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BEIJING SPECIALITY GAS RESEARCH AND DEVELOPMENT CENTRE

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PEOPLE'S REPUBLIC OF CHINA

Report on the Activities of Computer Software*

Prepared for the Government of the People's Republic of China
by the United Nations Industrial Development Organization,
acting as executing agency for the United Nations Development Programme

Based on the work of Mr. Robert McCarty
Expert of Equation of State for Gases Computer Programme

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United Nations Industrial Development Organization
Vienna

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Based on the arrangements of UNDP for the 4th aided project "Beijing speciality gas research & development center". the computer software expert Mr. Robert Mccarty came to China in June 16-July 4 of 1988 for helping our Inst. to develop computer software in the application field of gas mixing under different PVT conditions. and in according our Inst. real reuirements, Mr. Mccarty gave technical consultations and directions, he had finished his work satisfactorily.

During his two weeks stay, the project manager, technical persons of China side have discussed extensively with Mr.Mccarty about software technology and technical applications. Both sides have made some modifications and adjustments about the preliminary soft wares, so that it can accomodate to our Inst. practical requirements, it will promote further developing the applications in gas mixing by using computer software and increase the precision of mixed gases.

More details are as follows:

1. Train our Inst. personnel to operate the computer and the "fluid pack" program.

a) Mr.Mccarty gave us a brief introduction about the application of computer in different trades and developing trends.

b) He gave us a lecture about the formation of "fluid pack" including the establishment of PVC state equation.

through a large portion of experimental data, revise those parameters which influence the PVT equation, to establish a comlete mathematical module which is congruent to the real conditions and then use FORTRAN language to edit the "fluid pack" program.

c) To illustrate and put on a demonstration to our Inst.'s technical persons for the application of "fluids pack".

2. He gave directions to our Inst's technical persons in regarding how do use partial pressure method to mix gases. In this case, originally planned to prepare 6 mixed gases, ie.

a) $0.6\%C_3H_8 + 4\%CO + N_2$

b) $5\%CH_4 + 40\%N_2 + Ar$

c) $0.3\%CO + 20\%O_2 + N_2$

d) $10\%He + 20\%O_2 + 70\%N_2$

e) $1\%He + 5\%CH_4 + H_2$

f) $66\%CO_2 + 34\%Ar$

Owing to the limited time, we prepare only one mixed gas $1\%He + 5\%CH_4 + H_2$, after analyzing to check the accuracy of that by means of computer blending.

The compared results with gravimetric blending are shown in Table I.

A general requirement of blending gas by partial pressure method is to keep the relative error within 5%(see table I), obviously , in using the computer program to blend gas by partial pressure method, the precision is not sufficient and satisfy. through discussions, we all condemn that in the program, owing the neglection the consideration of temperature and filling speed, the relative error raises higher.

3. Mr.Mccarty brought here14 kinds of programs, see Table II, among which, he illustrated the 4 programs of MIPROPS,DDMIX, SUPERZ, AIRCV, and he made further improvements about DDMIX & SUPERZ, more details, see TableIII.

4. Mr.Mccarty gave us a lecture including all staff members of our Inst.. the topic is "Calculation of the thermophysics properties of mixed gases".

Since Mr. Mccarty came to China, however, the time is short but the content is substantial, the coorperation between two sides is very pleasant, he completed not only the specified task, but

also effectively to edit out DDFILL & ZFILL programs which are simple but practical, it gives convenience for our Inst. work.

Through the exchanging views in technology and concrete analysis of our Inst. concrete situations, both sides consider that the computer software edited for partial pressure method filling must have further modifications, for instance, the influences of temperature and filling speed to the mixed gas precision must be paid attention systematically. therefore, we hope that Mr.Mccarty will do such research work continuously and supply to us those relevant informations. Mr.Mccarty is very pleasnat to accept our request. In the mean time, we earnestly hope that UNIDO & UNDP will help Mr.Mccarty's work continuously, as soon as the conditions are riped, we hope Mr.Mccarty will come to China again for directing the development of computer software by means of partial pressure method and finnally to pursue the fruitful results.

Regards

Beijing speciality gas
research Institute

July 15, 1988

cc: Foreign economic affairs section of Beijing municipal Chemical industry corp.

Foreign economic affairs section of Beijing municipal economic trade bureau

China international economic & technologic exchange eenter

Resident representative of UNDP in China

TABLE I

composition	theoretical required value	analytical results (partial pressure method) %	relative error (partial pressure method)%	analyssis standard
He	1	1.08	8	1.08
CH_4	5	5.4	8	5.5
H_2 (equilibrium gas)	94	93.52	0.51	93.42

TABLE II

No.	contents	remarks
1.	MIPROPS.	physical parameters of relevant gases
2.	DDMIX,EXE,DDHELP	physical parameters of relevant gas mixers
3.	MIX.FOR,DDMIX.FOR,DDDAT.FOR, DDPRPS.FOR,,MSGGEN.FOR,DDMES. AG.FOR	" " "
4.	PA.COM,PX.COM,CSE.COM,CSE.XEX, CSE.HLP	
5.	DATABASP.317,EDIT.294	package and auto-edit
6.	PC-WRITE(1 of 2),078	
7.	PCWRITE(2 of 2).627	
8.	LLSQ.553,ELEMENTARYC.429, UNIFORTH.454,ASSEMBLY.114	429 is the program used in teaching
9.	STAT.MATH.180,MATH.PACK.394,L LINPACK.554.555	Mathematics statics
10.	SIMPLIFIED.472, NEW.FIG.FORTH. 685	this is a language which is not popular used
11.	F77L2 .ARC, HELP.EXE, MATH.ARC	Calculating the property of H_2 by matrix
12.	BWRFITS.ARC,PA.COM,PX.COM, BWR.ARC.,AIRCV.ARC, TABCODF.ARC	physical parameters of some gases
13.	STEAM.ARC,PKARC.COM,PKXARC .COM,MBPROP.FOR,NH_3PROP. EXE,NH_3SAT.FOR,N.EXE.SP-NBS-7.FOR,BP.NBS.FOR	characteristics of NH_3 steam
14.	SUPERZR.FOR,SUPERZR.EXE	Physical parameters of gases & gas mixers

TABLE III

name	gas kind selected	actions	remarks
DDFILL	$C_1, C_2, C_3, i\text{-}C_4, C_4, CO_2,$ AR, $N_2, O_2, CO, H_2S, C_5, i\text{-}C_5$ $C_6, i\text{-}C_6, C_7$	as the composition, temperature, pressure of each component are known, then the filling pressure of each gas can be obtained	this is the simplified program of DDMIX
ZFILL	$N_2, CO_2, H_2S, H_2O, He, CH_4,$ $C_2, C_3, C_4, i\text{-}C_4, C_5, i\text{-}C_5,$ $C_6, C_7, C_8, C_9, C_{10}, O_2$ CO, H_2	1. the critical tem. & pressure of pure gases can be found. 2. the temp. range of saturated gases can be found. 3. components which beyond DDFILL can be made.	
MIPROPS	$H_2, N_2, O_2, Ar, NF_3, CH_4,$ $C_2H_6, C_2H_4, C_3H_8, i\text{-}C_4H_{10}$ $N\text{-}C_4H_{10}$	1. The critical temp., pressure of pure gases can be found. 2. the temp. range of saturated pure gases can be found, also those parameters within the temp. range under saturated conditions. 3. as far two of the density, temp., pressure are known the relevant parameters of pure gas can be obtained.	
DDMIX	same to DDFILL	1. the relevant physical parameters can be obtained from the temp., pressure, composition of the component. 2. the equilibriur and physical parameters under bubbling point, dew point can be found.	
SUPERZ	same to ZFILL	the relevant parameters can be obtained from the composition, temp. pressure of mixed gases.	mainly for gas mixtures
AIRCN	$CH_4, C_2H_6, C_4, N_2,$ $C_5, i\text{-}C_5, O_2, Ar$	the relevant parameters can be obtained from the mixed gases.	mainly for liqu mixtures

S G F I L L I N S T R U C T I O N S

This program was written to operate with a minimum amount of input on the part of the user. To keep the input to an absolute minimum, certain assumptions have been made about the source and recieving cylinders. The program must have: The temperature and pressure of the source cylinders, The total volume of the source cylinders, The desired pressure in the recieving cylinder at the end of the filling process, The total volume of the recieving cylinder, The total heat capacity of the recieving cylinder, and a so called "equilibrium constant" for each gas. This information is contained in the file, BOTTLE.DAT, and therefore, the file BOTTLE.DAT must be present on the same disk drive when using either of the programs SGFILL or SGCHANG. The numbers in BOTTLE.DAT are from my memory about of the equipment in Beijing. These numbers may all be changed by running the accompanying program named SGCHANG. Before you proceed any further run the program SGCHANG to make sure the necessary information about the source and recieving cylinders is correct. Go now to the instructions for SGCHANG.

A sample run of SGFILL is included. The information which must be input by the user is marked in green, both here and on the sample run. To start the program one must enter

SGFILL

Information about the program then comes up on the screen. The allowable components are listed and the computer askes for the total number of components of the desired mixture. The user must then enter that number.

3

The computer then asks for the number and mole fraction of each fluid, one at a time. Enter the number from the table at the top of the screen which corresponds to a fluid you want to be in the mixture. Enter the desired mole fraction of that fluid after the fluid number, separate the two numners by a comma. The order in which you enter the fluids is not important, the computer chooses the most efficient order, or in some cases the only possible order. The computer will also tell you when a mixture is not possible.

The last few lines give the order and cut off pressure for each fluid.

S G C H A N G I N S T R U C T I O N S

Make sure the files BOTTLE.DAT and SGCHANG.EXE are on the current disk drive. Activate the program by entering SGCHANG. The program then writes information to the screen. Sample runs of this program are included, and the information which must be furnished by the user is highlighted in green. Match the sample runs now with the rest of these instructions. The last few lines written to the screen gives a value for the heat capacity of the recieving cylinder (bottle) and an opportunity to change the value if you wish. A notation to "see instruction no 1" referrs to the following.

Instruction No 1.

The heat capacity of the reieiving cylinder is based on the assumption that the cylinder is iron, the heat capacity of iron is 0.11 calories per gram per degree k, and the recieving cylinder weighs 5 pounds. If any of these assumptions are wrong, calculate a new heat capacity and instead of entering a N as seen in the sample run, enter a Y and the computer will ask for a new heat capacity. Enter the new heat capacity and the computer will move on to the next question which is the desired pressure at the end of the preparation process. If whatever the current value is (writeen on the screen) is not correct, change this value in the same manner. The third question is about the total capacity of the recieving cylinder, answer this question in the same way.

The computer then writes a table to the screen which lists the balance of the information which is necessary for SGFILL to run properly. This table is fairly self explanitary. The "COMPONENT NUMBER" is the same number used in SGFILL to designate a particular pure fluid. The corresponding fluid is given in the far right column. The pressure and temperature are the values of the pure fluid source cylinder at the beginning of the injection. The capacity is the total capacity of the source cylinder. The E CONSTANT is the number which in all probability will have to be adjusted on the bases of the composition analysis of mixtures prepared by using SGFILL. This number determines how much of the compression heat is transferred to the wall of the recieving cylinder. When this number is 1.0, the program assumes that all of the heat due to compression has been transferred to the cylinder and when this number is 2.0 the program assumes that none of the heat due to compression has been transferred to the cylinder. The program has been given the value of 1.1 for all fluids which means that 90% of the available heat due to compression has been transferred to the recieving cylinder. A higher number for the E CONSTANT will cause the composition of the corresponding gas to be higher in a mixture and a lower E CONSTANT will result in a lower composition of that gas in the mixture.

Instruction No 2.

If you want to change any of these numbers, enter a Y if the numbers are correct enter a N.

Instruction No 3.

You have a choice of two ways to change the numbers in the table. If you want to change anything other than the E CONSTANT, you must choose the direct change option. To do this enter a Y. Two sample runs have been included to illustrate the two change options. If the direct change option is chosen, an entire line must be changed. Follow the instructions from the program and study the example in the sample run.

Instruction No 4.

A second option to the direct change option is provided to allow changing the E CONSTANT only. This option was provided to allow the use of actual experimental data. For example if a mixture was prepared according to the sample run of SGFILL, and a composition analysis of that mixture revealed a composition of .099 for hydrogen when the original composition was specified as .1, these numbers were used in the second sample print out of SGCHANG. Study the first example of SGCHANG and then look at the second example of SGCHANG, note that the E CONSTANNT for hydrogen was changed by the first example, and that the second example changes the E CONSTANT for hydrogen back to its original value.

The last question from the computer gives you a chance abort the changes if you think you have done something wrong.

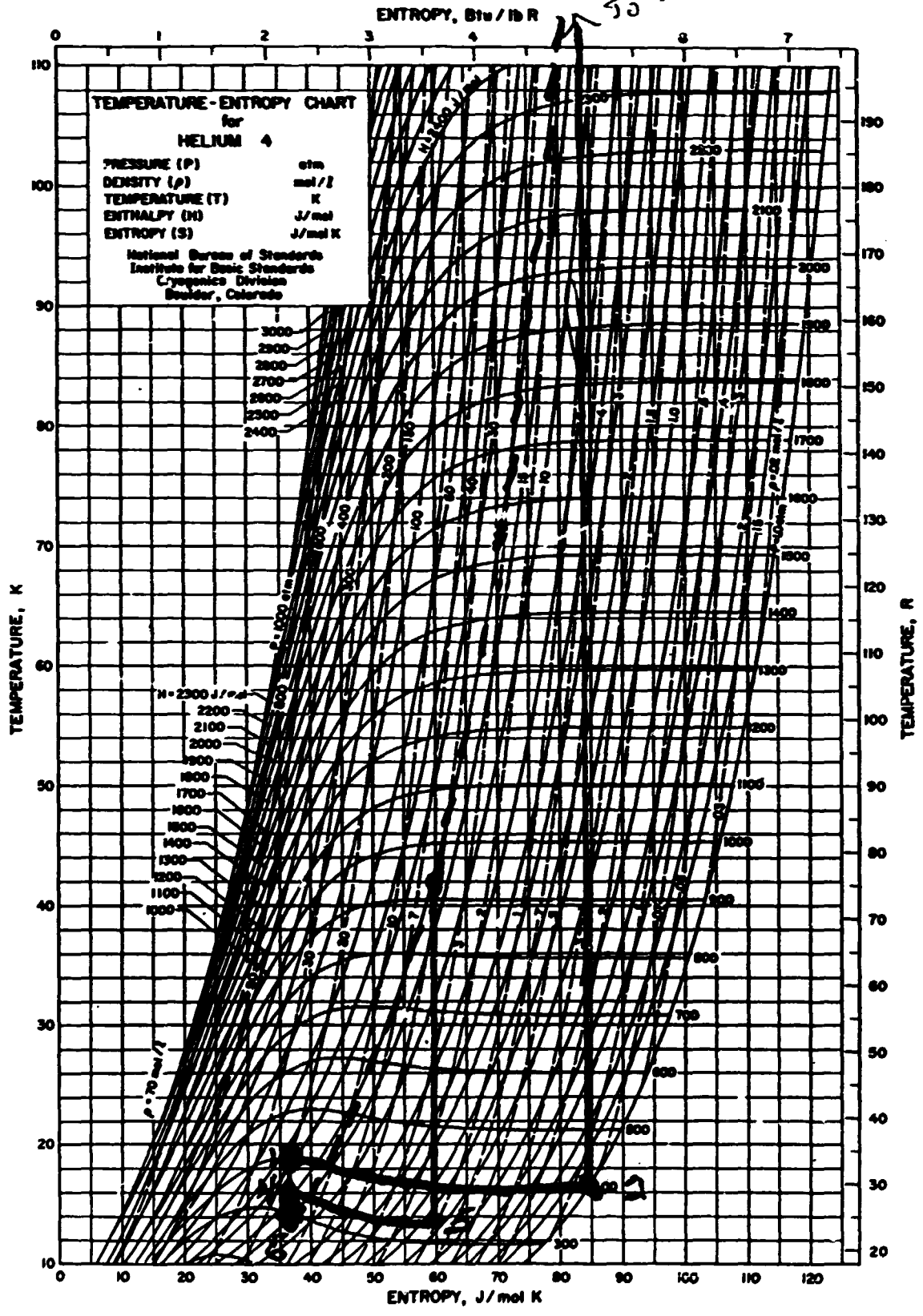

FIGURE 37. Temperature-entropy diagram for helium between 10 and 110 K

```
s1;50H13:25:52.64       Thu 12-01-1988uA:\>SGFILL
  THIS IS A COMPUTER PROGRAM WRITTEN BY ROBERT D.MCCARTY FOR THE BEIJING
SPECIALTY GAS RESEARCH INSTITUTE.  THE PROGRAM IS DESIGNED TO AID THE
PREPARATION OF GASEOUS MIXTURES BY INJECTING PURE GASES INTO A RECEIVING
CYLINDER, OF SPECIFED SIZE, ONE AT A TIME, IN A SEQUENCE SPECIFIED BY THIS
PROGRAM.   THE ALLOWABLE GASES ARE AS FOLLOWS.

1=HYDROGEN, 2=NITROGEN, 3=OXYGEN,4=ARGON,5=NITROGEN TRIFLOURIDE 6=METHANE,

7=ETHANE, 8=ETHYLENE, 9=PROPANE, 10=ISO PENTANE,11=NORMAL PENTANE,

12=DEUTTERIUM, 13=HELIUM, 14=CARBON DIOXIDE, 15=CARBON MONOXIDE


ENTER THE NUMBER OF COMPONENTS IN THE MIXTURE

3
ENTER COMPONENT NUMBER,AND MOL FRACTION
1,.1
ENTER COMPONENT NUMBER,AND MOL FRACTION
2,.2
ENTER COMPONENT NUMBER,AND MOL FRACTION
3,.7

DENSITY OF TARGET MIXTURE IS  4.088 MOLES/LITER


THE REQUIRED MASS OF H2   IS  .41 MOLES
THE REQUIRED MASS OF N2   IS  .82 MOLES
THE REQUIRED MASS OF O2   IS 2.86 MOLES


  TEMP OF FIRST COMPONENT AT END OF ISENTROPIC PATH      355. KELVIN
TEMP OF FIRST COMPONENT AFTER HEAT LOSS TO CYLINDER      304. KELVIN


INJECT O2   INTO RECIEVING CYLINDER TO A PRESSURE OF   6.99  MPA
INJECT N2   INTO RECIEVING CYLINDER TO A PRESSURE OF   9.12  MPA
INJECT H2   INTO RECIEVING CYLINDER TO A PRESSURE OF  10.33  MPA
Stop - Program terminated.
```

```
s1;50H13:26:51.52        Thu 12-01-1988uA:\>SGCHANG
 THIS PROGRAM ALLOWS THE USER TO CHANGE THE PERFORMANCE  OF THE PROGRAM
"SGFILL" WITHOUT RECOMPILING THE PROGRAM. THIS IS ACCOMPLISHED
BY CHANGING CERTAIN CONSTANTS WHICH DETERMINE THE AMOUNT OF HEAT
THAT IS TRANSFERRED FROM THE GAS IN THE RECIEVING CYLINDER
TO THE WALLS OF THE RECIEVING CYLINDER AS EXPLAINED IN THE
ACCOMPANYING LETTER .


PROCEED NOW BY REFERRING TO THE INSTRUCTION SHEET FOR THIS PROGRAM


THE PROGRAM IS CONFIGURED AS FOLLOWS


   THE HEAT CAPACITY OF THE RECIEVING BOTTLE IS       953. JOULES

DO YOU WANT TO CHANGE THIS NUMBER ?  SEE INSTRUCTION NO 1
ENTER Y OR N
N
THE FINAL DESIRED PRESSURE OF THE RECIEVING CYLINDER IS       10.0 MPA

DO YOU WANT TO CHANGE THIS NUMBER ?  SEE INSTRUCTION NO 1
ENTER Y OR N
N
THE CAPACITY OF THE RECIEVING CYLINDER IS  1.0 LITERS

DO YOU WANT TO CHANGE THIS NUMBER ?  SEE INSTRUCTION NO 1
ENTER Y OR N
N
THE STARTING PRESSURE, TEMPERATURE , CAPACITY AND EQUILIBRIUM CONSTANTS

OF THE SOURCE BOTTLES ARE:

COMPONENT PRESSURE TEMPERATURE  CAPACITY E CONSTANT
 NUMBER     MPA       DEG K      LITERS
    1       40.00     300.00     100.00     1.10      H2
    2       40.00     300.00     100.00     1.10      N2
    3       40.00     300.00     100.00     1.10      O2
    4       40.00     300.00     100.00     1.10      AR
    5       40.00     300.00     100.00     1.10      NF3
    6       40.00     300.00     100.00     1.10      CH4
    7       40.00     300.00     100.00     1.10      C2H4
    8       40.00     300.00     100.00     1.10      C2H6
    9       40.00     300.00     100.00     1.10      C3H8
   10       40.00     300.00     100.00     1.10      IC4
   11       40.00     300.00     100.00     1.10      NC4
   12       40.00     300.00     100.00     1.10      D2
   13       40.00     300.00     100.00     1.10      HE
   14       40.00     300.00     100.00     1.10      CO2
   15       40.00     300.00     100.00     1.10      CO
DO YOU WANT TO CHANGE ANYTHING IN THE ABOVE TABLE ?
SEE INSTRUCTION NO 2, ENTER Y/N

Y
YOU HAVE A CHOICE BETWEEN A DIRECT CHANGE IN THE NUMBERS  AND A CHANGE BASED
DATA OBTAINED FROM A PREVIOUS ATTEMPT  AT PREPARING A MIXTURE
SEE INSTRUCTION NO 3

DO YOU WANT A DIRECT CHANGE ? ENTER Y/N

N
```

BY USING DATA FROM THE EXPERIMENTALY DETERMINED COMPOSITIOIN OF A MIXTURE
PREPARED BY USING THE PROGRAM "SGFILL". SEE INSTRUCTION NO 4

ENTER THE NUMBER OF CHANGES TO BE MADE

1
THE STARTING PRESSURE, TEMPERATURE , CAPACITY AND EQUILIBRIUM CONSTANTS

OF THE SOURCE BOTTLES ARE:

COMPONENT NUMBER	PRESSURE MPA	TEMPERATURE DEG K	CAPACITY LITERS	E CONSTANT	
1	40.00	300.00	100.00	1.10	H2
2	40.00	300.00	100.00	1.10	N2
3	40.00	300.00	100.00	1.10	O2
4	40.00	300.00	100.00	1.10	AR
5	40.00	300.00	100.00	1.10	NF3
6	40.00	300.00	100.00	1.10	CH4
7	40.00	300.00	100.00	1.10	C2H4
8	40.00	300.00	100.00	1.10	C2H6
9	40.00	300.00	100.00	1.10	C3H8
10	40.00	300.00	100.00	1.10	IC4
11	40.00	300.00	100.00	1.10	NC4
12	40.00	300.00	100.00	1.10	D2
13	40.00	300.00	100.00	1.10	HE
14	40.00	300.00	100.00	1.10	CO2
15	40.00	300.00	100.00	1.10	CO

ENTER FLUID NUMBER, SPECIFIED COMPOSITION, AND EXPERIMENTAL COMPOSITION

1,.1,.099
DO YOU WANT THE CHANGES (IF ANY) TO BE PERMANANT ? Y/N
Y