ and (0/90) are required for the next correction. C_1 and C_2 both denote cancellations.

Logical Schedule for Programme III

A logical schedule for the computation of all system components x_i $(i=1,2,...,10)$ can be written in this way:



where A_1 denotes computation procedures for x_1, x_2, x_7, x_9 and x_{10} while A_2 denotes such procedures for x_3, x_4, x_5, x_6 and x_8 $\downarrow$(*)-denotes perforation of x_3, x_4, x_5, x_6, x_8 and (3/90) as well as x_1, x_2, x_7, x_9, x_{10} and (3/90).

V — EMPLOYMENT OF THE UNIVAC-60 MACHINE

The UNIVAC-60 is an electronic computing machine operating on the perforated cards principle. It consists of an electronically powered arithmetical unit and an input-output unit partly mechanical, partly electronic. The operation speed depends upon the arithmetical operations which take place. The length of time required for individual operations is as follows:

addition	10 msec	
subtraction	10 msec	
multiplication	50 msec	for two five-digit numbers
division	50 msec	for two five-digit numbers

The length of time for mechanical passage is as long as 200 msec, permitting a card flow of 9000 cards per hour, depending on numbers and types of operations.

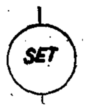
Capacity of the UNIVAC-60

Electronic storage	6×10 digits
Input storage	90 digits
Output storage	90 digits
Constants	27 digits
Selectors	18
Programme steps	20
Elements	12

Symbols used in a current programme schedule are as follows:

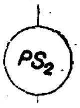
$\sigma[H_3]\times[S_3]==>[S_5]$ — denoting that the first value is the element N_3, while the second value is located in the storage space S_3. The multiplication result is contained in the storage space $[S_5]$. If letters *a* and *b* are found adjacent to the programme step number, they denote that the programme step is used twice, i. e., *a*, for the first passage, and *b*, for the second passage following the selection.

$[S_2]\,[S_3]$ — cancellation of values kept in storage spaces S_2 and S_3.

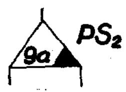


$[S_4]\,[S_5]$ — perforation of cards with results contained in storage spaces S_4 and S_5.

— sorting.

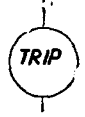


— shifting the selector control into „SELECTOR" position. The UNIVAC-60 machine has four *PS* (Programme Selector) controls. The programme card should contain special indication, such as „SEL. HOLD" adjacent to the PS_2 control symbol if the selector control is to be left in the „SELECTOR" position after the „TRIP" order is given.



— selector. The selector number is written inside the symbol, whereas another indication appearing adjacent to it denotes the selector control to be used. The selector side is that side of the symbol triangle bearing the indication.

— start of programme.



— end of programme and discharge of the card into the output storage space.

Operation of the UNIVAC-60 *Computing machine*

The card set up is such as to make unnecessary any reproduction of data from one card to another. In addition, no sorting of cards is necessary. In other words, when all cards are properly set up, and the machine starts its operation, the procedure goes on until the whole job is done. For each solution, three or four corrections have been made, but it is also possible to make any additional number of corrections, if required. Should k corrections be made for any one solution, then it is necessary to have $k+1$ cards, ensuring that only the first card has the symbol (0/90) and the assumed values for $x^{1/2}$ and σ.

The problem of balance of a gaseous mixture is of such a nature that system components of a related problem group should be found where a_i are permanent constants, while K_i are variable parameters. Let n be the number of related problems, and k the number of corrections required for the solution of each problem, then the total number of cards used to solve the related group is $n(k+1)$. Only the first one of all $n(k+1)$ cards used, has been perforated as an assumed value for $x^{1/2}$. Since a related group contains n related problems, their cards arranged either in accordance with decreasing or increasing values for K_i, it has been found suitable to employ the corrected value for $x^{1/2}$ of the previous problem as an assumed value for the next problem of the same related group. In other words, the computed values for $x^{1/2}$ and x, respectively, obtained from the first correction, are to be used as assumed ones for the next corrections.

Assuming the values for $x^{1/2}$ instead of x is one of the great facilities in solving this problem. In this way, the solution is obtained much more readily, programme making is less complicated and the employment of the machine memory capacity more efficient. On the strength of the great number of problems solved by the UNIVAC-60 computing machine, we may draw the conclusion that the time required for each solution is one minute.

Fig. 1 represents a current diagram for programme (I). It should be noted that when the first correction for $x^{1/2}$ is worked out, storages S_2 and S_3 are not cancelled, thus permitting, as mentioned before, that computed values for $x^{1/2}$ from a preceding problem be used as an assumed value for the next one belonging to the same related group of problems. When working out the second, third, etc., corrections, storages S_2 and S_3 are cancelled.

The programme selector PS_1 permits the selection of values in programme steps 3 through 15, and together with the programme selectors

PS_2 and PS_4, makes it possible to use the iterative method of correcting the value for $x^{1/2}$; on the other hand, the programme selector PS_3 is used to determine whether the values for x should be decreased or increased.

The elements and storages used for programme (I) have the following values:

$$[N_1] ==> x^1/_2 \text{ assumed}, \quad [N_2] ==> 0, \quad [N_3] ==> \frac{K_3^2}{2},$$

$$[N_4] ==> \left(\frac{\sigma}{p}\right)^{1/2} \text{ or } |F| = 10^{-4}, \quad [N_5] ==> a_1, \quad [N_6] ==> K_{10},$$

$$[N_7] ==> K_1 \text{ or } 10^{-3}, \quad [N_8] ==> a_3, \quad [N_9] ==> 2K_6,$$

$$[N_{10}] ==> K_7, \quad [N_{11}] ==> K_9 \text{ or } a, \quad [N_{12}] ==> a_4,$$

$$[S_1] ==> z, \quad [S_2] ==> x^{1/2}, \quad [S_3] ==> x^{1/2}, \quad [S_4] ==> y.$$

The values read directly from the cards are:

$$x^{1/2} \text{ assumed' } K_1, \ \frac{K_3^2}{2}, \ 2K_6, \ K_7, \ K_9, \ K_{10} \text{ and } \left(\frac{\sigma}{p}\right)^{1/2},$$

while those read from the programme discs are

$$a_1; \ a_3; \ a_4; \ a; \ 0; \ 10^{-4} \text{ and } 10^{-3}.$$

The current diagram for Programme (II) is shown in Fig 2. The first step in this programme is designed to shift the selector 2, if (0/90) exists. If such a step does not exist, the selector might not be shifter into position „SELECTOR" and the programme would follow a wrong course. The result of the 13th programme step operation is always negative and it is used to perforate (1/90). The programme will follow the course of this programme step only if the computed value for σ gives the required accuracy. Should the contrary be the case, the value for $(\sigma/p)^{1/2}$ is worked out and the card is sorted. For the next cards, namely those for a solution, the programme either follows the 20th programme step or not, depending on whether the solution has given the accuracy required for σ. If the preceding solution is corrected, the following card is perforated at $(\sigma/p)^{1/2}$, σ and (0/90), since the result of the arithmetical operation in the 20th programme step is always negative. Connection with the „SEL. HOLD" position is interrupted when the PS_3 starts to operate.

The elements and storages used for programme (II) have following values:

$$[N_1] ==> K_1, \text{ or } 1, \quad [N_2] ==> y, \quad [N_3] ==> a_3, \quad [N_4] ==> x^{1/2},$$

$$[N_5] ==> \left(\frac{\sigma}{p}\right)^{1/2}, \quad [N_6] ==> K_7 \text{ or } |\sigma_p - \sigma_i| = 4 \times 10^{-3}, \quad [N_7] ==> a_1,$$

$$[N_8] \Longrightarrow \sigma \text{ or } a, \quad [N_9] \Longrightarrow a_4, \; [N_{10}] \Longrightarrow K_9, \; [N_{11}] \Longrightarrow 2,$$

$$[N_{12}] \Longrightarrow p, \quad [S_2] \Longrightarrow \sigma, \; [S_3] \Longrightarrow \left(\frac{\sigma}{p}\right)^{1/2}.$$

The elements read directly from the cards in this programme are: $x^{1/2}$, y, K_1, K_7, K_9, σ_i and $(\sigma/p)^{1/2}$, while those read from the programme panel are:

$$a_1;\; a_3;\; a_4;\; a;\; p;\; 2;\; 1 \text{ and } 4\times 10^{-3}$$

The current diagram for programme (III) is shown in Fig. 3. This programme is used only when the values for x, y and z are found from all problems. Such solutions are perforated into the cards bearing the sign (1/90). Two empty cards should be inserted next to each of these cards, on which solutions for x_i $(i=1,2,\ldots,10)$ will be perforated, the computations and perforations for x_3, x_4, x_5, x_6 and x_8 taking place during the first passage, and those for x_1, x_2, x_7, x_9 and x_{10} during the second passage. The programme for determining all the ten components is set up by means of Equations (17 through 26). The elements and storages used have the following values:

$$[N_1] \Longrightarrow \left(\frac{\sigma}{p}\right)^{1/2}, \; [N_2] \Longrightarrow 2K_6, \quad [N_3] \Longrightarrow y, \quad [N_4] \Longrightarrow z,$$

$$[N_5] \Longrightarrow K_{10}, \quad [N_6] \Longrightarrow K_7, \quad [N_7] \Longrightarrow K_9, \; [N_8] \Longrightarrow x^{1/2}$$

$$[N_9] \Longrightarrow K_1, \quad [N_{10}] \Longrightarrow a_3, \quad [N_{11}] \Longrightarrow 2 \quad [N_{12}] \Longrightarrow a_4,$$

$$[S_1] \Longrightarrow x_8, \text{ or } x_9, \quad [S_3] \Longrightarrow x_5, \text{ or } x_{10}, \quad [S_4] \Longrightarrow x_6, \text{ or } x_7,$$

$$[S_5] \Longrightarrow x_3, \text{ or } x_1, \quad [S_6] \Longrightarrow x_4, \text{ or } x_2 ..$$

The following values are read directly from the cards

$$x^{1/2},\; y,\; z,\; K_1,\; 2K_6,\; K_7,\; K_9,\; K_{10} \text{ and} \left(\frac{\sigma}{p}\right)^{1/2},$$

while those read from the discs are:

$$a_3,\; a_4 \text{ and } 2.$$

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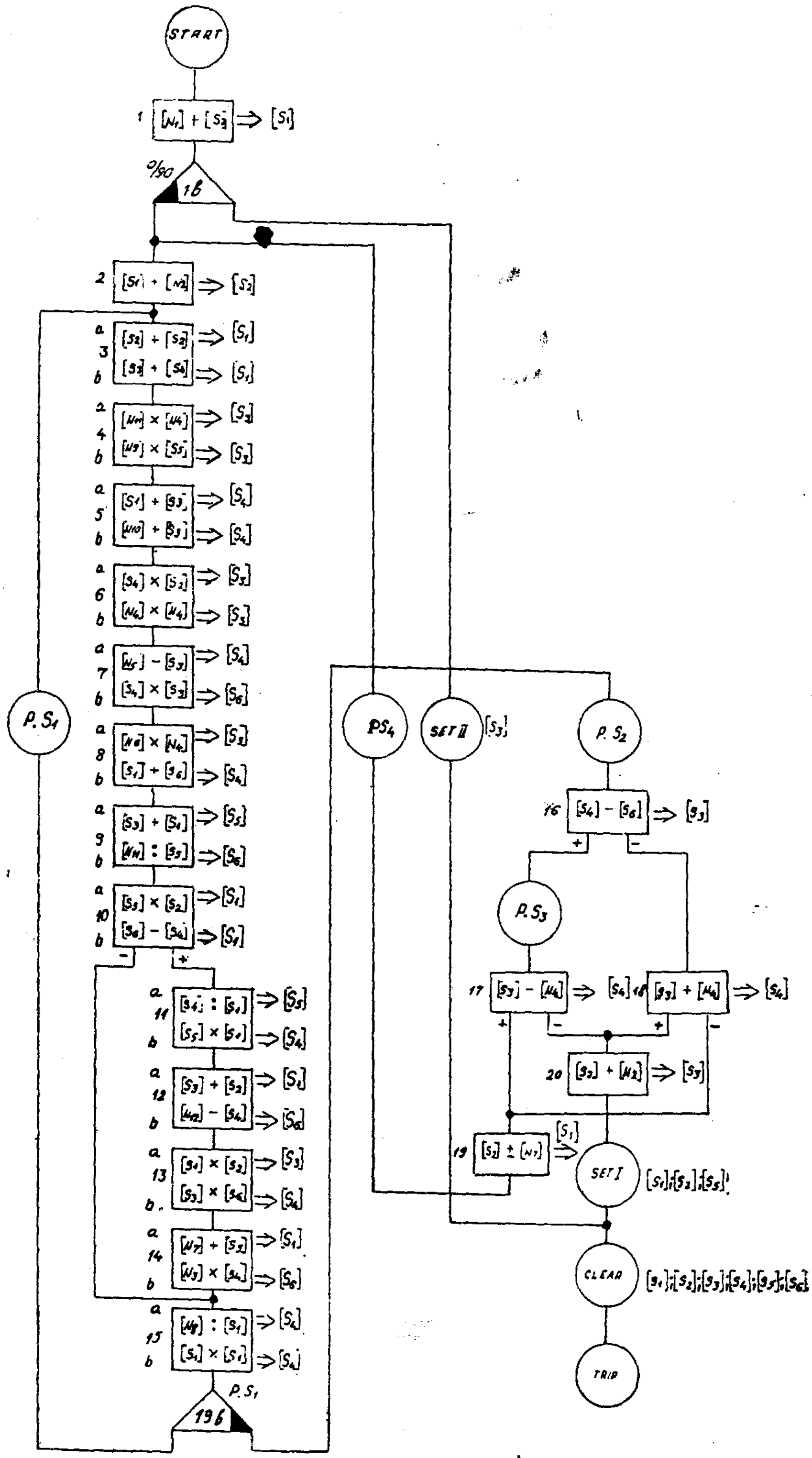

Fig. 1

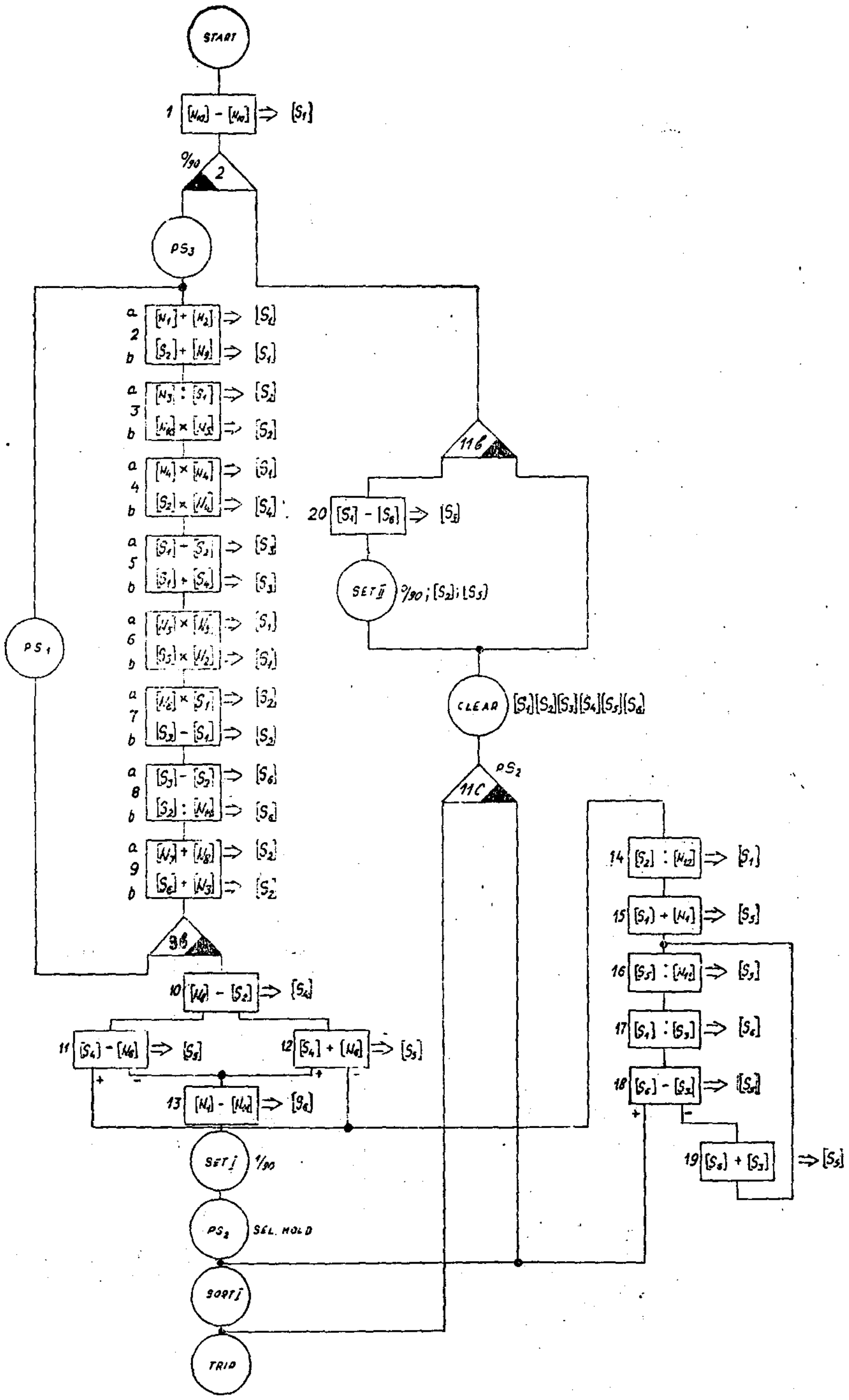
START
PS3
PS1
SET I
PS2
SEL. HOLD
SORT I
TRIP
SET II
CLEAR
11b
11C
9b

Fig. 2

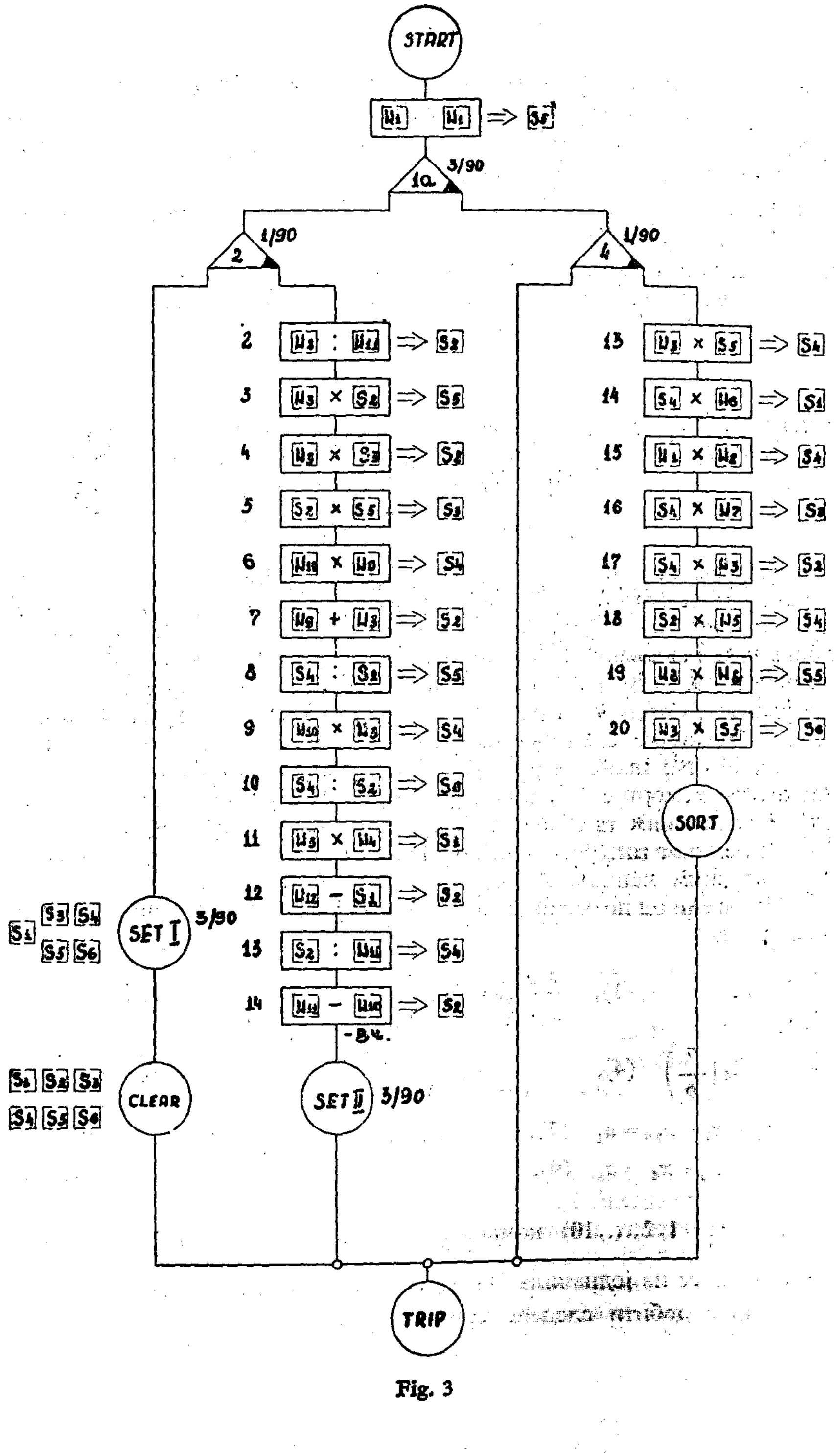

Fig. 3

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РЕШЕЊЕ СИСТЕМА ЈЕДНАЧИНА РАВНОТЕЖЕ ГАСНИХ ПРОДУКАТА САГОРЕВАЊА ПОМОЋУ ДИГИТАЛНЕ МАШИНЕ „UNIVAC-60"

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Решење проблема равнотеже у гасној смеши се врло често среће у пракси технолога и хемичара који раде на проучавању састава горива. Овај проблем је дефинисан системом нелинеарних алгебарских једначина чије решавање, ако се користе стоне машине, захтева велики нумерички посао који траје више дана и праћен је субјективним грешкама калкуланата. Отуда је за решавање овог проблема неопходно користити модерна техничка средства као што су дигиталне рачунске машине. До сада је овај проблем решаван помоћу дигиталних машина великих капацитета меморије [1], али како многи инжењери који се у својој пракси баве овим проблемом немају на располагању овакве машине, то је од великог интереса показати како се овај проблем може решавати на дигиталним машинама малог капацитета меморије.

Полазећи од познатих једначина са којима је дефинисана равнотежа гасне смеше

$$\frac{x_2 \cdot x_3}{x_1 \cdot x_4} = K_1 \quad (1), \qquad \frac{x_1 \cdot x_8}{x_2 \cdot x_6^{1/2}} = K_3\left(\frac{\sigma}{p}\right)^{1/2} \quad (2), \qquad \frac{x_1^2 \cdot x_5}{x_2^2} = K_6\left(\frac{\sigma}{p}\right) \quad (3),$$

$$\frac{x_1 \cdot x_9}{x_2} = K_7\left(\frac{\sigma}{p}\right) \quad (4), \qquad \frac{x_{10}}{x_1^{1/2}} = K_9\left(\frac{\sigma}{p}\right)^{1/2} \quad (5), \qquad \frac{x_1^{1/2} \cdot x_7}{x_2} = K_{10}\left(\frac{\sigma}{p}\right)^{1/2} \quad (6),$$

$$2x_1 + 2x_2 + x_7 + x_{10} = a_1 \quad (7), \qquad x_2 + x_3 + 2x_4 + 2x_5 + x_7 + x_8 + x_9 = a_2 \quad (8),$$

$$x_3 + x_4 = a_3 \quad (9), \qquad 2x_6 + x_8 = a_4 \quad (10),$$

где су x_i $(i = 1, 2, \ldots, 10)$ компоненте састава а $\sigma = \sum_{i=1}^{10} x_i$, није тешко показати да се из једначина (1—10), елиминисањем x_3, x_4, x_5, x_6, x_7, x_9 и x_{10}, могу добити следеће три једначине

$$y = \frac{a_1 - x^{1/2}[2x^{1/2} + K_9(\sigma/p)^{1/2}]}{x^{1/2}[2x^{1/2} + K_{10}(\sigma/p)^{1/2}]} \tag{11}$$

$$z = \frac{a}{y} - \frac{a_3}{K_1 + y} - x^{1/2}\left[x^{1/2} + K_{10}\left(\frac{\sigma}{p}\right)^{1/2}\right] - \left(\frac{\sigma}{p}\right)(K_7 + 2K_6 y) \tag{12}$$

$$F(y, z) \equiv z^2 - {}^1/_2 K_2^3 \left(\frac{\sigma}{p}\right)(a - yx) = 0, \tag{13}$$

које смо назвали радним једначинама. У једначинама (11—13) задржане су све ознаке из једначина (1—10) осим $x = x_1$, $y = \frac{x_2}{x_1}$, $z = \frac{x_8}{x_2/x_1}$ и $a = a_2 - a_3$.

Једначине (11—13) су много погодније за прорачун компонената сагоревања од оних једначина које су дате у [1], [2] и [3]. Израчунавање x, y и z може се извршити са задовољавајућом тачношћу ако се искористи тзв. метод покушаја и грешке који се састоји у следећем: претпостави се вредност $x^{1/2}$ и израчуна y помоћу једначине (11), затим се претпостављено $x^{1/2}$ и израчунато y уврсти у једначину (12) и израчуна z и најзад, ако израчунато y и z задовоље, према једначини (13), услов

$$|F(y, z)| \leqq \varepsilon_1, \tag{14}$$

онда, на тај начин, добијене вредности за x, y и z претстављају тражено решење. Ако услов (14) није задовољен, увећава се или смањује претпостављено $x^{1/2}$ за неку малу вредност и поступак се наставља изнова све док се не постигну за x, y и z резултати жељене тачности. Међутим, како је $\sigma = f(x_i)$, $i = 1, 2, \ldots, 10$, нумеричка обрада овог проблема према ауторима [1], [2] и [3] је била веома гломазна и захтевала је посао од више дана рачунања на стоним машинама или употребу машина великих капацитета меморије. Познато је да се σ може приближно одредити претходним термодинамичким прорачуном и та вредност за $\sigma = \sigma_p$ се користи као претпостављена полазна вредност. Ми смо израз за $\sigma = f(x_i)$ свели на облик $\sigma = f(x, y, z)$ који зависи само од x, y и z

$$\sigma = \frac{1}{2}\left\{a_1 + a + a_4 - y\left[x + \frac{a_3}{K_1 + y} - K_7\left(\frac{\sigma}{p}\right)\right] + K_9\left(\frac{\sigma}{p}\right)^{1/2} x^{1/2}\right\} + a_3 \tag{15}$$

тако се никада не рачунају компоненте x_i $(i = 1, 2, \ldots, 10)$ пре него што се помоћу вредности x, y и z које задовољавају услов (14) не израчуна $\sigma = \sigma_i$ према једначини (15). Ако је испуњен услов

$$|\sigma_p - \sigma_i| \leqq \varepsilon_2, \tag{16}$$

онда се рачунају вредности свих десет компонената x_i, а ако није, онда се место $\sigma = \sigma_p$ уноси у једначине (11—13) нова вредност $\sigma = \sigma_i$ и цео поступак тече изнова све док не буду испуњени услови (14) и (16). Оба ова поступка су конвергентна. На овај начин, постигнуто је да се систем нелинеарних алгебарских једначина равнотеже у гасној смеши може успешно решавати и на дигиталним машинама малих капацитета меморије као што је и „UNIVAC-60", а ако се врши решавање на стоним шинама, такође се постиже уштеда у времену. Састављању програма смо пришли преко логичких шема које омогућују лакши увид и брже схватање целине проблема и начина на који се решава.

Из великог броја примера које смо решили на „UNIVAC 60" и практичне примене добијених резултата, показало се да је довољно усвојити $\varepsilon_1 = 10^{-4}$ и $\varepsilon_2 = 4 \times 10^{-4}$. У пракси се јавља потреба за решавање више група сродних задатака, нарочито када је у питању састављање (*i*, *s*) *T* дијаграма. У случају када једна група има 20—30 сродних задатака, време прорачуна свих 10 конпонената за све задатке целе групе није прелазило 30 мин., што значи да за сваки задатак, понаособ, коришћењем „UNIVAC-60", није уторшено време веће од једног минута. Коришћење израчунатих конпонената за састављање (*i*, *s*) *T* дијаграма не претставља нумеричке тешкоће.