296
4-24-68

MASTER

MOLE REACTION-FORTRAN-IV DATA
REDUCTION PROGRAM FOR GAS-GAS
AND GAS-SOLID REACTIONS

THE DOW CHEMICAL COMPANY
ROCKY FLATS DIVISION
P. O. BOX 888
GOLDEN, COLORADO 80401
U.S. ATOMIC ENERGY COMMISSION
CONTRACT AT(29-1)-1106

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

Printed in the United States of America

Available from

Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151

Price: Printed Copy \$3.00; Microfiche \$0.65

May 21, 1968

RFP-1107
UC-32 MATHEMATICS
AND COMPUTERS
TID-4500

MOLE REACTION-FORTRAN-IV DATA
REDUCTION PROGRAM FOR GAS-GAS
AND GAS-SOLID REACTIONS

Robert W. Loser

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor, transmits, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

THE DOW CHEMICAL COMPANY
ROCKY FLATS DIVISION
P. O. BOX 888
GOLDEN, COLORADO 80401
U. S. ATOMIC ENERGY COMMISSION
CONTRACT AT(29-1)-1106

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

CONTENTS

Abstract.....	1
Introduction.....	1
Experimental Procedure	1
Mathematical Methods	2
Program Description	4
Input Data	4
Output Data	4

ACKNOWLEDGMENT

The author wishes to express sincere appreciation to D. K. Strangfeld for his conscientious support which made possible the development of the program.

MOLE REACTION-FORTRAN-IV DATA REDUCTION PROGRAM FOR GAS-GAS AND GAS-SOLID REACTIONS

Robert W. Loser

Abstract. The Mole Reaction-FORTRAN IV Program represents a comprehensive evaluation of gas pressure data from gas-gas and gas-solid reactions. The program reduces the pressure, volume, temperature and sample volume, and the composition data to give the rate of change in the concentration of residual gases in a reaction and the total change in moles of each gas for a number of reactions. From the initial reactant and temperature-dependent input data, the reactions are evaluated by gas law equations and the formation or consumption of key gases is presented.

INTRODUCTION

The Mole Reaction-FORTRAN IV Program was written for rapid and concise reduction of gas-pressure data from a gas-gas or gas-solid reaction. The program is applicable to any experiment utilizing a reaction chamber containing reactant gases and a quantity of solid material (for a gas-solid reaction). The gas-pressure data obtained from the reaction consist of gas analyses by percent by volume, pressure, temperature, and the time of the reaction. With the volume of the reaction chamber and the names of the gases fed into a computer, the program produces the following information:

1. The initial total pressure of the gases in the reaction chamber at time (zero hours).
2. The initial concentration in moles of each gas in the reaction chamber.
3. The reaction number and the time of the reaction.
4. An indication as to whether the total pressure of the gases in the reaction chamber increased, decreased, or remained unchanged since the previous timed reaction, and if applicable, an indication of how much the total pressure changed.
5. The concentration in moles of each gas in the reaction chamber after the reaction.
6. The rate of change in the concentration of each gas in moles per liter per second, with and

without loss due to sampling, and the total sample loss in moles of each gas for each sample obtained.

A general application of the ideal gas law is made to reduce the gas pressure data.

EXPERIMENTAL PROCEDURE

The experimental procedure is a typical procedure for monitoring the gaseous product of a gas-gas or gas-solid reaction in a closed system. Figure 1 illustrates the vacuum system used for the experiment.

One or more reactant gases are injected into the vacuum system through Valve A. Valve B is open. The total pressure of the gas in the system can be measured by the pressure gauge in the expansion reservoir. The first gas sample is obtained through Valve C for the initial concentrations. Closing Valve B and at time (zero hours), a reaction in the reaction chamber is initiated and sustained by elevating the temperature of the reaction chamber. During the reaction, the expansion reservoir is evacuated by opening Valve A to a vacuum pump. After a definite period of time, the reaction becomes arrested by momentarily decreasing the temperature of the reaction chamber. Valve A is closed. Opening Valve B, the residual gases are expanded into the expansion reservoir. The pressure is recorded. Valve B is then closed and the temperature elevates once again. The reaction is re-initiated. Valve C is opened and a second gas sample collected. Finally, with Valve A opened, the expansion reservoir is evacuated.

The expansion of the residual gases is repeated as often as necessary for as many samples needed to complete the study of the gas-gas or gas-solid reaction.

Table I gives an example of the gas-pressure data obtained as input data for the data-reduction program.

FIGURE 1. Vacuum System for Gas-Gas and Gas-Solid Reaction.

TABLE I. Gas-Pressure Data.

Gases under Surveillance, Analyses by Volume Percent

Sample No.	Expanded Pressure (mercury millimeters)	Gas 1 (percent)	Gas 2 (percent)	Gas 3 (percent)	Gas 4 (percent)	Gas 5 (percent)	Reaction Time (hours)	Reaction Chamber Temperature (°C)
1	100.00	0.00	0.03	0.16	0.04	99.61	0.0	*25
2	100.40	0.05	0.02	1.17	0.06	98.60	3.0	25
3	96.20	0.03	0.04	1.50	0.18	97.87	6.5	25
4	92.02	0.02	0.00	2.10	0.07	97.53	21.5	25
5	88.04	0.02	0.00	4.23	0.06	95.75	68.5	25
6	84.59	0.04	0.05	5.57	0.05	93.80	187.5	25
7	80.72	0.03	0.03	7.20	0.07	92.00	354.5	25
8	77.69	0.03	0.04	7.24	0.09	91.12	497.0	25

Expansion Reservoir Volume. = 17.5 milliliters

Expansion Reservoir Temperature = 25°C

Reaction Chamber Volume = 383.3 milliliters

*Ambient temperature

MATHEMATICAL METHODS

1. The initial total pressure of the gases in the reaction chamber is equal to the first pressure readings taken before the reaction is initiated. (See Table II, FORTRAN Notation, for variable names.)

For example, since the first expansion is that of the reactant gases being injected into the vacuum system:

$$PR_1 = PEXP_1$$

2. The gases expand from the reaction chamber into the expansion reservoir at time $(j + 1)$, if no reaction takes place between time (j) and time $(j + 1)$. The total pressure of the gases then is given by:

$$PCALC_j = \frac{PEXP_j \times \frac{VR}{TR_{(j+1)}}}{\frac{VR}{TR_{(j+1)}} + \frac{VEXP}{TEXP}}$$

TR_1 corresponds to PR_1

$j = 1, 2, \dots, m$, where m is the number of gas samples obtained after the first sample (the first sample being obtained before any reaction).

The variable $PCALC_j$ is compared to $PEXP_{(j+1)}$ (the observed pressure) to compute the results of the reaction.

TABLE II. FORTRAN Notation.

Variable Name	Explanation
ADMDT	The actual change in moles of each gas per liter per second from the reaction and from loss due to the expansion.
AMOLE	An intermediate variable for the total number of moles of the gases in the reaction chamber.
BMOLE	The number of moles of each gas in the reaction chamber.
CMOLE	An intermediate variable for the total number of moles of the gases lost in the expansion.
JJ	The variable name for the input device.
KK	The variable name for the output device.
KRET	The dummy variable name of a DO statement.
LAB1, LAB2	Gas formulae.
NGAS	The number of gases under surveillance.
NSAMP	The number of samples taken for the analysis.
NXP	The number of experiments to be processed.
PCALC	The anticipated total pressure in torr of the gases expanded into the evacuated expansion reservoir after the reaction, assuming no changes by the reaction in the partial pressures of the gases.
PCENT	The volume percent of each gas analyzed.
PEXP	The observed total pressure in torr of the gases expanded into the reservoir.
PR	The calculated total pressure in torr of the gases in the reaction chamber giving rise to PEXP (except for the first value when the reaction chamber is filled with the gases).
R	Gas constant divided by 1.333×10^3 dynes per square centimeter per torr, a pressure conversion factor.
SAMOLE	An intermediate variable for the number of moles of each gas lost in the expansion.
SAMPLE	The accumulative sum of the moles of each gas lost in the expansion.
SUMSAM	An intermediate variable for accumulative sum.
TDMDT	The total change in moles of each gas per liter per second from the reaction.
TEXP	The ambient temperature in $^{\circ}$ Kelvin of the expansion reservoir.
TIME	The reaction time in seconds (converted from hours).
TITLE	Experiment identification.
TR	The temperature in $^{\circ}$ Kelvin of the reaction chamber.
VEXP	The volume of the expansion reservoir in milliliters.
VR	The volume of the reaction chamber in milliliters.

3. The actual total pressure of the gases in the reaction chamber after the reaction has occurred is computed by applying a P-V-T correction to the measured pressure $PEXP(j+1)$ as follows:

$$PR(j+1) = PEXP(j+1) \times \frac{\frac{VR}{TR(j+1)} + \frac{VEXP}{TEXP}}{\frac{VR}{TR(j+1)}}$$

$j = 1, 2, \dots, m$, where m is the number of gas samples obtained after the first sample.

4. The number of moles of each of the gases in the reaction chamber is determined by:

$$BMOLE_{k,j} = PR_j \times \frac{VR}{R \times TR_j} \times PCENT_k$$

$k = 1, 2, \dots, n$, where n is the number of gases under surveillance.

$j = 1, 2, \dots, m$, where m is the number of gas samples.

5. The change in the concentration of each gas in moles per liter per second from the reaction, but without corrections for loss due to sample removal, is determined by:

$$TDMDT(j+1) = \frac{(BMOLE_k(j+1) - BMOLE_{k,j})}{TIME(j+1) - TIME_j} \times \frac{1000}{VR}$$

$k = 1, 2, \dots, n$, where n is the number of gases under surveillance.

$j = 1, 2, \dots, m$, where m is the number of gas samples obtained after the first sample.

6. The number of moles of each of the gases removed from the reaction by sampling the expansion reservoir is determined by:

$$SAMOLE_{k,j} = PEXP(j+1)$$

$$\times \frac{VEXP}{(R \times TEXP)} \times PCENT_k$$

$k = 1, 2, \dots, n$, where n is the number of gases under surveillance.

$j = 1, 2, \dots, m$, where m is the number of gas samples obtained after the first sample.

7. The actual change in the concentration of each gas in moles per liter per second from the reaction corrected for loss due to the removal of samples is determined by:

$$\text{ADMDT}_{k, (j+2)} = \frac{[\text{BMOLE}_{k, (j+2)} + \text{SAMOLE}_{k, (j+1)} - \text{BMOLE}_{k, (j+1)}]}{\text{TIME}_{(j+2)} - \text{TIME}_{(j+1)}} \times \frac{1000}{\text{VR}}$$

$$\text{ADMDT}_{k, 2} = \text{TDMDT}_{k, 2}$$

$k = 1, 2, \dots, n$, where n is the number of gases under surveillance.

$j = 1, 2, \dots, m$, where m is the number of gas samples obtained between the first and final samples.

PROGRAM DESCRIPTION

The source-program deck consists of 115 executable and nonexecutable statements (see Table III). The DIMENSION statements require 7864 bytes of core storage. Statement numbers 1 through 21 are FORMAT statement numbers, two-digit statement numbers greater than 21 are IF and GO TO statement numbers, and three-digit statement numbers are DO statement numbers. Processing the source program in an IBM SYSTEM 360, Model 40, requires approximately 1.5 minutes for translating the source program into an object program. The object program can process up to 25 different gas samples with each sample consisting of 12 gases. Typical running time of the program is approximately 3 minutes, including the translation time and depending upon the number of sets of input data and the output device used.

The source program was written to process input data entirely. With modification of the READING section, the program can be used for real-time processing. Table IV shows the source-program flow chart.

Input Data: The gas-pressure data obtained from a gas-gas or gas-solid reaction are punched into cards for a card read-punch, input-output device. Data fields have been restricted to ten columns except for the title card, formulae cards, and control number cards. Each experiment or job has a title card and more than one experiment can be processed during the execution of the program. The input-data cards are described in Column 2.

The seven card types complete the make-up of the input deck. A field format layout of each card type is shown in Figure 2.

Output Data: The results of a gas-gas or gas-solid reaction are obtained through a line-printer output

device. A line printer consisting of no less than 120 columns per line is sufficient for a complete print-out. The program will first edit the input data, then generate one sheet of output data per sample. Each sheet will show the initial concentration followed by the changes caused by the reaction. Results of the first reaction are shown in Figure 3.

Input Data

- Card Type 1 – Indicates the number of experiments to be processed. Care must be taken to use the right-hand portion of the 5-column field for low-order digits. Only one Card Type 1 is required.
- Card Type 2 – The 72-column title card. Each job will require a title card. Column 1 of the 72-column field is reserved for the digit 1 for carriage control.
- Card Type 3 – Indicates reaction chamber volume, expansion-reservoir volume and expansion-reservoir temperature in three 10-column fields, respectively.
- Card Type 4 – Indicates the number of samples and the number of gases under surveillance in two 5-column fields, respectively. Care must be taken to use the right-hand portions of the fields for low-order digits.
- Card Type 5 – Supplies the gas formulae in two 3-column fields. There is one card for each formula used.
- Card Type 6 – Indicates pressure, time, and reaction chamber temperature in three 10-column fields, respectively. This card type will be repeated for each sample.
- Card Type 7 – Indicates the analysis of a gas in one 10-column field. There is one card for each gas under surveillance. The cards must correspond sequentially to the formulae of the gases supplied by Card Type 5. Care must be taken not to transpose the cards within a sample or among the samples. This card type will be repeated for each gas in each sample.

TABLE III. Source Program.

```

C MOLE REACTION FORTRAN---A DATA REDUCTION PROGRAM
C FOR GAS-GAS AND GAS-SOLID REACTIONS.
C
C
C DIMENSION TITLE(18),LAB1(12),LAB2(12),PEXP(25),TIME(25),TR(25) 1
C DIMENSION PCENT(12,25),PR(25),BMOLE(12,25),PCALC(24),TDMDT(12,25) 2
C DIMENSION SAMOLE(12,25),SAMPLE(12,25),ADMDT(12,25) 3

1 FORMAT(I5) 4
2 FORMAT(18A4) 5
3 FORMAT(3F10.4) 6
4 FORMAT(2I5) 7
5 FORMAT(2A3) 8
6 FORMAT(F10.4) 9
7 FORMAT('OPRESSURE',2X,'TIME',3X,'TEMP',1X,12(2X,2A3)) 10
8 FORMAT('O',F8.3,F7.2,1X,F6.2,12F8.4) 11
9 FORMAT('ORÉACTION CHAMBER VOLUME=',F7.2,3X,'EXPANSION RESERVOIR', 12
11X,'VOLUME=',F6.2,3X,'TEMPERATURE OF THE RESERVOIR=',F7.2) 13
10 FORMAT('OINITIAL PRESSURE IN REACTION CHAMBER=',F8.3,1X,'TORR', 14
11X,'AT TIME',F7.2,1X,'HOURS') 15
11 FORMAT('OINITIAL REACTANTS'/(1X,I2,2X,2A3,E12.4,1X,'MOLES'))/ 16
12 FORMAT(' REACTION NUMBER',I3,5X,'REACTION TIME',F7.2,1X,'HOURS') 17
13 FORMAT(' EXPANDED PRESSURE AFTER THE REACTION=',E13.5,1X,'TORR') 18
14 FORMAT(' THE EXPANDED PRESSURE WAS CALCULATED TO BE',E13.5,1X, 19
1'TORR') 20
15 FORMAT(' THE INCREASE IN PRESSURE INDICATES THAT GAS WAS', 21
11X,'GENERATED IN THE REACTION CHAMBER') 22
16 FORMAT(' THE PRESSURE IN THE REACTION CHAMBER DID NOT CHANGE') 23
17 FORMAT(' THE DECREASE IN PRESSURE INDICATES THAT GAS WAS', 24
11X,'CONSUMED IN THE REACTION CHAMBER') 25
18 FORMAT(' PRESSURE OF THE GAS IN THE REACTION CHAMBER BEFORE', 26
11X,'EXPANSION=',E13.5,1X,'TORR') 27
19 FORMAT('O',4X,'REACTION',17X,'CHANGE IN MOLES/LITER/SEC', 28
13X,'CHANGE IN MOLES/LITERS/SEC',3X,'TOTAL SAMPLE') 29
20 FORMAT(' ',4X,'PRODUCTS',6X,'MOLES',34X,'WITH LOSS DUE TO', 30
11X,'SAMPLING',3X,'LOSS IN MOLES')/ 31
21 FORMAT(1X,I2,2X,2A3,4X,E11.4,10X,E12.5,16X,E12.5,9X,E12.5) 32
JJ=1 33
KK=3 34

```

(continued)

(Table III - continued)

```

C
C   READING THE INPUT DATA.
C
  READ(JJ,1)NXP                                     35
  DO 100 KRET=1,NXP                                  36
  READ(JJ,2)TITLE                                    37
  READ(JJ,3)VR,VEXP,TEXP                             38
  READ(JJ,4)NSAMP,NGAS                                39
  READ(JJ,5)(LAB1(J),LAB2(J),J=1,NGAS)                40
  DO 105 I=1,NSAMP                                    41
  READ(JJ,3)PEXP(I),TIME(I),TR(I)                     42
  READ(JJ,6)(PCENT(K,I),K=1,NGAS)                     43
105  CONTINUE                                         44
C
C   EDITING THE INPUT DATA.
C
C
  WRITE(KK,2)TITLE                                     45
  WRITE(KK,7)(LAB1(J),LAB2(J),J=1,NGAS)                46
  DO 110 I=1,NSAMP                                    47
  WRITE(KK,8)PEXP(I),TIME(I),TR(I),(PCENT(K,I),K=1,NGAS) 48
110  CONTINUE                                         49
  WRITE(KK,9)VR,VEXP,TEXP                             50
C
C   COMPUTATION.
C
C
  DO 115 J=1,NSAMP                                    51
  TIME(J)=TIME(J)*3600.0                               52
115  CONTINUE                                         53
  R=0.6237059E+05                                       54
  PR(1)=PEXP(1)                                         55
  AMOLE=PR(1)*VR/(R*TR(1))                             56
  DO 120 K=1,NGAS                                       57
  BMOLE(K,1)=AMOLE*PCENT(K,1)                          58
120  CONTINUE                                         59
  DO 125 J=2,NSAMP                                     60
  PCALC(J-1)=(PEXP(J-1)*VR/TR(J))/(VR/TR(J)+VEXP/TEXP) 61
  PR(J)=PEXP(J)*(VR/TR(J)+VEXP/TEXP)/(VR/TR(J))        62
  AMOLE=PR(J)*VR/(R*TR(J))                             63
  DO 130 K=1,NGAS                                       64
  BMOLE(K,J)=AMOLE*PCENT(K,J)                          65
  TDMDT(K,J)=(BMOLE(K,J)-BMOLE(K,J-1))/(TIME(J)-TIME(J-1)) 66
  1*1000.0/VR                                           67
130  CONTINUE                                         68
  CMOLE=PEXP(J)*VEXP/(R*TEXP)                          69
  DO 135 K=1,NGAS                                       70
  SAMOLE(K,J)=CMOLE*PCENT(K,J)                         71
135  CONTINUE                                         72

```

(Table III - continued)

125	CONTINUE	73
	DO 140 K=1,NGAS	74
	SUMSAM=0.0	75
	DO 145 J=2,NSAMP	76
	SUMSAM=SUMSAM+SAMOLE(K,J)	77
	SAMPLE(K,J)=SUMSAM	78
145	CONTINUE	79
140	CONTINUE	80
	DO 150 J=3,NSAMP	81
	DO 155 K=1,NGAS	82
	ADMDT(K,J)=(BMOLE(K,J)-BMOLE(K,J-1)+SAMOLE(K,J-1))/(TIME(J)-	83
	1 TIME(J-1))*1000.0/VR	84
155	CONTINUE	85
150	CONTINUE	86
	DO 160 K=1,NGAS	87
	ADMDT(K,2)=TDMDT(K,2)	88
	SAMPLE(K,1)=0.0	89
160	CONTINUE	90
C		
C	WRITING THE RESULTS	
C		
	TIME(1)=TIME(1)/3600.0	91
	DO 165 J=2,NSAMP	92
	WRITE(KK,2)TITLE	93
	WRITE(KK,10)PR(1),TIME(1)	94
	WRITE(KK,11)(K,LAB1(K),LAB2(K),BMOLE(K,1),K=1,NGAS)	95
	TIME(J)=TIME(J)/3600.0	96
	I=J-1	97
	WRITE(KK,12)I,TIME(J)	98
	WRITE(KK,13)PEXP(J)	99
	WRITE(KK,14)PCALC(J-1)	100
	IF(PCALC(J-1)-PEXP(J))30,32,34	101
30	WRITE(KK,15)	102
	GO TO 36	103
32	WRITE(KK,16)	104
	GO TO 36	105
34	WRITE(KK,17)	106
36	WRITE(KK,18)PR(J)	107
	WRITE(KK,19)	108
	WRITE(KK,20)	109
	WRITE(KK,21)(K,LAB1(K),LAB2(K),BMOLE(K,J),TDMDT(K,J),ADMDT(K,J),	110
	1SAMPLE(K,J-1),K=1,NGAS)	111
165	CONTINUE	112
100	CONTINUE	113
	STOP	114
	END	115

TABLE IV. Source Program Flow Chart.

(Table IV - continued)

(continued)

(Table IV - continued)

*CARD TYPE 6 and CARD TYPE 7 are repeated for each sample.

FIGURE 2. Field Format Layout of Card Typea.

EXPERIMENT NO. 1 FOR R AND D

INITIAL PRESSURE IN REACTION CHAMBER = 100.000 TORR AT TIME 0.0 HOURS

INITIAL REACTANTS

1 GAS 1 0.0 MOLES

2 GAS 2 0.6183E-06 MOLES

3 GAS 3 0.3298E-05 MOLES

4 GAS 4 0.8245E-06 MOLES

5 GAS 5 0.2053E-02 MOLES

REACTION NO. 1 REACTION TIME 3.00 HOURS

EXPANDED PRESSURE AFTER THE REACTION = 0.10040E 03 TORR

THE EXPANDED PRESSURE WAS CALCULATED TO BE: 0.95634E 02 TORR

THE INCREASE IN PRESSURE INDICATES THAT GAS WAS GENERATED IN THE REACTION CHAMBER

PRESSURE OF THE GAS IN THE REACTION CHAMBER BEFORE EXPANSION = 0.10498E 03 TORR

REACTION PRODUCTS	MOLES	CHANGE IN MOLES PER LITER PER SECOND	CHANGE IN MOLES PER LITER PER SECOND WITH LOSS DUE TO SAMPLING	TOTAL SAMPLE LOSS IN MOLES
1 GAS 1	0.1082E-05	0.26136E-09	0.26136E-09	0.0
2 GAS 2	0.4328E-06	*-0.44828E-10	*-0.44828E-10	0.0
3 GAS 3	0.2532E-04	0.53192E-08	0.53192E-08	0.0
4 GAS 4	0.1298E-05	0.11447E-09	0.11447E-09	0.0
5 GAS 5	0.2134E-02	0.19438E-07	0.19438E-07	0.0

* The negative sign indicates gas consumption.

FIGURE 3. Results of the First Reaction.