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REPORT NO.
TDR-69(2240-51)TR-2

The Aerospace Corporation Computer Programs for the Solution of Multielement Chemical Equilibria

28 JUNE 1962

Prepared by
S. A. GREENE
Materials Sciences Laboratory
and
H. J. VALE
Computation and Data Processing Center

Prepared for DEPUTY COMMANDER AEROSPACE SYSTEMS
AIR FORCE SYSTEMS COMMAND
UNITED STATES AIR FORCE
Inglewood, California

LABORATORIES DIVISION • AEROSPACE CORPORATION
CONTRACT NO. AF 04(695)-69

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ABSTRACT

Work has been completed on a generalized method for the analytical solution of complex multielement chemical equilibria under all conditions of pressure, temperature, and mass balance. The programs are written for the IBM 7090 and use a unique technique of majors and minors to guarantee automatic convergence. Variations of the basic solution method are applied to problems in chemical synthesis, thermal stability, and chemical compatibility. The programs are also used to obtain theoretical rocket propellant performance and Mollier diagrams.

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NOMENCLATURE

a	speed of sound
$a_{i,j}$	number of atoms of ith element in jth chemical constituent
A	area
c	specific heat
c^*	characteristic velocity
c_p^t	total specific heat of mixtures
C	molar heat capacity
C_F	thrust coefficient
(c_j)	coefficient matrix of the jth constituent based on element columns (column matrix)
$(C.M.)^{-1}$	inverted coefficient matrix of major products based on element rows
F	free energy
g	gravitational constant
h	specific enthalpy
H	molar enthalpy
ΔH_f	heat of formation
H_o^o	arbitrary constant associated with elements
H_T^o	sum of sensible energy and heat of formation
I_s	specific impulse
J	mechanical equivalent of heat
K	equilibrium constant

$\dot{m}$	weight flow rate
M	molecular weight
n	moles
N	weight of gas or solid
p	pressure
(p_m)	partial pressure matrix of major products based on element rows (row matrix)
R	gas constant
S	molar entropy
s	specific entropy
T	temperature
u	velocity
v	specific volume
x_g	weight fraction of gases
γ	isentropic exponent
ϵ	area ratio
ρ	density
σ_i	total number of atoms of ith element in system

Superscripts

g	gaseous species
s	condensed species

Subscripts

e	exit conditions
g	gaseous species

p	constant pressure
s	condensed species
t	throat conditions
v	constant volume

I. INTRODUCTION

The position of equilibrium in complex (multielement) chemical systems can be computed from first principles. Given selected thermodynamic and thermochemical data associated with reactants and all possible products, the distribution between products and reactants may be uniquely determined at all pressures, temperatures, and stoichiometries. Required data include: heat capacity, entropy, and heat of formation of products and reactants.

The thermodynamic equations that describe systems which contain many elements cannot be solved in closed form and require iterative procedures. These procedures use thermodynamic properties of constituents as input data. It is the purpose of this report to outline the capabilities and applications of a unique computational procedure for the solution of multielement chemical equilibria. The approach uses a technique of majors and minors to assure automatic convergence.

II. OUTLINE OF PROGRAM

Computer programs which solve complex chemical equilibria may be divided into two categories. One type defines equilibria between constituents and their atomic gases; the other, between the constituents which are present in major quantity and the remainder of the products. These are known as methods of minors and majors, respectively.

The former has the advantage of being general in approach, but it is logically complex. It also leads to numerical difficulties at low temperatures where the concentrations of atomic gases become vanishingly small. The latter has the advantage of rapid and certain convergence provided products are selected which are indeed present in major quantity. However, during expansion (and cooling) of equilibrium products, the major products generally change and provision must be made to examine and reselect major products.

The program system described herein combines the flexibility of the minors approach with the convergence advantages of the majors technique. The detailed logic and numerical methods utilized by the program will not be presented here, but they will be the subject of a future report. The calculational procedure is qualitatively the following:

a) The problem is solved at 3000 K using the minors technique. At 3000 K, the concentration of atomic gases is adequately high and convergence is assured.

   Since iterative procedures are utilized, it is necessary to initiate the problem with an estimate of the concentrations of atomic gases. These estimates are stored internally within the program and obviate guesses by the program user. Mass balance and pressure balance equations are applied, and the solution at 3000 K is attained even though the initial atomic gas concentration guesses may be incorrect by factors of 10^{10}.

b) When initial convergence has been attained, a generalized major product selection routine is given control. A set of major products may be defined as that list of products in which each element appears at least once and which contains the majority of the elements.* As many major products are chosen as there are elemental types. Only gaseous products are considered as candidates. The routine can select a new set of major products at any time during the problem solution.

A. Basic Equations

Some of the basic equations which are solved in the program may be represented by the following:

1. Conservation of Atomic Types (Mass Balance)

$$\sigma_i = \sum_{j=1}^{\beta} a_{i,j} n_j \qquad (1)$$

2. Conservation of Pressure

$$p = \sum_{j=1}^{\beta} p_j \qquad (2)$$

3. Chemical Equilibrium

$$K_j = \frac{p_j}{\prod_{i=1}^{n} (p_i)^{a_{i,j}}} \qquad (3)$$

*The mathematically rigorous definition will be presented in the previously mentioned, future report.

or using matrix notation for the generalized major product solution

$$\ln K_j = \ln p_j - (C.M.)^{-1} (C_j) (p_m)$$

and, since

$$\Delta F = \Delta H - T\Delta S = -RT \ln K \tag{4}$$

we have

$$\ln K_j = \frac{-\Delta H}{RT} + \frac{\Delta S}{R} \tag{5}$$

4. Conservation of Static Enthalpy

$$h = \sum_{j=1}^{\beta} n_j (H_T^o)_j \tag{6}$$

B. Minors Technique

Using the method of minors, equilibrium constants for constituents are computed in terms of equilibrium between the constituents and their atomic gases. To illustrate, consider the system H, O, OH, and H_2O; equilibria are set up in terms of

$$OH = O + H \tag{7}$$

$$H_2O = O + 2H \tag{8}$$

The thermodynamic state of the system is fixed by specifying the total amounts of the elements, σ_i, and the total pressure, p. The state of the system can be redefined in terms of pressure, temperature, and concentrations of atomic gases, from which the concentration of the chemical constituents may be computed.

For solution at a given temperature, estimates of the concentration of atomic gases are made from which concentration of constituents follow; the mass balance and total pressure restraints are, of course, taken into account. The equilibrium constants for OH and H_2O are, respectively,

$$\ln K_{OH} = -\left[\frac{(H_T^o)_{OH} - (H_T^o)_H - (H_T^o)_O}{RT}\right] + \left[\frac{(S_T^o)_{OH} - (S_T^o)_H - (S_T^o)_O}{R}\right] \quad (9)$$

$$\ln K_{H_2O} = -\left[\frac{(H_T^o)_{H_2O} - 2(H_T^o)_H - (H_T^o)_O}{RT}\right] + \left[\frac{(S_T^o)_{H_2O} - 2(S_T^o)_H - (S_T^o)_O}{R}\right] \quad (10)$$

From the $\ln K_j$ values, the partial pressures of the jth chemical constituents are computed using Eq. (3). Where the problem is one of combustion at constant pressure, and a flame temperature is sought, the restraint of Eq. (6) must be considered.

Estimates of concentration (and temperature, when necessary) are repeated until convergence is obtained; the iteration controls and sequencing are complex and are beyond the scope of this report.

C. Majors Technique

Each element in a problem requires a major product, and all elements must be represented in the major products at least once. If we select H_2O and H as the major products in the system H, O, OH, and H_2O, then

$$H_2O - H - OH \quad (11)$$

$$H_2O - 2H = O \tag{12}$$

and all products are represented. Equations (9) and (10) then become

$$\ln K_{OH} = -\left[\frac{(H_T^o)_{OH} - (H_T^o)_{H_2O} + (H_T^o)_H}{RT}\right] + \left[\frac{(S_T^o)_{OH} - (S_T^o)_{H_2O} + (S_T^o)_H}{R}\right] \tag{13}$$

$$\ln K_{H_2O} = -\left[\frac{(H_T^o)_O - (H_T^o)_{H_2O} + 2(H_T^o)_H}{RT}\right] + \left[\frac{(S_T^o)_O - (S_T^o)_{H_2O} + 2(S_T^o)_H}{R}\right] \tag{14}$$

For each nonmajor product, one equilibrium constant needs to be computed.

D. Program Construction

The program is coded in the FORTRAN system and will run on any IBM 7090 EDPM with two on-line channels of at least 7-tape units per channel. The program will consider up to 150 chemical constituents and a maximum of 15 chemical elements per problem.

Each complete program consists of an input or precomputation section, the main computation program, and an output program. A schematic is shown in Fig. 1.

When the program recognizes the chemical elements involved in the problem, the thermodata tape is searched, and all constituents which contain these elements are transferred into core with their corresponding tabular thermodynamic data. A program sophistication allows the program user to specify these constituents which are to be considered, if he so desires.

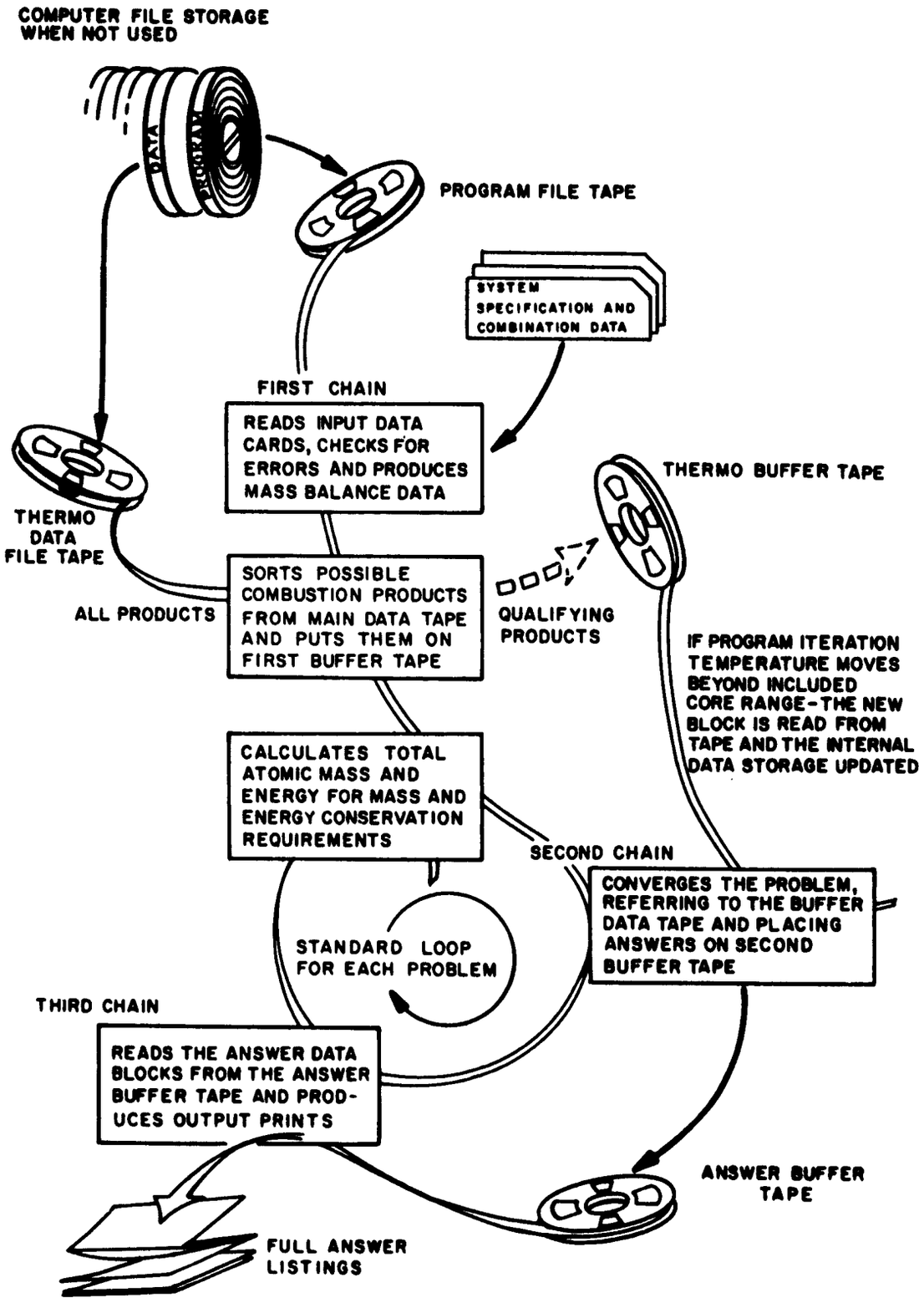

Fig. 1. Program Construction

The technique for the solution of chemical equilibria is sufficiently general and independent of application so that it may be incorporated into a variety of special purpose programs. To date, the following computation programs are included:

1) Chemical Equilibria,

2) Adiabatic Flame Composition,

3) Mollier Diagrams, and

4) Theoretical Rocket Propellant Performance.

In the FORTRAN programming system, all main programs form chain links and use the same program library and thermodynamic data reference tapes.

The precomputation, or input, program produces the mass balance and data verification sheets. The input data consists of the following information:

1) tape unit specification of all tapes including input, output, data library, and program library;

2) titles;

3) control indicators to select the proper computation program;

4) ingredient formulation consisting of name, elements, and coefficients contained and heat of formation of the ingredient;

5) combination ratio of ingredients: either moles of each, mole per cent, weight per cent, or mixture ratio;

6) specifically included or excluded constituents - optional; and

7) any specific data applicable to the computation chain involved, such as enthalpy-entropy boundaries in the Mollier diagram.

All control is internal within each computational program; no computer console settings are required. The only special treatment involved is the loading of the thermodynamic reference tape and the program library. All iteration loops are checked for iteration limits, and an exit procedure is initiated in case of excessive loopings.

The programs named above use a basic solution block consisting of four subroutines. These perform the functions of examining major products, building and solving the iteration matrices, and applying the matrix answers. The same subroutines are used in all main calculation programs. The varying types of solutions are obtained by means of control indicators set in the main program and used in the basic block. The basic block can construct and solve any of the following equation systems:

1) constant temperature solution of mass balance and pressure balance equations;

2) solution of mass and pressure balance equations plus an enthalpy balance-seeks a flame temperature;

3) system (1) plus entropy balance (isentropic expansion to assigned pressure);

4) constant total enthalpy solution and entropy balance (expansion to assigned mach number);

5) constant entropy point solution (to obtain $(\partial p/\partial \rho)_s$ for acoustic velocity determinations); and

6) constant pressure point solution (to obtain $(\partial n/\partial T)_p$ for C_p determination).

The only program using all the available matrices is the Rocket Propellant Performance Program. The Chemical Equilibria, Mollier Diagram, and Adiabatic Flame Composition Programs use combinations of (1) and (2).

III. THERMODYNAMIC DATA

From Eqs. (9) and (10) we see that thermodynamic data required for the solution of equilibrium constants include entropy and enthalpy. Since

$$H_T^o = \Delta H_f^o + \int_o^T C_p \Delta T \tag{15}$$

we find that H_T^o is the sum of the sensible enthalpy and chemical energy (heat of formation). Aside from entropy, we require heat capacity and heat of formation data.

Data which are currently available to the Computer Program include the important products of the elements listed in Table 1. While ionic species are not yet included, provision has been made for their incorporation (E is electron). Data on the thermodynamic data tape are composed of heat of formation and heat capacity, enthalpy, and entropy in tabular form from 0 to 6000 K in 100 deg increments. Table 2 illustrates a dump of a constituent contained on the tape.

A. JANAF Thermochemical and Thermodynamic Data Tables

In order to furnish Department of Defense contractors with consistent tables of thermodynamic and thermochemical data, the Joint Army-Navy-Air Force Thermochemical Panel was established in 1960. Under AF 33(616)-6149 and numerous other contracts, thermodynamic data were to be compiled, generated, evaluated, and disseminated in tabular form and on IBM cards. Main contributors include the Dow Chemical Co. (who issue the Tables), National Bureau of Standards, U. S. Bureau of Mines (Bartlesville), and the University of Wisconsin. Table 3 illustrates the format of the tables, while Table 4 shows data documentation observed on their reverse side.

Table 1

Elements Contained on Thermodynamic Data Tape

MAR 29, 1962

AEROSPACE CORP.

THERMODYNAMIC DATA LISTING OF 62 3/28/62

ELEMENTS CONTAINED ON THIS TAPE ARE AS FOLLOWS

H	34.72039986
HE	0.
C	92.21359921
N	1.88579999
O	2.05544999
MG	253.54669952
AL	233.62509918
SI	250.18759918
AR	0.
K	-20.02899981
CA	-44.55899954
BR	2.50000000
RB	-19.02899981
ZR	389.66699982
E	61.48099995

NUMBER OF ELEMENTS=30 NUMBER OF PRODUCTS=278

Table 2

Example of Tabular Data Contained on Thermodata Tape

MAR 29, 1962

AEROSPACE CORP.

THERMODYNAMIC DATA CARDING OF TITLE

RECORD 240 OF TAPE NO. 47

STATE INDICATOR 1

T	CP	H	S	T	CP	H	S	T	CP	H	S
0.	0.	-4.[illegible]									
50.00	15.[illegible]	-4.[illegible]									
100.00	15.880	-3.987	62.922	2000.00	25.752	43.097	131.748	4100.00	25.814	97.264	150.261
150.00	17.621	-2.875	68.230	2100.00	25.759	45.672	133.004	4200.00	25.815	99.845	150.883
200.00	20.538	-2.143	75.621	2200.00	25.766	48.249	134.203	4300.00	25.816	102.427	151.491
[illegible]											
298.15	22.843	0.	[illegible]								
300.00	22.[illegible]	[illegible]									
400.00	24.007	2.393	91.102	2600.00	25.785	58.559	138.509	4700.00	25.819	112.754	153.787
500.00	24.611	4.826	96.530	2700.00	25.789	61.138	139.482	4800.00	25.820	115.336	154.331
600.00	24.963	7.307	101.051	2800.00	25.792	63.717	140.420	4900.00	25.820	117.918	154.863
[illegible]											
1000.00	25.509	17.427	113.964	3200.00	25.802	74.036	143.865	5300.00	25.822	128.247	156.869
1100.00	25.564	19.981	116.398	3300.00	25.804	76.616	144.659	5400.00	25.823	130.829	157.372
1200.00	25.607	22.539	118.624	3400.00	25.806	79.197	145.429	5500.00	25.823	133.411	157.866
[illegible]											
1600.00	25.705	32.805	126.006	3800.00	25.811	89.520	148.300	5900.00	25.825	143.741	159.659
1700.00	25.720	35.376	127.565					6000.00	25.825	146.323	160.093

Table 3

JANAF Thermodynamic Data Table

Beryllium (Be)

(Ideal Gas) Mol. Wt. = 9.013

T, °K.	C_p° (cal. mole^{-1}deg.$^{-1}$)	S° (cal. mole^{-1}deg.$^{-1}$)	$-(F^\circ-H^\circ_{298})/T$ (cal. mole^{-1}deg.$^{-1}$)	$H^\circ-H^\circ_{298}$ (kcal. mole^{-1})	ΔH_f° (kcal. mole^{-1})	ΔF_f° (kcal. mole^{-1})	Log K_p
0	.000	.000	INFINITE	-1.481	77.241	77.241	INFINITE
100	4.968	27.118	34.062	-.984	77.728	79.029	-103.060
200	4.968	30.561	32.990	-.488	78.087	72.177	- 78.867
298	4.968	32.545	32.545	.000	78.255	69.231	- 50.745
300	4.968	32.576	32.545	.009	78.257	69.175	- 50.302
400	4.968	34.005	32.760	.506	78.315	66.137	- 36.134
500	4.968	35.114	33.108	1.003	78.307	63.093	- 27.576
600	4.968	36.019	33.520	1.500	78.262	60.053	- 21.873
700	4.968	36.785	33.933	1.996	78.187	57.024	- 17.803
800	4.968	37.449	34.332	2.493	78.089	54.007	- 14.753
900	4.968	38.036	34.711	2.990	77.969	51.004	- 12.385
1000	4.968	38.557	35.070	3.487	77.825	48.015	- 10.493
1100	4.968	39.031	35.409	3.984	77.658	45.042	- 8.949
1200	4.968	39.465	35.729	4.481	77.466	42.085	- 7.664
1300	4.968	39.861	36.032	4.977	77.251	39.146	- 6.581
1400	4.968	40.229	36.319	5.474	77.012	36.223	- 5.654
1500	4.968	40.572	36.591	5.971	76.748	33.318	- 4.854
1600	4.968	40.892	36.850	6.468	73.706	30.511	- 4.167
1700	4.968	41.193	37.097	6.965	73.510	27.817	- 3.576
1800	4.968	41.477	37.332	7.461	73.309	25.135	- 3.052
1900	4.968	41.746	37.557	7.958	73.103	22.464	- 2.584
2000	4.969	42.001	37.773	8.455	72.892	19.804	- 2.164
2100	4.969	42.243	37.980	8.952	72.676	17.155	- 1.785
2200	4.970	42.474	38.179	9.448	72.454	14.516	- 1.442
2300	4.972	42.695	38.371	9.946	72.229	11.889	- 1.130
2400	4.974	42.907	38.556	10.443	71.998	9.271	- .844
2500	4.977	43.110	38.736	10.941	71.761	6.661	- .582
2600	4.982	43.306	38.906	11.438	71.521	4.069	- .342
2700	4.988	43.494	39.072	11.937	71.278	1.473	- .119
2800	4.997	43.675	39.234	12.437	.000	.000	.000
2900	5.007	43.851	39.390	12.937	.000	.000	.000
3000	5.021	44.021	39.541	13.438	.000	.000	.000
3100	5.037	44.186	39.688	13.941	.000	.000	.000
3200	5.057	44.346	39.832	14.446	.000	.000	.000
3300	5.081	44.502	39.971	14.953	.000	.000	.000
3400	5.109	44.654	40.106	15.462	.000	.000	.000
3500	5.142	44.802	40.238	15.975	.000	.000	.000
3600	5.179	44.948	40.367	16.491	.000	.000	.000
3700	5.221	45.090	40.493	17.010	.000	.000	.000
3800	5.268	45.230	40.616	17.535	.000	.000	.000
3900	5.320	45.368	40.736	18.064	.000	.000	.000
4000	5.378	45.503	40.853	18.599	.000	.000	.000
4100	5.440	45.637	40.968	19.140	.000	.000	.000
4200	5.508	45.768	41.081	19.687	.000	.000	.000
4300	5.581	45.899	41.192	20.242	.000	.000	.000
4400	5.658	46.028	41.300	20.804	.000	.000	.000
4500	5.741	46.156	41.406	21.374	.000	.000	.000
4600	5.828	46.283	41.511	21.952	.000	.000	.000
4700	5.919	46.410	41.614	22.539	.000	.000	.000
4800	6.014	46.535	41.715	23.136	.000	.000	.000
4900	6.113	46.660	41.815	23.742	.000	.000	.000
5000	6.215	46.784	41.913	24.359	.000	.000	.000
5100	6.320	46.909	42.010	24.985	.000	.000	.000
5200	6.428	47.033	42.105	25.623	.000	.000	.000
5300	6.538	47.156	42.198	26.271	.000	.000	.000
5400	6.650	47.279	42.292	26.930	.000	.000	.000
5500	6.765	47.402	42.384	27.601	.000	.000	.000
5600	6.877	47.525	42.475	28.283	.000	.000	.000
5700	6.993	47.648	42.566	28.976	.000	.000	.000
5800	7.109	47.771	42.655	29.681	.000	.000	.000
5900	7.224	47.894	42.741	30.398	.000	.000	.000
6000	7.340	48.019	42.828	31.126	.000	.000	.000

September 30, 1961

JANAF THERMOCHEMICAL DATA

Compiled and Calculated by THE DOW CHEMICAL COMPANY, THERMAL LABORATORY, Midland, Michigan

Table 4

Data Table Documentation

BERYLLIUM (Be) (IDEAL GAS) MOL. WT. = 9.013

ΔH°_{f0} = 77.241 kcal. mole^{-1} $\Delta H^\circ_{f\ 298.15}$ = 78.25 ± 0.5 kcal. mole^{-1}

Ground State Configuration $^1S_0$ $S^\circ_{298.15}$ = 32.545 cal. deg.$^{-1}$ mole^{-1}

Electronic Levels and Multiplicities

ϵ_i, cm.$^{-1}$	g_i	ϵ_i, cm.$^{-1}$	g_i	ϵ_i, cm.$^{-1}$	g_i
0.0	1	67943	15	73089	3
21980	9	68781	5	73141	1
42565	3	69009	3	73520	5
52082	3	69322	1	73608	1
54677	1	69634	9	73803	15
56432	5	70606	15	73867	5
58791	9	71002	5	73930	1
59696	9	71162	3	74071	15
60187	3	71320	1	74117	5
62054	15	71483	9	74163	1
64428	5	71499	1	74269	15
64507	3	72030	15	74301	5
65245	1	72251	5	74416	15
65949	9	72355	3	74443	5
67228	3	72448	1	73430	15
		72882	15		
		73017	5		

Heat of Formation.

Derived from a third law analysis of the vapor pressure data. See Be crystal for references.

Heat Capacity and Entropy.

Electronic levels and multiplicities from C. E. Moore, Natl. Bur. Standards Circ. 467 (1949).

These data are used almost exclusively. Data are updated biannually by the Panel, and working meetings are held triannually. Information on almost 550 solid, liquid, and gaseous constituents are available over the 0 to 6000K range or where applicable.

While the tabular data are currently available only to 6000 K, no difficulties are anticipated in extending this range. The Tables may simply be extended by appropriate calculation or a simple routine utilized within the computational program which would extrapolate data to temperatures greater than 6000 K. There is no limit to the maximum temperature, provided ionic* species are considered.

B. Calculation of Thermodynamic Data

The bases for thermodynamic data calculation are standard to statistical mechanics.

Assignments for ideal monoatomic gases include translation and electronic contributions.

For ideal diatomic gases, contributions from translation, rotation, vibration, and electronic transitions are included. When available, spectroscopic constants are utilized; otherwise, appropriate molecular models are used. Anharmonicity corrections are made when adequate data are available.

For linear polyatomic molecules, anharmonic corrections are neglected.

The rigid rotator, harmonic oscillator approximation is utilized for nonlinear polyatomic molecules, and anharmonic corrections are neglected.

Thermodynamic data of condensed phases rest upon either measured or estimated heat capacity data. Heats of transition are either experimentally determined or theoretically estimated and are included in enthalpy and entropy totals.

*The present computation system automatically adds a charge balance equation when ionic species are included in the problem.

C. Determination of Thermochemical Data

Generally, the most important thermodynamic or thermochemical datum is the heat of formation of the constituent. Heats of formation are directly obtained from calorimetric measurements or indirectly from bond energy contributions as estimated from spectroscopic data or calorimetric data. Second law heats are utilized as indirect estimates when necessary.

D. Thermodata Tape Monitor Programs

Programs which maintain and update the thermodata tape are independent of the calculational program. The monitor routines will alter any of the data as given in Table 2 as well as add or delete elements or constituents. In every case of data alteration, the tape identification number is updated as the first action. Where different individuals require their specific data tapes, a number of tapes may be written.

IV. PROGRAM APPLICATIONS

The development of the capability to predict chemical equilibria in systems under analytical or experimental investigation is a valuable adjunct to problems involving chemical synthesis, materials development and testing, laboratory flames, chemical propulsion, and aerodynamics. Whenever possible, thermodynamic calculations should be applied to experimental programs. Consideration of the thermodynamics of the situation can save a great deal of experimentation in terms of a priori analysis.

A. Chemical Synthesis

Experimental attempts to create new molecules through synthesis or high temperature equilibration can be placed on a sound basis by computing the equilibrium composition of products under specified reaction conditions. For illustrative purposes, consider the synthesis of nitric oxide (NO) by the high temperature equilibration (over a catalyst) of an arbitrarily chosen equimolar mixture of nitrogen and oxygen. (See Tables 5 - 10.) Input data to the program include the following which must be specified:

1) molar or weight concentrations of reactants;

2) total pressure(s) at equilibration; and

3) temperature(s) at equilibration.

For an example (only a few points are illustrated), 69 temperatures from 6000 to 300 K were computed at a total pressure of 1 atm in 2.6 min. Between 6000 and 1000 K, temperature increments were 100 K; 1000 to 500 K, increments were 50 K; and 500 to 298.16 K, increments were 25 K.

Table 5 shows the problem definition and mass balance sheets followed by an automatic statement of the products selected for consideration and their heats of formation (Table 6). Tables 7 - 10 show the computed equilibria at various temperatures. Included are their reactant and product concentrations and their individual heat capacities (CP), enthalpies, entropies, and free

Table 5

Problem Definition and Input Verification

AEROSPACE CORPORATION
EXAMPLE
CHEMICAL SYNTHESIS

COMPONENT	WEIGHT PERCENT	MOLES	MOLE PERCENT
N2	46.682883	1.00000000	50.00000000
O2	53.319114	1.00000000	50.00000000

ELEMENTS	MOLES	MASS BALANCE (MOLES/GM)
N	1.0000	0.33324447E-01
O	1.0000	0.33324447E-01

INPUT VERIFICATION

COMPONENT N2
N 2.0000 NUMBER OF ELEMENTS 1 HEAT OF FORMATION (KCAL/MOLE)= 0.
COMPONENT O2
O 2.0000 NUMBER OF ELEMENTS 1 HEAT OF FORMATION (KCAL/MOLE)= 0.

Table 6

Products Selected from Thermodata Tape

N_2/O_2

********** PRODUCTS CHOSEN ARE THE FOLLOWING		
N	HEAT OF FORMATION	112.96504402
C	HEAT OF FORMATION	59.55014181
NO	HEAT OF FORMATION	21.59794998
NO2	HEAT OF FORMATION	8.09150577
N2	HEAT OF FORMATION	-0.00000024
N2O	HEAT OF FORMATION	19.49022865
C2	HEAT OF FORMATION	0.
C3	HEAT OF FORMATION	33.99998856

Table 7

Equilibration of N_2 and O_2 at 6000 K

TAPE 40 7/14/61

EXAMPLE CHEMICAL SYNTHESIS

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 6000.00
SYSTEM ENTHALPY (KCAL/GM) 4.6096
SYSTEM ENTROPY (CAL/GM-DEG) 3.1499
SYSTEM GAS CP 0.33923

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
N	0.11853045	6.1000	144.6299	51.8219	-[illegible]
O	0.61826207	5.3234	90.5893	53.6547	-[illegible]
NO	0.01134531	9.3128	75.7274	75.1873	-375.3966
NO2	0.00000000	13.8657	90.1947	86.6732	-429.8443
N2	0.25086433	9.1652	53.0095	69.9966	-366.9698
N2O	0.00000039	14.8357	106.[illegible]689	91.8208	[illegible]
O2	0.00099743	10.2790	57.5892	74.8098	-[illegible]
O3	0.00000000	13.8840	117.2317	95.3925	[illegible]

Table 8

Equilibration of N_2 and O_2 at 3500 K

TAPE 40 7/14/61

EXAMPLE

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 3500.00
SYSTEM ENTHALPY (KCAL/GM) 1.7033
SYSTEM ENTROPY (CAL/GM-DEG) 2.5035
SYSTEM GAS CP 0.31220

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
N	0.00014004	5.0855	130.8096	48.8670	-40.2250
O	0.25614005	5.0412	77.6383	50.8695	-100.6861
NO	0.06762285	9.0458	52.7646	70.2430	-193.0860
NO2	0.00000057	13.7798	55.6100	79.2188	-221.6557
N2	0.40204521	8.9268	30.3832	65.1239	-197.5503
N2O	0.00000259	14.7067	69.1995	83.8529	-221.2
O2	0.27404840	9.7620	32.3856	69.4683	-210.7
O3	0.00000030	13.8326	82.5691	87.9205	-225.

Table 9

Equilibration of N_2 and O_2 at 2700 K

TAPE 40 7/14/61

EXAMPLE CHEMICAL SYNTHESIS

PRESSURE (ATM) 1.0000

SYSTEM GAS CP 0.30336

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
NO	0.03821791	8.9285	45.5722	67.9105	-137.7862
NO2	0.00000073	13.6931	44.6165	75.6531	-159.6468
N2	0.47479122	8.8006	23.2881	62.8229	-146.3338

Table 10

Equilibration of N_2 and O_2 at 2600 K

EXAMPLE CHEMICAL SYNTHESIS

PRESSURE (ATM) 1.0000

SYSTEM GAS CP 0.30213

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
NO	0.03321348	8.9103	44.6803	67.5739	-131.0118
NO2	0.00000071	13.6766	43.2490	75.1366	-152.1072
N2	0.47942264	8.7792	22.4091	62.4913	-140.0682

energies (H-TS). System enthalpies, entropies, and heat capacities (frozen equilibria) are also tabulated. From the example, it was concluded that a maximum concentration of NO for the given stoichiometry and pressure would be attained at approximately 3500 K.

It should be noted that the program can yield adiabatic flame temperatures. Since the enthalpy* of NO at 298.16 K is

$$h = \frac{\Delta H_f + H_o^o}{M}$$

$$= \frac{+ 21.60 + \left[(1)(1.89) + (1)(2.06)\right]}{30}$$

$$= 0.85 \qquad (16)$$

0.85 kcal/gm, we would calculate that the adiabatic decomposition flame temperature of NO (initially at 298.16 K) is between 2600 and 2700 K (see Tables 9 and 10). Plots of system H vs T over small temperature intervals are linear, and linear interpolation is justified.

B. High Temperature Stability

In many cases it is desired to predict the thermal stability or compatibility of refractories or other materials at elevated temperatures in reactive and inert atmospheres. Tables 11 - 14 illustrate thermodynamic computations of the refractory beryllium oxide in gaseous nitrogen and water vapor. The calculations refer to the stoichiometries

Stability - $BeO + N_2$

Compatibility - $BeO + H_2O$

in closed systems and predict the distribution of products which would be

* ΔH_f from Table 6 and H_o^o from Table 1.

Table 11

Equilibration of BeO and N_2 at 3000 K

EXAMPLE STABILITY

PRESSURE (ATM) 1.0000

SYSTEM GAS CP 0.17128

PRODUCT		MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
O		0.00039491	5.0042	75.1275	50.0955	-75.1590
BEO		0.00006144	9.0667	186.9448	66.1427	-11.4834
BE2O2		0.00027947	19.6799	214.2788	100.0176	-85.7739
BE3O3		0.00001945	28.8561	337.6335	122.8522	-330.9231
NO		0.00042605	8.9773	48.2583	68.8539	-158.3034
NO2		0.00000000	13.7336	48.7308	77.0980	-182.5632
O3		0.00000000	13.8047	75.8593	85.1902	-181.7114
BE	COND	0.	7.5000	152.8641	18.6747	96.8400
BEO	COND	0.49201348	16.0000	36.7120	33.9904	-65.2593

Table 12

Equilibration of BeO and N_2 at 2300 K

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EXAMPLE

STABILITY

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 2300.00
SYSTEM ENTHALPY (KCAL/GM) 0.6324
SYSTEM ENTROPY (CAL/GM-DEG) 1.6356
SYSTEM GAS CP 0.16412

PRODUCT		MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
BE		0.00000177	4.9737	219.1303	42.6955	[illegible]
N		0.00000001	4.9724	124.7971	46.7649	[illegible]
O		0.00000019	4.9797	71.6350	48.7700	-40.5359
BEO		0.00000001	8.9637	180.6317	63.7470	34.0136
BE2O2		0.00000007	19.5481	200.5430	94.8046	-17.5075
BE3O3		0.00000308	31.1472	196.4684	119.5868	[illegible]
BE4O4		0.00000001	42.7463	232.5267	143.4614	[illegible]
BE5O5		0.00000000	54.6851	273.9357	177.3572	[illegible]
BE6O6		0.00000000	66.3691	290.9825	205.1475	-180.8567
NO		0.00000157	8.8475	42.0162	66.4853	-110.9001
NO2		0.00000000	13.6140	39.1538	73.4635	-129.8122
N2		0.50000106	8.7030	19.7863	61.4195	[illegible]
N2O		0.00000000	14.4644	51.6686	77.7227	[illegible]
O2		0.00000000	9.1960	20.9920	69.4904	[illegible]
O3		0.	13.7319	66.0182	82.1311	-122.8834
BE	COND	0.	7.5000	147.6141	16.6819	109.2457
BEO	COND	0.49999137	13.2650	13.7487	25.3134	-44.4720
BE3N2	COND	0.	36.9400	326.6920	71.5225	[illegible]

Table 13

Equilibration of BeO and H_2O at 3000 K

IIPE 42 3/28/62

EXAMPLE COMPATIBILITY

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 3000.00
SYSTEM ENTHALPY (KCAL/GM) 2.4215
SYSTEM ENTROPY (CAL/GM-DEG) 2.5834
SYSTEM GAS CP 0.31756

PRODUCT		MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
H		0.03150771	4.9681	100.2338	38.8625	-16.3537
BE		0.00002944	5.0206	222.6223	44.0207	90.5603
O		0.01386432	5.0042	75.1275	50.0955	-75.1590
BEH		0.00000028	9.2248	267.0258	60.7734	84.7055
BEOH		0.00808124	13.3067	159.0052	77.5020	-73.5009
OH		0.04662143	8.7772	68.2372	61.3567	-115.8329
H2		0.07233034	8.8592	90.6492	48.4670	-54.7518
BE(OH)2		0.00024693	25.4912	106.4419	96.5781	-183.2925
H2O		0.34987881	13.1300	43.6948	68.3292	-161.2928
BEO		0.00006698	9.0667	186.9448	66.1427	-11.4834
BE2O2		0.00030470	19.6799	214.2788	100.0176	-85.7739
BE3O3		0.00335041	31.4108	218.3756	127.9007	-165.3265
BE4O4		0.00002782	43.1417	262.6054	154.8762	-202.0233
BE5O5		0.00001466	55.0747	312.3694	191.9433	[illegible]
BE6O6		0.00002120	66.8561	337.6335	222.8522	-330.9231
O2		0.02749057	9.5510	27.5559	67.9797	-176.3832
O3		0.00000000	13.8047	75.6593	85.7902	-181.7114
BE	COND	0.	7.5000	152.8051	18.8747	[illegible]
BEO	COND	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Table 14

Equilibration of BeO and H_2O at 2300 K

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EXAMPLE COMPATIBILITY

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 2300.00
SYSTEM ENTHALPY (KCAL/GM) 1.1691
SYSTEM ENTROPY (CAL/GM-DEG) 2.1177
SYSTEM GAS CP 0.29046

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
H	0.00071371	4.9681	96.7561	37.5424	10.4085
BE	0.00000000	4.9717	219.1303	42.6955	120.9307
O	0.00023155	4.9797	71.6350	48.7700	-40.5359
BEH	0.00000000	9.0251	260.6341	58.3485	126.4326
BEOH	0.00003609	12.9609	149.7986	74.0095	-20.4231
OH	0.00448672	8.4710	62.1918	59.0639	-73.6551
H2	0.01085225	8.4279	84.5911	46.1712	-21.6026
BE(OH)2	0.00005935	24.6401	88.8786	89.9163	-117.9288
H2O	0.48290771	12.4826	34.7142	64.9241	-114.6113
BEO	0.00000001	8.9637	180.6317	63.7470	34.0136
BE2O2	0.00000008	19.5481	200.5430	94.8046	-17.5075
BE3O3	0.00000310	31.1472	196.4684	119.5868	-78.5812
BE4O4	0.00000001	42.7463	232.5267	143.4614	-97.4345
BE5O5	0.00000000	54.6851	273.9357	177.3572	-133.9857
BE6O6	0.00000000	66.3691	290.9825	205.1475	-180.8567
O2	0.00438121	9.1940	20.9920	65.4904	-129.6358
O3	0.00000000	13.7319	66.0182	82.1311	-122.8834
BE COND	0.	7.5000	147.6141	16.6819	109.2457
BEO COND	0.49632816	13.2650	13.7487	25.3134	-44.4720

observed after an infinite length of time. The tables show that in nitrogen condensed BeO decomposition proceeds through the formation of the gaseous BeO polymers. In water vapor, the gaseous hydroxides play a major role. The partial pressures of the constituents are simply their mole fractions multiplied by the total pressure.

C. Composition of Flames

The computer programs can be of great value to problems which investigate flame phenomena. Input data to the program would consist of oxidizer and fuel stoichiometry and ambient pressure. These conditions would define a premixed flame or a rocket exhaust jet. The actual flame temperature at a given stoichiometry and pressure would easily be calculable from the thermodynamic and thermochemical data of the oxidizer and fuel.

Tables 15 and 16 list the flame compositions of the system tetrafluoroethylene-oxygen ($C_2F_4 + 2O_2$) at ambient pressure. The calculations were made in support of a laboratory program which will investigate the flame in order to give insight into the phenomonology of Teflon ablation in air. One of the surprising results is the extremely high concentration of fluorine atoms. For a given stoichiometry and pressure, this program does not automatically compute the adiabatic flame temperature; these would be hand calculated as shown in Section IV. A., Chemical Synthesis. Oxidizer and fuel enthalpy is 1.00 kcal/gm which yields an adiabatic flame temperature between 2000 - 2100 K.

Calculations, such as those illustrated in Tables 15 and 16, would appear to be an aid toward the prediction of the radiative signatures of rocket exhaust jets. Since the flame composition and temperature is predicted, the concentration of the emitters from first principles has been established. These calculations are, of course, based on thermodynamic equilibrium and do not recognize the existence of excited emitters or other nonequilibrium phenomena.

Table 15

Composition of $C_2F_4 + 2O_2$ Flame at 2100 K

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EXAMPLE COMPOSITION OF FLAME

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 2100.00
SYSTEM ENTHALPY (KCAL/GM) 1.0983
SYSTEM ENTROPY (CAL/GM-DEG) 1.8427
SYSTEM GAS CP 0.29550

PRODUCT		MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
C		0.	5.0190	272.4479	47.4336	172.1534
O		0.00049996	4.9780	70.6392	48.3170	-30.8266
F		0.40420459	4.9985	59.5857	48.0112	-41.2377
CO		0.00184855	8.6976	82.2459	62.2309	-48.4391
F2CO		0.20028078	19.3169	38.6264	93.6449	-158.0279
CO2		0.23104442	14.5545	25.5867	74.6296	-131.1354
CF		0.00000000	8.9902	213.7748	66.8969	73.2914
CF2		0.00000057	13.6306	131.9879	82.9792	-42.2685
CF3		0.00017057	19.5379	89.4253	95.4412	-111.0013
CF4		0.03025556	25.2808	42.0275	104.5984	-177.6292
C2		0.	8.8632	395.8423	64.8127	259.7357
C2F2		0.00000000	20.3789	230.3255	95.6084	29.5478
C3		0.	14.5196	490.7030	80.1757	322.3339
O2		0.13124537	9.0840	19.1642	64.6591	-116.6198
O3		0.00000000	13.6970	63.2751	80.8834	-106.5801
F2		0.00044961	9.2294	78.9273	65.1427	-57.8724
C	SOLID	0.	5.7899	101.1032	10.0039	80.0950

Table 16

Composition of $C_2F_4 + 2O_2$ Flame at 2000 K

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EXAMPLE COMPOSITION OF FLAME

PRESSURE (ATM) 1.0000

[illegible] 0.8795

[illegible] 1.7363

SYSTEM GAS CP 0.29409

PRODUCT		MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
[illegible]						
[illegible]						
F		0.29347803	5.0014	59.0857	47.7672	-36.4487
CO		0.00062659	8.6636	81.3777	61.8074	-42.2372
F2CO		0.25186038	19.2632	36.6973	92.7037	-148.7101
[illegible]						
[illegible]						
[illegible]						
CF3		0.00012941	19.5045	87.4732	94.4888	-101.5044
CF4		0.06008898	25.2259	39.5021	103.3663	-167.2305
C2		0.	8.8390	394.9572	64.3808	266.1956
[illegible]						
[illegible]						
[illegible]						
O3		0.00000000	13.6757	61.9065	80.2157	-98.5249
F2		0.00038378	9.2063	78.0056	64.6930	-51.3804
C	SOLID	0.	5.7577	100.5232	9.7202	81.0827

[illegible]

For the premixed flame, the specification of oxidizer and fuel stoichiometry is reasonable since one expects and observes predicted flame temperatures, radiation, and compositions. However, many processes of interest to the aerospace sciences, such as ablation, must be approximated by a diffusion flame. There is transport of material through the boundary layer, and the flame stoichiometry is not well defined. However, flame temperatures near the theoretical maximum are often observed in diffusion flames although there is no true final flame temperature.

D. Problems Which Contain Many Elements

Tables 17 - 19 illustrate a problem which contains six elements. As seen from the Tables, condensed phases may appear and disappear. Computation time is somewhat increased over that with fewer elements; there are no increased computational difficulties.

E. Mollier Diagrams

Isobaric and isothermal curves on an enthalpy-entropy plane for a given stoichiometry result in a Mollier diagram. Such diagrams are of general utility in power-plant design and thermodynamic analysis. Mollier diagrams are usually presented for single constituents, but the computer routines described in this report are general in nature. Thus, data for the Mollier diagrams can be easily and automatically computed for systems which contain numerous constituents.

Printouts from the current Mollier Diagram Program are illustrated in Tables 20 - 22 and are produced at various pressure and temperature intervals specified by the program user. In practice, points are generated by computing points at equally spaced temperatures along an isobar. When computations have been completed for a temperature range and pressure, the program proceeds to the next pressure. The following data are printed out at each pressure and temperature:

Table 17

Equilibration of ClO_3F and $LiBH_4$ at 6000 K

EXAMPLE — MANY ELEMENTS

PRESSURE (ATM) 1.0000

SYSTEM GAS CP 0.47670

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
B	0.05563164	5.1684	338.7987	51.5967	29.2183
O	0.26133049	5.3234	90.5893	53.6547	-231.3391
F	0.07563834	4.9721	79.0044	53.2406	-240.4390
BH	0.00001112	9.7471	375.6626	65.8729	-19.5748
HBO2	0.00000010	19.7094	183.3224	106.8963	-458.0555
OH	0.00065825	9.3715	95.6000	67.6558	-310.3347
LI2O2H2	0.	31.4436	333.9850	136.8087	-486.8670
H2O	0.00000089	13.8585	84.9382	77.8258	-382.0164
BR3	0.00000000	19.6700	399.4451	91.0485	-146.8459
LIF	0.00112163	9.7552	135.5407	74.3703	-310.6808
LICL	0.00041737	9.7329	143.2809	77.7841	-323.4235
LI2	0.00000209	10.8840	368.2439	75.5337	-84.9585
LI3F3	0.	31.7447	305.3110	159.1736	-649.7306
BO	0.02203546	9.1702	232.7430	73.3037	-207.0791
BOF	0.00019269	14.8558	147.9871	94.9632	-421.7923

Table 17 (continued)

Equilibration of ClO_3F and $LiBH_4$ at 6000 K

BF		0.01691830	9.3628	212.1393	73.3251	-227.8112
BFCL		0.000CCCC2	14.8719	215.9025	96.8694	-365.3140
BFCL2		0.000000C0	19.8391	172.4157	124.1388	-572.4171
BF2		0.0000C019	14.8568	185.3677	91.4544	-363.3589
BF2CL		0.00000000	19.8872	140.4777	[illegible]	[illegible]
BF3		0.00000000	19.8134	108.5409	113.8400	[illegible]
BCL		0.00008159	9.5003	275.3773	77.3523	[illegible]
BCL2		0.000000C0	14.8867	248.5889	100.0540	-351.7353
BCL3		0.000000C0	19.8487	204.1350	125.5247	-549.0134
B2		C.00000092	9.5540	601.4428	74.3603	155.2807
B2O2		0.00000018	20.7809	356.3155	[illegible]	[illegible]
B2O3		0.00000000	25.6933	284.3730	129.7708	[illegible]
B3O3F3		0.	49.5572	329.5833	211.6226	-940.1525
B3O3CL3		0.	49.5742	416.6441	218.7822	-896.0490
CLO		0.00000553	9.5990	84.8461	80.6010	-398.7600
O2		0.C0017820	10.2790	57.5892	74.8898	-391.7494
O3		0.00000000	[illegible]	117.2917	[illegible]	[illegible]
CLF		0.00000059	[illegible]	76.8042	[illegible]	[illegible]
F2		0.00000002	9.9366	116.3530	75.1539	[illegible]
CL2		0.C0000051	9.6721	62.8723	80.3121	-419.0002
LIOH	COND	0.	20.7400	172.6040	73.5736	-268.8375
LI	LIQUID	0.	6.2920	169.4127	28.5358	-1.8018
LIF	COND	0.	15.3100	[illegible]	[illegible]	[illegible]
LICL	LIQUID	0.	14.4000	124.2750	[illegible]	[illegible]
LI2C	COND	0.	23.0000	261.9430	78.9050	-211.4889
B	SOLID	0.	7.5000	219.9530	21.9231	88.4147
B2O3	COND	0.	32.0000	234.9160	106.4809	-403.9691

Table 18

Equilibration of ClO_3F and $LiBH_4$ at 1200 K

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EXAMPLE MANY ELEMENTS

PRESSURE (ATM) 1.0000
TEMPERATURE (DEG K) 1200.00
SYSTEM ENTHALPY (KCAL/GM) 1.0558
SYSTEM ENTROPY (CAL/GM-DEG) 1.6277
SYSTEM GAS CP 0.20548

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
H	[illegible]	[illegible]	91.2911	34.3102	[illegible]
LI	[illegible]	[illegible]	[illegible]	40.0613	[illegible]
B	0.	4.9683	314.7809	43.5683	262.4990
O	0.000CCC00	4.9898	66.1561	45.5292	11.5211
F	0.00000000	5.0521	55.0689	45.2013	0.8274
CL	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
LIH	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
LIOH	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
BH	0.	8.1946	331.3595	51.3183	269.7776
HBO2	0.00081556	17.0794	91.2904	76.5195	-0.5331
OH	0.00000012	7.5478	53.3203	53.8497	-11.2993
BF	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
HCL	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
H2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
LI2O2H2	0.00000000	26.6628	188.1199	88.8069	81.5516
H2O	0.38153469	10.4343	21.9440	57.4403	-46.9844
BH3	0.	15.9753	308.4417	61.1935	235.0095
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
LIO	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
LIF	0.00008C64	8.9230	90.4362	59.4121	19.1417
LICL	0.00633576	9.0041	98.1639	62.8035	22.7998
LI2	0.	9.3019	319.7529	59.6012	248.2314
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
LI3F3	0.00000183	30.5756	153.8976	108.6002	23.5773
BO	0.	8.3247	189.8064	59.0628	118.9310
BOF	0.00027346	13.9127	77.5220	71.5014	-8.2797
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Table 18 (continued)

Equilibration of ClO_3F and $LiBH_4$ at 1200 K

BF		0.00000000	8.6199	168.3780	58.7919	97.8271
BFCL		0.00000000	14.1661	145.1125	73.2532	57.2086
BFCL2		0.00000035	19.1023	77.8035	92.5397	-33.2441
BF2		0.00000000	13.8492	114.9162	68.0042	33.3112
BF2CL		0.00007474	18.8438	46.1378	86.5018	-80.0000
BF3		0.00584036	18.5562	14.5076	82.5259	-84.9238
BCL		0.	8.8948	230.9861	62.5872	155.8819
BCL2		0.	14.4888	177.4614	76.2717	85.9353
BCL3		0.00000000	19.3081	109.3066	93.8193	-3.2766
B2		0.	8.8219	556.9736	59.5924	485.4627
B2O2		0.	19.1277	258.0459	80.0813	162.9468
B2O3		0.00000002	22.9040	163.5131	89.7321	58.8568
B3O3F3		0.00136311	46.8039	94.0041	133.0970	-63.1189
B3O3CL3		0.00000000	47.2005	180.6678	140.0596	12.5964
CLO		0.00000000	8.9060	40.1783	65.7610	-38.7349
O2		0.00000019	8.5270	11.2245	59.7364	-60.4592
O3		0.	13.2875	51.8844	73.3137	-30.2568
CLF		0.00000000	8.9659	31.6378	63.8193	-44.9608
F2		0.	8.9553	70.7297	60.0525	-1.3353
CL2		0.00000433	9.0158	17.9096	65.3691	-60.5334
LIOH	COND	0.	20.7400	73.0520	40.1916	24.8221
LI	LIQUID	0.	6.8680	137.8284	17.8361	116.4251
LIF	COND	0.17017145	15.3100	28.6926	25.8203	-2.2981
LICL	LIQUID	0.07085097	14.4000	55.1550	36.1516	11.7789
LI2O	COND	0.	22.0008	139.6024	33.4789	98.8977
B	SOLID	0.	6.5010	179.8204	8.1611	170.0271
B2O3	COND	0.11341250	32.0000	81.3160	54.9789	15.3413

Table 19

Equilibration of ClO_3F and $LiBH_4$ at 500 K

TAPE 43 4/2/62

EXAMPLE MANY ELEMENTS

PRESSURE (ATM) 1.0000

SYSTEM GAS CP 0.24322

PRODUCT	MOLE FRACTION	CP	ENTHALPY	ENTROPY	H-TS
B	0.	4.9691	311.3030	39.2184	291.6938
O	0.	5.0808	62.6440	41.1312	42.0784
F	0.	5.2822	51.4754	40.6924	31.1292
BH	0.	7.1084	325.9911	44.6768	303.6527
HBO2	0.00000000	12.9458	80.5017	63.2914	40.8560
OH	0.	7.0492	48.2632	47.5568	24.4848
LI2O2H2	0.	19.3366	171.3033	68.3330	137.2148
H2O	0.29436745	8.4156	15.3554	49.3337	-9.3115
BH3	0.	10.0476	299.0417	49.8290	274.1272
LIF	0.	8.1887	84.3708	51.8719	58.4349
LICL	0.00000000	8.5204	91.9785	55.0970	64.4308
LI2	0.	8.9430	313.3483	51.6133	287.5416
LI3F3	0.	26.1724	133.4943	83.3525	91.8181
BO	0.	7.2301	184.3114	52.2633	158.1797
BOF	0.	11.8842	68.3289	60.1335	38.2621

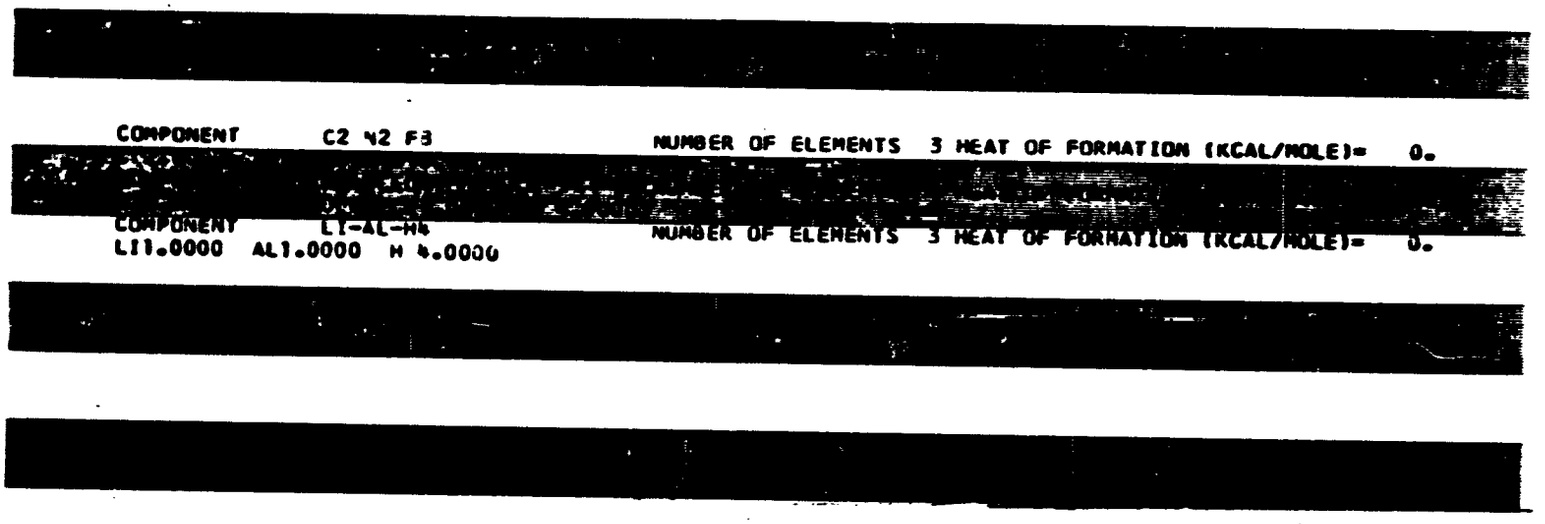
Table 19 (continued)

Equilibration of ClO_3F and $LiBH_4$ at 500 K

BF		0.	7.5812	162.6226	51.6611	136.7921
BFCL		0.	11.9531	135.7296	61.6567	104.9013
BFCL2		0.00000000	16.6498	65.0125	76.6948	26.6651
BF2		0.	10.9861	105.9355	56.9534	77.4588
BF2CL		0.00000000	15.0144	33.6833	73.1164	-2.8798
BF3		0.00000170	14.9659	2.4144	67.6285	-31.3998
BCL		0.	8.2484	224.9146	55.0336	197.3478
BCL2		0.	13.0347	167.6518	64.0924	135.6056
BCL3		0.	17.2981	96.2489	77.6117	57.4430
B2		0.	7.9795	551.0082	52.1846	524.9159
B2O2		0.	15.9590	249.8022	64.7415	213.2914
B2O3		0.	16.5620	149.1609	72.1991	113.0693
B3O3F3		0.00000004	37.5451	63.4297	95.4347	19.7123
B3O3CL3		0.	39.1973	149.5135	101.5925	98.7172
CLO		0.	8.2262	34.1088	58.2120	5.0028
O2		0.	7.4310	5.5652	52.7300	-20.7997
O3		0.	11.2393	42.2817	62.4087	11.0889
CLF		0.	8.3615	29.5140	54.1987	-2.3894
F2		0.	8.1918	64.6914	52.4981	38.4084
CL2		0.00000001	8.6236	11.6940	57.6192	-17.1156
LIOH	COND	0.	15.2010	54.5124	16.9772	46.0238
LI	LIQUID	0.	7.0650	132.9503	11.7501	127.0753
LIF	COND	0.30040062	11.8318	19.2206	14.1931	12.1241
LICL	LIQUID	0.00022576	14.4096	45.0250	23.5448	38.3028
LI2O	COND	0.	16.6270	125.3189	16.7000	116.9460
B	SOLID	0.	4.4970	175.8348	3.3012	174.1843
B2O3	COND	0.	21.0000	54.6790	22.2682	43.5449

Table 20

Input Verification of Mollier Diagram Program System Is $C_2N_2F_8/NH_4ClO_4/LiAlH_4$



COMPONENT C2 N2 F8 NUMBER OF ELEMENTS 3 HEAT OF FORMATION (KCAL/MOLE)= 0.

COMPONENT LI-AL-H4 NUMBER OF ELEMENTS 3 HEAT OF FORMATION (KCAL/MOLE)= 0.
LI1.0000 AL1.0000 H 4.0000

Table 21

Products Selected from Thermodata Tape
$C_2N_2F_8/NH_4ClO_4/LiAlH_4$

H	HEAT OF FORMATION	52.09024620
LI	HEAT OF FORMATION	37.35074234
F	HEAT OF FORMATION	18.86126733
AL	HEAT OF FORMATION	78.59363123
CL	HEAT OF FORMATION	28.94370773
HCN	HEAT OF FORMATION	31.18438339
CHO	HEAT OF FORMATION	-1.14804840
HFCO	HEAT OF FORMATION	-91.51711845
NH	HEAT OF FORMATION	81.27510738
HNO	HEAT OF FORMATION	14.08901262
CH	HEAT OF FORMATION	10.05754995
HCL	HEAT OF FORMATION	-22.05139947
H2	HEAT OF FORMATION	0.
LI2O2H2	HEAT OF FORMATION	-168.77707100
CH2F2	HEAT OF FORMATION	-102.95857539
C2H2	HEAT OF FORMATION	54.12521935
NH2	HEAT OF FORMATION	42.67289829
NH3	HEAT OF FORMATION	-11.06597092
CH4	HEAT OF FORMATION	-17.92509698
LIO	HEAT OF FORMATION	12.88809967

Table 21 (continued)

Products Selected from Thermodata Tape

$C_2N_2F_8/NH_4ClO_4/LiAlH_4$

LI2	HEAT OF FORMATION	48.30184937
LI2O	HEAT OF FORMATION	-37.60570145
LI2F2	HEAT OF FORMATION	-215.64668846
FCN	HEAT OF FORMATION	-12.83328724
CLCN	HEAT OF FORMATION	34.13969326
CO	HEAT OF FORMATION	-26.45284939
CO2	HEAT OF FORMATION	-94.09119892
CF	HEAT OF FORMATION	74.74216461
CCL3F	HEAT OF FORMATION	-71.77709389
CF3CL	HEAT OF FORMATION	-171.93898773
CF4	HEAT OF FORMATION	-217.95817184
ALC	HEAT OF FORMATION	212.05507278
C2F2	HEAT OF FORMATION	-51.36782265
AL2C2	HEAT OF FORMATION	-30.89197540
C3	HEAT OF FORMATION	189.82765579
ALN	HEAT OF FORMATION	107.68692780
N2	HEAT OF FORMATION	-0.00000024
N2O	HEAT OF FORMATION	19.49022865
AL2O	HEAT OF FORMATION	-36.87511826
CLO	HEAT OF FORMATION	25.45765376
O2	HEAT OF FORMATION	0.

Table 21 (continued)

Products Selected from Thermodata Tape

$C_2N_2F_8/NH_4ClO_4/LiAlH_4$

O3		HEAT OF FORMATION	33.99998856
ALF		HEAT OF FORMATION	-58.90781593
ALCLF		HEAT OF FORMATION	-119.01047516
ALFCL2		HEAT OF FORMATION	-180.70163155
CLF		HEAT OF FORMATION	-12.63953829
F2		HEAT OF FORMATION	-0.00000095
ALF2		HEAT OF FORMATION	-155.85352516
ALF2CL		HEAT OF FORMATION	-234.49999237
ALF3		HEAT OF FORMATION	-283.70128632
ALCL		HEAT OF FORMATION	-10.20645714
ALCL2		HEAT OF FORMATION	-76.90002060
ALCL3		HEAT OF FORMATION	-137.92339706
AL2		HEAT OF FORMATION	106.14785004
CL2		HEAT OF FORMATION	-0.00004923
LIOH	COND	HEAT OF FORMATION	-116.66994953
LI	LIQUID	HEAT OF FORMATION	-0.00000381
LIALO2	COND	HEAT OF FORMATION	-284.31109619
LIF	COND	HEAT OF FORMATION	-146.17592049
LICL	LIQUID	HEAT OF FORMATION	-94.46419048
LI2O	COND	HEAT OF FORMATION	-143.04864693
LI3N	COND	HEAT OF FORMATION	-51.57710266
C	SOLID	HEAT OF FORMATION	-0.00000191
ALN	SOLID	HEAT OF FORMATION	-74.92989922
AL2O3	COND	HEAT OF FORMATION	-400.60654449
ALF3	COND	HEAT OF FORMATION	-355.20355988
AL	COND	HEAT OF FORMATION	-0.00000191
ALCL3	LIQUID	HEAT OF FORMATION	-162.33645058

Table 22

Printout of Mollier Diagram Program

AEROSPACE CORPORATION

•••••••••••••••••• EXPERIMENTAL PROBLEM•••••••••••••••••••••• ••••••••••••••••••••

COMPONENT	WEIGHT PERCENT	MOLES	MOLE PERCENT
C2 N2 F8	25.000000	1.00000000	7.83635980
NH4 CLO4	29.999999	2.08384553	16.32976317
LI-AL-H4	44.999999	9.67718183	75.83387756

ELEMENTS	MOLES	MASS BALANCE (GM/GM)
H	3.6865	0.57641358E-01
LI	0.7583	0.11657063E-01
C	0.1567	0.24505240E-02
N	0.3203	0.50037806E-02
O	0.6532	0.10213026E-01
F	0.6269	0.98020960E-02
AL	0.7583	0.11857083E-01
CL	0.1633	0.25532567E-02

999.999992	6000.000000	12.97377777	4.21359318	107	2
999.999992	5900.000000	12.73574269	4.17358738	107	3
999.999992	5800.000000	12.48963666	4.13151771	107	4
999.999992	5700.000000	12.23521221	4.08726454	107	5
999.999992	5600.000000	[illegible]	[illegible]	107	6
999.999992	5500.000000	11.70104063	3.99185136	107	7
999.999992	5400.000000	11.42306077	3.94084072	107	8
999.999992	5300.000000	11.13930571	3.88782489	107	9
999.999992	5200.000000	[illegible]	3.83330726	107	10
999.999992	5100.000000	[illegible]	3.77794516	107	11
999.999992	5000.000000	10.28565863	3.72207639	107	12
999.999992	4900.000000	10.01015544	3.66636980	107	13
999.999992	4800.000000	9.74322355	3.61134657	107	14
999.999992	4700.000000	9.48773396	3.55756792	107	15
999.999992	[illegible]	[illegible]	[illegible]	107	16
999.999992	4500.000000	[illegible]	3.45525599	107	17
999.999992	[illegible]	[illegible]	3.40728612	107	18
999.999992	4300.000000	8.60365856	3.36138326	107	19
999.999992	4200.000000	8.41797650	3.31776053	107	20
999.999992	4100.000000	8.24484944	3.27597478	107	21
999.999992	[illegible]	[illegible]	[illegible]	107	22

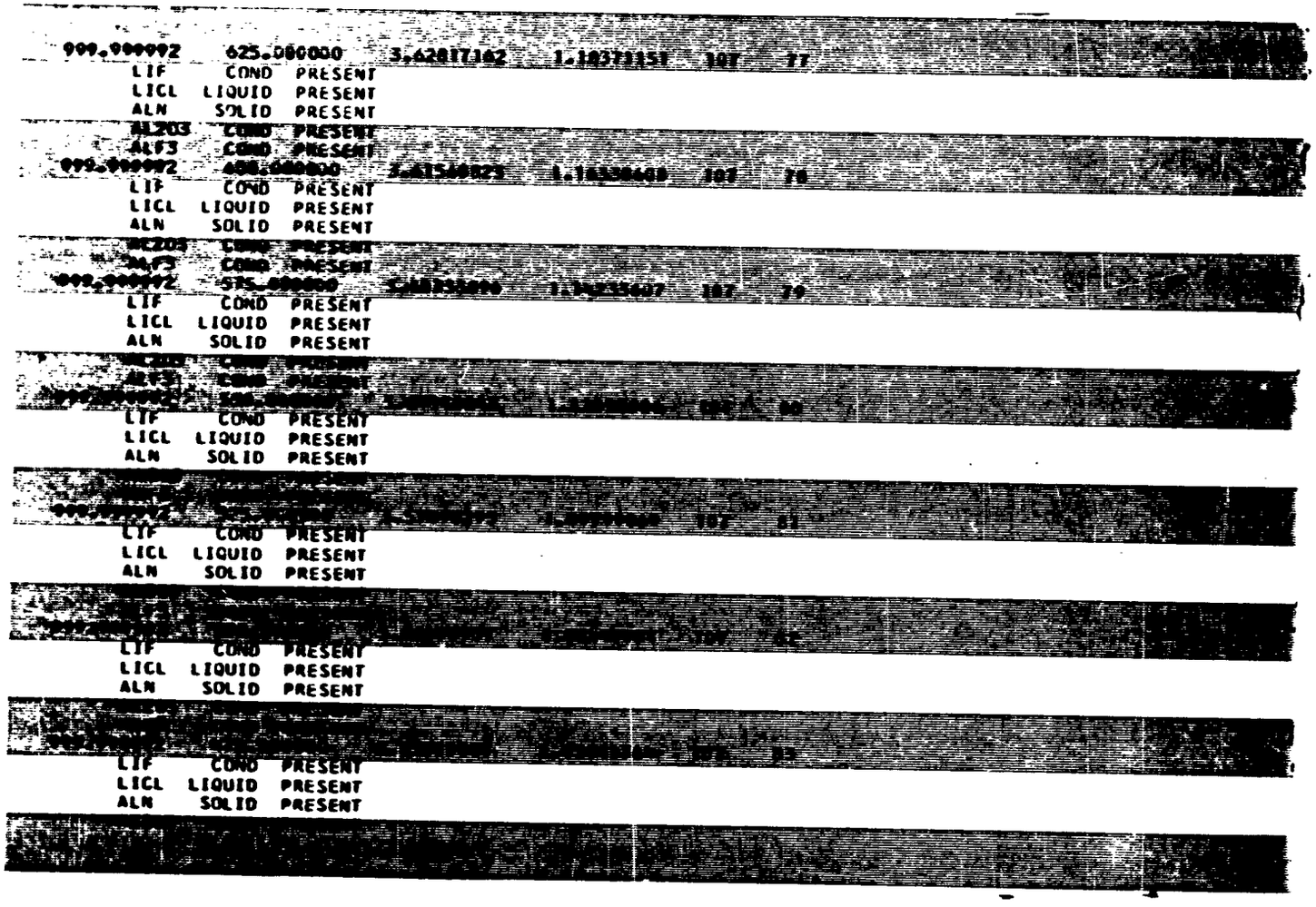
Table 22 (continued)

Printout of Mollier Diagram Program

```
      ALN     SOLID   PRESENT
      AL2O3   COND    PRESENT
999.999992   1650.000000    4.49478042    1.94306967    107    49
      LIF     COND    PRESENT
      LICL    LIQUID  PRESENT
      ALN     SOLID   PRESENT
      AL2O3   COND    PRESENT
999.999992   1600.000000    4.45473081    1.91845532    107    50
      LIF     COND    PRESENT
      LICL    LIQUID  PRESENT
      LIF     COND    PRESENT
      LICL    LIQUID  PRESENT
      ALN     SOLID   PRESENT
      LICL    LIQUID  PRESENT
      ALN     SOLID   PRESENT
      AL2O3   COND    PRESENT
      ALN     SOLID   PRESENT
      AL2O3   COND    PRESENT
999.999992   1400.000000    4.27145827    1.79521561    107    54
      AL2O3   COND    PRESENT
999.999992   1350.000000    4.18825179    1.73466489    107    55
      LIF     COND    PRESENT
      ALF3    COND    PRESENT
999.999992   1300.000000    4.10526317    1.67208366    107    56
      LIF     COND    PRESENT
```

Table 22 (continued)

Printout of Mollier Diagram Program



Column	Datum
1	Pressure
2	Temperature
3	Enthalpy
4	Entropy
5	Indicator
6	Point Number

When condensed phases appear, the program notes their presence and identifies them (see Table 22).

The subscript COND refers to a constituent whose thermodynamic data over the range 0 to 6000 K is associated with both solid and liquid phases. The data list the melting point to the nearest 100 deg, and the entropy, heat capacity, and enthalpy are discontinuous. System composition data are deleted in order to reduce the amount of output but may be produced as an option. The temperature interval selected for each isobar is identical, facilitating the construction of isotherms on the diagram.

Applications of Mollier diagrams of complex systems are numerous. In the aerospace sciences, obvious application involves determination of theoretical rocket propellant performance and the solution of a host of aerodynamic problems. Most important in the latter case is ablation and the calculation of the thermodynamic and transport properties of flowing, reacting gas mixtures. Since the viscosity and thermal conductivity of a gas mixture is of importance, gas composition must be known before its transport properties can be computed. The ability to treat flow with chemical reaction is mandatory for the solution of contemporary aerodynamic problems.

While each point computed by the Mollier Diagram Program is an equilibrium one, shifting equilibrium parameters such as heat capacity, isentropic exponent, and speed of sound necessary for some aerodynamic calculations are not computed. The program could be modified to compute these

parameters, but computer time would be increased sharply. However, the following section will illustrate how the parameters may be derived from the current program which will be modified slightly.

F. Calculation of the Velocity of Sound

The velocity of sound is

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\frac{p}{\rho}\left(\frac{\partial \ln p}{\partial \ln \rho}\right)_s} \tag{17}$$

and γ the isentropic exponent is

$$\gamma = \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_s = -\frac{v}{p}\left(\frac{\partial p}{\partial \rho}\right)_s \tag{18}$$

Using the Bridgman formulas, Eq. (18) is

$$\gamma = -\frac{v}{p}\,\frac{\frac{C_p}{T}}{\frac{C_p}{T}\left(\frac{\partial v}{\partial p}\right)_T - \left(\frac{\partial v}{\partial T}\right)_p^2} \tag{19}$$

Since

$$pv = \frac{RT}{M} \tag{20}$$

differentiation yields

$$p\,dv + v\,dp = \frac{R}{M}\,dt - \frac{RT}{M^2}\,dM \tag{21}$$

and substitution in Eq. (19)

$$\gamma = \frac{c_p}{c_p \left[1 + \left(\frac{\partial \ln M}{\partial \ln p}\right)_T\right] - \frac{R}{M}\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_p\right]^2} \tag{22}$$

where c_p, the shifting equilibrium heat capacity, is

$$c_p = \left(\frac{\partial h}{\partial T}\right)_p \cong \frac{h_2 - h_1}{T_2 - T_1} \tag{23}$$

For a nonreacting gas mixture (frozen equilibrium)

$$\left(\frac{\partial \ln M}{\partial \ln p}\right)_T = \left(\frac{\partial \ln M}{\partial \ln T}\right)_p = 0 \tag{24}$$

and Eqs. (22) and (17) are reduced to

$$\gamma = \frac{c_p}{c_p - \frac{R}{M}} \tag{25}$$

and

$$a^2 = pv\,\gamma = \frac{RT}{M}\,\gamma \tag{26}$$

Molecular weight changes are primarily caused by reassociation of high temperature species; the degree of dissociation is related exponentially to temperature and is much less sensitive to pressure. At static temperatures below, e.g., 1500 K, molecular weight changes become negligible and Eq. (25) may be utilized. At temperatures below approximately 1500 K, frozen and shifting equilibrium parameters are essentially identical. Table 23 illustrates values for frozen and shifting γ in the oxygen/hydrogen system.

Table 23

Comparison of Frozen and Shifting γ in O_2/H_2 Mixtures (60 psia)

T($^{\circ}$K)	γ	
	Shifting	Frozen
1183	1.3395	1.3396
1514	1.3077	1.3079
2089	1.2550	1.2649
2329	1.2267	1.2510
2828	1.1605	1.2265
3015	1.1386	1.2182
3217	1.1174	1.2077

In order to evaluate the shifting equilibrium isentropic exponent and the speed of sound for areas on a Mollier diagram, we need information on

1) enthalpy
2) molecular weight
3) pressure
4) temperature
5) volume

These will be tabulated for each point; for a given isobar, the molecular weight, enthalpy, and specific volume will be found on the printout. The speed of sound and isentropic exponent may then be evaluated graphically.

A section of a Mollier diagram is illustrated in Fig. 2, and we wish to calculate the isentropic exponent in the area of p_1 and T_1 from Eq. (22). Evaluation of $(\partial \ln M)/(\partial \ln p)_T$ and $(\partial \ln M)/(\partial \ln T)_p$ would be made over the interval p_o, T_1 - p_2, T_1 and p_1, T_2 - p_1, T_o, respectively, as $(\Delta \ln M)/(\Delta \ln T)_p$. c_p is simply read from the printout as the difference in h between p_1, T_2 - p_1, T_o. For the speed of sound we need, in addition, pv at p_1, T_1. Since the data are printed out along an isobar

$$v = \frac{RT}{Mp} \tag{27}$$

Use of Correct M When System Contains Condensed Phases

Let

$$\gamma = \frac{c_p}{c_v} \tag{28}$$

and for a system which contains a condensed phase

$$\gamma = \frac{N_g c_p^g + N_s c_p^s}{N_g c_v^g + N_s c_v^s} \tag{29}$$

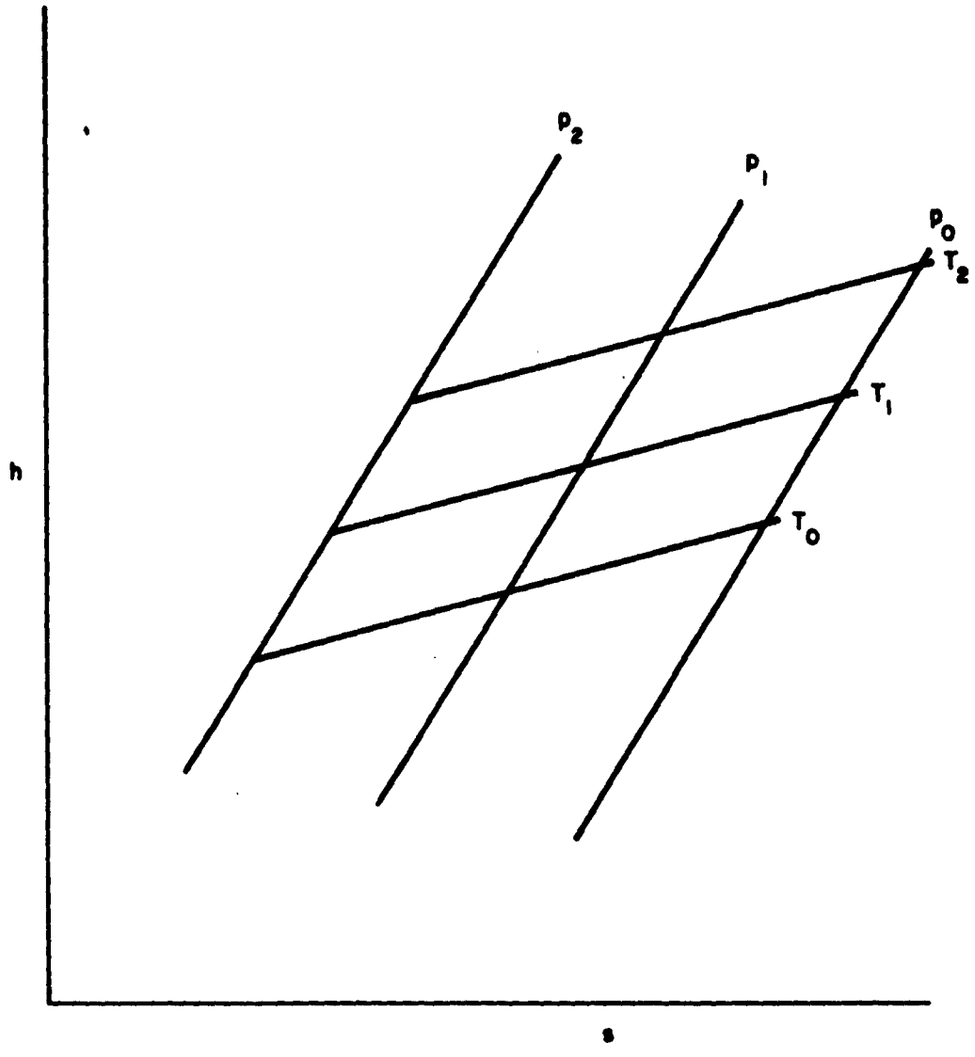


Fig. 2. Mollier Diagram

Since

$$N_s c_v^s = N_s c_p^s \tag{30}$$

and

$$c_p - c_v = \frac{R}{M} \tag{31}$$

then Eq. (29) is

$$\gamma = \frac{N_g c_p^g + N_s c_p^s}{N_g c_p^g - N_g \frac{R}{M} + N_s c_p^s} = \frac{c_p^t}{c_p^t + X_g \frac{R}{M}} \tag{32}$$

where

c_p^t = total specific heat of mixtures

N = weight of gas or solid

X_g = weight fraction of gases

M = molecular weight of mixture

Thus, the M used in a two-phase system is actually M/X_g.

G. Theoretical Rocket Propellant Performance Calculations

The solution of complex chemical equilibria is a fundamental requirement for the computation of theoretical rocket propellant performance. Every parameter of performance may be computed from a thermodynamic analysis of combustion products at selected pressure planes within the thrust chamber.

1. Performance Parameters

Generally, performance parameters which characterize a given propellant system are

a) I_s specific impulse

b) c^* characteristic velocity

c) C_F thrust coefficient

d) ϵ area ratio

Items (a) and (c) are a function of the area ratio, and it is usually desired that they be tabulated at numerous pressure ratios in order to predict altitude and vacuum performance. Also, it is advantageous to include tabular material for the calculation of performance resulting from nonoptimum expansion.

2. Specific Impulse

Specific impulse is defined and calculated from the relation

$$I_s = \frac{u_e}{g} + \frac{A_e}{\dot{m}} (p_e - p_o) \tag{33}$$

Optimum specific impulse is established when the static pressure at the nozzle exit is equal to the ambient pressure, and Eq. (33) is

$$I_{opt} = \frac{u_e}{g} \tag{34}$$

When the thrust chamber is at a high altitude and the ambient pressure approaches a vacuum, Eq. (33) is

$$I_{vac} = \frac{u_e}{g} + \frac{A_e p_e}{\dot{m}} \tag{35}$$

Both I_{opt} and I_{vac} are a function of the nozzle expansion ratio (ϵ); the latter is defined by

$$\epsilon = \frac{A_e}{A_t} \tag{36}$$

Because the rocket engine is a heat engine in which the kinetic energy of the jet is created at the expense of combustion product enthalpy, it can easily be shown that

$$I_{opt} = \sqrt{\frac{2J}{g}} \sqrt{h_c - h_e} \qquad (37)$$

The calculation of I_{opt} from Eq. (37) involves the difference in combustion product enthalpy between the chamber and the exit pressure plane. The calculation proceeds on the basis of selecting a chamber pressure and assigning the ambient pressure to the pressure at the exit plane of the nozzle. Calculations are made with the following assumptions:

a) Propellants are injected into a combustion chamber at a prescribed chamber pressure.

b) Propellants are transformed adiabatically and isenthalpically into their combustion products at the prescribed chamber pressure.

c) Combustion is complete, and a mixture results which can be described by the perfect gas law.

d) Combustion products enter a de Laval nozzle; the contraction ratio (A_e/A_t) is infinite, and the velocity of gases entering the convergent portion of the throat is negligible.

e) Jet velocity at the throat is equal to the local speed of sound.

f) Expansion through the nozzle is adiabatic isentropic, frictionless, and one-dimensional.

g) Condensed phases exhibit a negligible volume and are in thermal equilibrium with gas particles while travelling with their identical velocities.

The expansion process may be treated exactly by the methods of classical thermodynamics with the assumptions of either frozen or shifting

equilibrium. For the former, we assume the composition of the chamber combustion products to be invariant with position in the nozzle. With the assumption of shifting equilibrium, combustion product composition continually changes and is required to reflect the temperature change during the nozzle expansion process. All performance parameters may be computed for the conditions of frozen and shifting equilibrium.

3. Area Ratio (ϵ)

Thrust chamber geometry is best characterized by the area ratio, ϵ. Utilizing the equation for the continuity of mass

$$\rho u A = \dot{m} \tag{38}$$

Eq. (36) becomes

$$\epsilon = \frac{(\rho u)_t}{(\rho u)_e} \tag{39}$$

The perfect gas law is

$$\rho = \frac{pM}{RT} \tag{40}$$

and ϵ is then

$$\epsilon = \frac{\left(\frac{pMu}{T}\right)_t}{\left(\frac{pMu}{T}\right)_e} \tag{41}$$

ϵ is seen to involve the evaluation of the properties of combustion products at the throat and exit pressure plane.

Procedures for evaluating throat properties are somewhat complicated, since the throat position is not uniquely known but encompasses only basic thermodynamics. The significance of Eq. (41) is that from a thermodynamic analysis of combustion products at selected stations in the thrust

chamber, data on the design of thrust chambers may be deduced. Given a propellant stoichiometry and enthalpy, chamber pressure, and exit pressure, an optimum impulse can be computed and the area ratio of the thrust chamber which is required to produce that exit pressure may also be computed.

Substituting Eqs. (34), (36), and (38) into Eq. (33)

$$I_\epsilon = I_{opt} + \frac{\epsilon}{(\rho u)_t} (p_e - p_o) \tag{42}$$

from which can be computed the specific impulse at any area ratio (viz, exit pressure) and for all conditions of nonoptimum expansion, $p_e \neq 0$. The special case, I_{vac}, namely, $p_o = 0$, is also included. The term $A_e/\dot{m} = \epsilon/(\rho u)_t$ can be expressed in more tractable terms. From Eqs. (34), (38), and (40),

$$\frac{A_e}{\dot{m}} = \left(\frac{RT}{pMu}\right)_e = \left(\frac{RT}{pM}\right)_e \frac{1}{I_{opt}\, g} \tag{43}$$

Thus, nonoptimum specific impulse can be computed but without specification of ϵ. However, the specification of the area ratio for optimum or nonoptimum specific impulse will always involve the determination of throat properties since ϵ can only be derived from Eq. (41).

4. Derived Performance Parameters - Thrust Coefficient and Characteristic Velocity

For reasons peculiar to the experimental evaluation of a propellant system in a thrust chamber, it is convenient to define parameters which yield insight into the efficiencies of the combustion and expansion process. Three parameters associated with the thrust chamber which may be experimentally measured are the chamber pressure, throat area, and propellant weight flow. As an excellent approximation for a given throat area, the chamber pressure is directly proportional to the propellant weight flow,

$$p_c \propto \frac{\dot{m}}{A_t} \tag{44}$$

Note that the term $p_c A_t/\dot{m}$ has the dimension of seconds, which are those of specific impulse; and we intuitively conclude that the term could be proportional to specific impulse. Utilizing the acceleration of gravity we find the familiar proportionately constant c^*

$$c^* = \frac{p_c A_t g}{\dot{m}} \tag{45}$$

to have the dimensions of velocity.

The characteristic velocity, c^*, has appeared quite often in the rocket literature and has been the source of much misunderstanding. Much of the confusion associated with the interpretation of c^* could be avoided if its lack of fundamental significance could be kept in mind. Unfortunately, c^* is neither the velocity of the jet at the throat nor at the exit plane, and the product of chamber pressure and throat area has no particular significance. We find Eq. (45) to be a general equation which states that for a given throat area and chamber pressure, propellant systems with higher c^* require less flow rate to produce a given chamber pressure. Equations (44) and (45) are statements of a relationship between chamber pressure and propellant flow rate for a given propellant system. The value of the parameter c^* is that while Eq. (45) may be evaluated experimentally, it may also be evaluated theoretically from a thermodynamic analysis of the propellants, and the results can be compared. Thus, one obtains an experimental indication of whether the particular design of hardware (injector or thrust chamber) permits the realization of near theoretical results. Use of Eqs. (38), (40), and (45) yields

$$c^* = p_c \left(\frac{RT}{pM}\right)_t \frac{g}{u_t} \tag{46}$$

c^* is a single valued function of propellant stoichiometry inlet conditions and chamber pressure and is independent of processes which take place beyond the throat. I_s is a function of propellant stoichiometry and chamber

pressure but includes the contribution of the expansion process. We define the coefficient of thrust

$$C_F = \frac{I_s g}{c^*} \tag{47}$$

and

$$I_s = \frac{c^* C_F}{g} \tag{48}$$

We define c^* and C_F to approximately separate the combustion and expansion efficiencies. Like I_s and c^*, C_F may be computed for both frozen and shifting equilibrium.

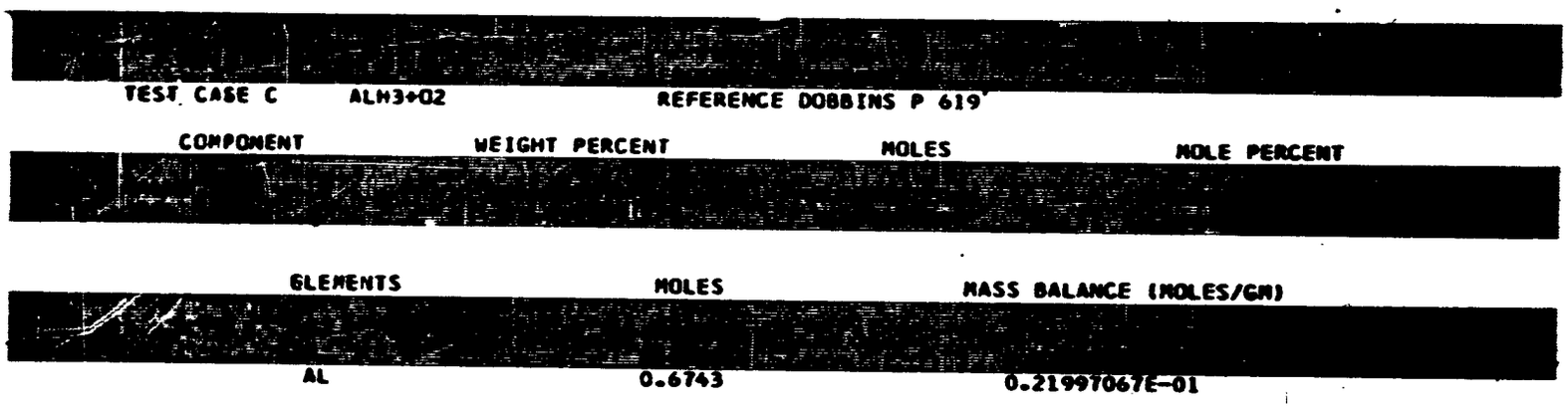
In general, c^*, which is determined experimentally, is less than c^* theoretical, while the reverse is true for the thrust coefficient. The reason is that combustion is usually not complete in the chamber and will occur to some extent in the nozzle. The result is a somewhat lower than theoretical chamber pressure. Hence, the experimental c^* is lower than theoretical, while the enthalpy converted to velocity in the nozzle is augmented by an additional enthalpy of combustion. It should be realized that the thrust coefficient is determined indirectly; thrust, chamber pressure, and propellant weight flow are measured directly, and the thrust coefficient is computed.

5. Theoretical Rocket Performance Printout

Tables 24 - 28 illustrate the output format of the Shifting Equilibrium Theoretical Rocket Performance Programs. Input data, such as propellant chemical formulas and heats of formation, are reiterated. Mass balance sheets are then produced, and propellant components are listed in weight per cent, moles, and mole per cent. A list of the combustion products selected and their heats of formation (kcal/mole) follows.

Table 24

Problem Definition and Input Verification



TEST CASE C ALH3+O2 REFERENCE DOBBINS P 619

COMPONENT	WEIGHT PERCENT	MOLES	MOLE PERCENT

ELEMENTS	MOLES	MASS BALANCE (MOLES/GM)
AL	0.6743	0.21997067E-01

Table 25

Products Selected from Thermodata Tape
AlH_3/O_2

PRODUCTS CHOSEN ARE THE FOLLOWING		
H	HEAT OF FORMATION	52.09024620
C	HEAT OF FORMATION	59.55014181
AL	HEAT OF FORMATION	78.59360123
CH	HEAT OF FORMATION	10.05754995
ALOH	HEAT OF FORMATION	-2.07924271
ALH	HEAT OF FORMATION	62.80041885
H2	HEAT OF FORMATION	0.
H2O	HEAT OF FORMATION	-57.79524899
ALO	HEAT OF FORMATION	17.98375702
AL2O	HEAT OF FORMATION	-36.87511826
O2	HEAT OF FORMATION	0.
AL2O2	HEAT OF FORMATION	-100.00292587
O3	HEAT OF FORMATION	33.99998856
AL2	HEAT OF FORMATION	106.14785004
AL2O3 COND	HEAT OF FORMATION	-400.60649872
AL COND	HEAT OF FORMATION	-0.00000191

Table 26

Thermodynamic Conditions for Each of 24 Expansion Planes

[redacted] SHIFTING EQUILIBRIUM EXPANSION-ROCKET PERFORMANCE [redacted]

THERMC DATA LIBRARY TAPE 43 4/2/62

[redacted] REFERENCE DOBBINS P 619

[redacted] CHAMBER PRESSURE = 1000 PSIA

TABLE ONE

THERMODYNAMIC CONDITIONS FOR EACH EXPANSION PLANE

[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	833.333	715.286	581.364	[redacted]	
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	
H (CAL/GM)	7661.3	7648.6	7602.9	7554.4	7490.8	7289.5	7099.0	6993.8
S (CAL/GM-DEG K)	2.619	2.619	2.619	2.619	2.619	2.619	2.619	2.619
CP (CAL/GM)	1.864	1.857	1.831	1.802	1.761	1.613	1.449	1.350
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
COND MOLES/100 GM	0.40180	0.40403	0.41201	0.42029	0.43088	0.46171	0.48607	0.49704

COMPOSITION-MOLES PER 100 GRAMS PROPELLANT

[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
AL	0.05870	0.05858	0.05815	0.05770	0.05709	0.05512	0.05311	0.05188
OH	0.01964	0.01908	0.01715	0.01522	0.01288	0.00695	0.00327	0.00195
ALOH	0.00110	0.00107	0.00096	0.00085	0.00073	0.00041	0.00021	0.00014
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
ALO	0.01006	0.00986	0.00915	0.00842	0.00750	0.00490	0.00294	0.00209
AL2O	0.65683	0.65486	0.64780	0.64048	0.63110	0.60378	0.58233	0.57284
O2	0.00007	0.00006	0.00005	0.00004	0.00003	0.00001	0.00000	0.00000
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]

Table 26 (continued)

Thermodynamic Conditions for Each of 24 Expansion Planes

[redacted] SHIFTING EQUILIBRIUM EXPANSION-ROCKET PERFORMANCE [redacted]

THERMC DATA LIBRARY TAPE 43 4/2/62

[redacted] REFERENCE ROUTINES P 619

[redacted] CHAMBER PRESSURE = [redacted] 1000 PSIA

TABLE ONE

THERMODYNAMIC CONDITIONS FOR EACH EXPANSION PLANE

[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	-73.460	58.704	48.887	29.392	26.939	25.[redacted]		
[redacted]	3042.071	2985.918	2936.075	2797.145	2741.[redacted]	2[redacted]		
H (CAL/GM)	6922.2	6867.7	6824.1	6707.0	6666.9	6633.5	6604.9	6558.4
S (CAL/GM-DEG K)	2.619	2.619	2.619	2.619	2.619	2.619	2.619	2.619
CP (CAL/GM)	1.281	1.227	1.184	1.068	1.028	0.996	0.968	0.924
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	24.584	24.678	24.751	24.994	25.[redacted]	25.[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
COND MCLES/100 GM	0.50340	0.50759	0.51053	0.51669	0.51823	0.51931	0.52008	0.52108

COMPOSITION-MCLES PER 100 GRAMS PROPELLANT

[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]
[redacted]	0.28059	0.27814	0.27629	0.27087	0.26913	0.26[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	0.00005	0.00004	0.00001	0.00001	0.00001	[redacted]	[redacted]
AL	0.05098	0.05023	0.04960	0.04769	0.04693	0.04626	0.04566	0.04459
OH	0.00131	0.00093	0.00069	0.00028	0.00019	0.00014	0.00011	0.00006
ALOH	0.00010	0.00008	0.00006	0.00003	0.00003	0.00002	0.00002	0.00001
[redacted]	0.00527	0.00495	0.00468	0.00385	0.00355	0.00[redacted]	[redacted]	[redacted]
H2	3.10802	3.12857	3.14135	3.17840	3.19033	3.19[redacted]	3.21[redacted]	[redacted]
H20	0.04421	0.03587	0.02994	0.01705	0.01363	0.01[redacted]	[redacted]	[redacted]
ALC	0.00159	0.00127	0.00105	0.00057	0.00045	0.00036	0.00030	0.00021
AL20	0.56745	0.56398	0.56160	0.55698	0.55599	0.55537	0.55499	0.55468
AL202	0.00003	0.00002	0.00002	0.00001	0.00001	0.00001	0.00001	0.00000
[redacted]	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	[redacted]	[redacted]
[redacted] COND	0.50340	0.50759	0.51053	0.51669	0.51823	0.51931	[redacted]	[redacted]

Table 26 (continued)

Thermodynamic Conditions for Each of 24 Expansion Planes

[redacted] EQUILIBRIUM EXPANSION-ROCKET PERFORMANCE [redacted]

THERMO DATA LIBRARY TAPE 43 4/2/62

[redacted] REFERENCE CONDITION P 615 [redacted]

TABLE ONE

THERMODYNAMIC CONDITIONS FOR EACH EXPANSION PLANE

[redacted] IPS(A)							
H (CAL/GP)	6480.9	6352.6	6231.2	6159.9	6111.1	6074.5	6010.9	5967.7
S (CAL/GP-DEG K)	2.619	2.619	2.619	2.619	2.619	2.619	2.619	2.619
CP (CAL/GM)	0.853	0.789	0.790	0.728	0.682	0.650	0.602	0.576
[redacted]								
COND MOLES/100 GM	0.52208	0.52236	0.52278	0.52320	0.52326	0.52321	0.52300	0.52277

COMPOSITION-MOLES PER 100 GRAMS PROPELLANT

[redacted]								
CH	0.00002	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
ALCH	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
ALH	0.00302	0.00245	0.00199	0.00190	0.00186	0.00184	0.00182	0.00182
[redacted]								
AL2O	0.55491	0.55605	0.55510	0.55476	0.55492	0.55520	0.55597	0.55669
AL2O2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
AL2	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001

Table 27

Optimum Specific Impulse Tabulation

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TABLE TWO

C_o = 6042 FT/SEC

1.0000	1000.0000	3803.7	7661.27	1.1163	0.	0.	0.
1.0400	961.5385	3791.4	7648.60	1.1162	2.3403	0.1765	33.15
3.4023	293.9188	3435.9	7289.46	1.1154	1.2481	0.9577	179.86
6.8046	146.9594	3239.1	7098.95	1.1169	1.8885	1.1777	221.19
10.2069	97.9729	3126.3	6993.77	1.1185	2.4914	1.2832	240.99
20.4137	48.9867	2936.1	6824.13	1.1222	4.1303	1.4370	269.89
34.0228	29.3920	2797.1	6707.01	1.1256	6.0949	1.5342	288.15
40.8275	24.4933	2747.7	6666.86	1.1270	7.0197	1.5662	294.15
100.0000	10.0000	2505.0	6480.89	1.1349	14.2280	1.7064	320.48
200.0000	5.0000	2371.2	6352.56	1.1393	25.4864	1.7967	337.45
1000.0000	1.0000	2076.4	6074.53	1.1543	100.7116	1.9784	371.57
1500.0000	0.6667	1968.8	6010.86	1.1612	140.1726	2.0177	378.95
2000.0000	0.5000	1892.6	5967.72	1.1659	177.1835	2.0439	383.87

Table 28

Altitude Specific Impulse

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TABLE THREE

2.0000	7.4192	226.25	50.63	0.38	276.88	1.2047	1.4742
3.0000	13.2326	252.36	42.58	0.56	294.94	1.3437	1.5704
4.0000	19.5596	268.21	38.41	0.75	306.62	1.4281	1.6326
7.0000	40.6800	294.03	32.32	1.31	326.35	1.5656	1.7376
8.0000	48.2773	299.47	31.12	1.50	330.59	1.5945	1.7602
9.0000	56.1055	304.10	30.13	1.69	334.22	1.6192	1.7796
12.0000	80.7187	314.78	27.92	2.25	342.70	1.6760	1.8247
13.0000	89.4599	317.25	27.29	2.44	344.54	1.6892	1.8345
14.0000	98.0377	319.90	26.82	2.63	346.72	1.7033	1.8461
17.0000	124.0584	326.76	25.74	3.19	352.50	1.7398	1.8769
18.0000	132.8278	328.69	25.45	3.38	354.15	1.7501	1.8856
19.0000	141.6450	330.45	25.19	3.57	355.64	1.7594	1.8936
22.0000	168.8478	332.85	24.47	4.13	357.33	1.7723	1.9026
23.0000	177.7663	334.23	24.30	4.32	358.53	1.7796	1.9090
24.0000	186.6984	335.56	24.14	4.51	359.71	1.7867	1.9152

Table 28 (continued)

Altitude Specific Impulse

THERMC DATA LIBRARY TAPE 43 4/2/62

TABLE THREE

27.0000	213.5770	339.26	23.74	5.07	363.00	1.8064	1.9328
28.0000	222.5639	340.39	23.63	5.26	364.02	1.8124	1.9382
29.0000	231.5645	341.48	23.52	5.45	365.00	1.8182	1.9434
32.0000	258.6483	344.44	23.24	6.01	367.68	1.8340	1.9577
33.0000	267.7037	345.33	23.15	6.20	368.49	1.8387	1.9620
34.0000	276.7727	346.18	23.07	6.39	369.25	1.8432	1.9660
37.0000	300.6509	346.18	23.11	6.95	369.29	1.8432	1.9663
38.0000	309.8335	346.86	23.03	7.14	369.90	1.8469	1.9695
39.0000	319.0865	347.53	22.96	7.32	370.49	1.8504	1.9727
42.0000	347.2682	349.48	22.71	7.89	372.20	1.8608	1.9818
43.0000	356.8029	350.11	22.63	8.08	372.75	1.8642	1.9847
44.0000	366.4081	350.73	22.55	8.26	373.28	1.8674	1.9875
47.0000	395.6463	352.50	22.31	8.83	374.81	1.8769	1.9957
48.0000	405.5332	353.07	22.23	9.01	375.30	1.8799	1.9983
49.0000	415.4905	353.63	22.15	9.20	375.77	1.8829	2.0008

The problem solved in the tables illustrates the typical three-table shifting equilibrium output format. While the selection of the chamber pressure is infinitely variable, computations are executed at 24 pressure ratios (Table 26). The initial pressure is that within the combustion chamber whereas the fifth pressure locates the exact position and conditions at the throat. At every pressure, the temperature, enthalpy, entropy, heat capacity, isentropic exponent (GAMMA), product molecular weights, and the concentration of combustion products are printed.

Table 27 lists the rocket performance data. Characteristic velocity is tabulated as is optimum specific impulse, expansion ratio (EPSILON), and thrust coefficient (CF) as a function of pressure ratio.

Table 28 lists altitude performance parameters as a function of 50 unit area ratios and is utilized to read the thrust coefficient (CF EPS) and specific impulse (I EPS) for an ambient pressure of zero as a function of area ratio. Optimum specific impulse (I OPT) is tabulated at the unit area ratio. The table affords the rapid and accurate calculation of specific impulse under any set of optimum and nonoptimum area ratios and altitude conditions. The exact equation for these effects is

$$\text{I EPS} = \text{I OPT} + A - Bp_o$$

$$= \frac{u_e}{g} + \left(\frac{RT}{Mu}\right)_e - \left(\frac{RT}{pMu}\right)_e p_o$$

$$= \text{I OPT} + \frac{p_e c^*\epsilon}{p_c g} - \frac{p_o c^*\epsilon}{p_c g} \qquad (49)$$

Table 29 illustrates a portion of the thermodynamic properties of the propellant system N_2O_4 with BeH_2. Solution was obtained with the presence of three condensed phases.

Table 29

Example with Three Condensed Phases

THERMC DATA LIBRARY TAPE 43 4/2/62

TABLE ONE

THERMODYNAMIC CONDITIONS FOR EACH EXPANSION PLANE

H (CAL/GM)	11301.0	11286.7	11233.6	11177.6	11105.1	10876.2	10653.9	10522.9
S (CAL/GM-DEG K)	3.816	3.816	3.816	3.816	3.816	3.816	3.816	3.816
CP (CAL/GM)	2.960	2.964	2.977	2.990	3.005	3.280	3.795	3.770
COND MOLES/100 GM	3.87746	3.87984	3.88864	3.89815	3.91102	3.86514	3.80511	3.84402

COMPOSITION-MOLES PER 100 GRAMS PROPELLANT

BEN	0.09150	0.08987	0.08409	0.07817	0.07082	0.05607	0.04732	0.03757
BECN	0.05075	0.04965	0.04574	0.04181	0.03701	0.02922	0.02359	0.01631
NN	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H2O	0.00082	0.00079	0.00069	0.00059	0.00048	0.00029	0.00018	0.00010
NH3	0.00004	0.00004	0.00003	0.00003	0.00002	0.00001	0.00001	0.00000
BEC	0.00004	0.00003	0.00003	0.00002	0.00002	0.00001	0.00001	0.00000
BE5O5	0.00001	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
BE6O6	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000
N2	0.00390	0.00384	0.00362	0.00339	0.00310	0.00266	0.00250	0.00198
BE3N2 CCND	0.44165	0.44171	0.44193	0.44216	0.44246	0.44291	0.44307	0.44360

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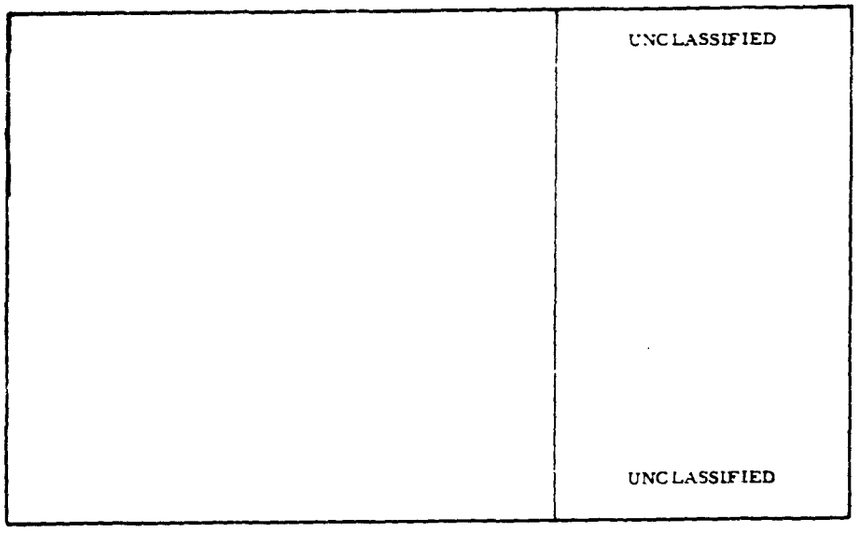
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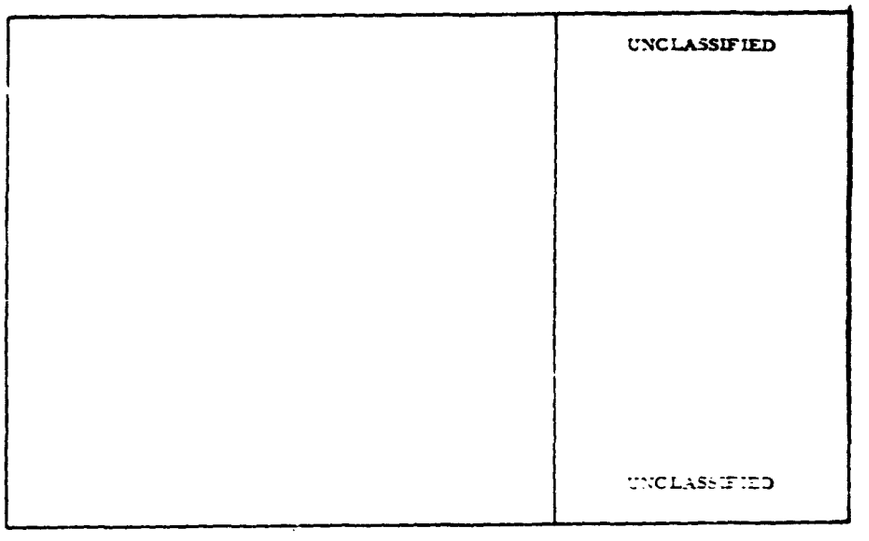
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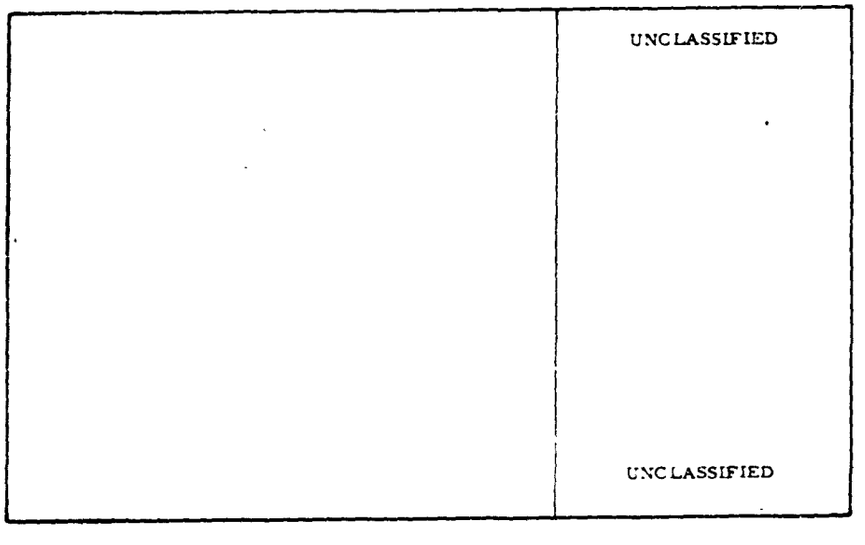
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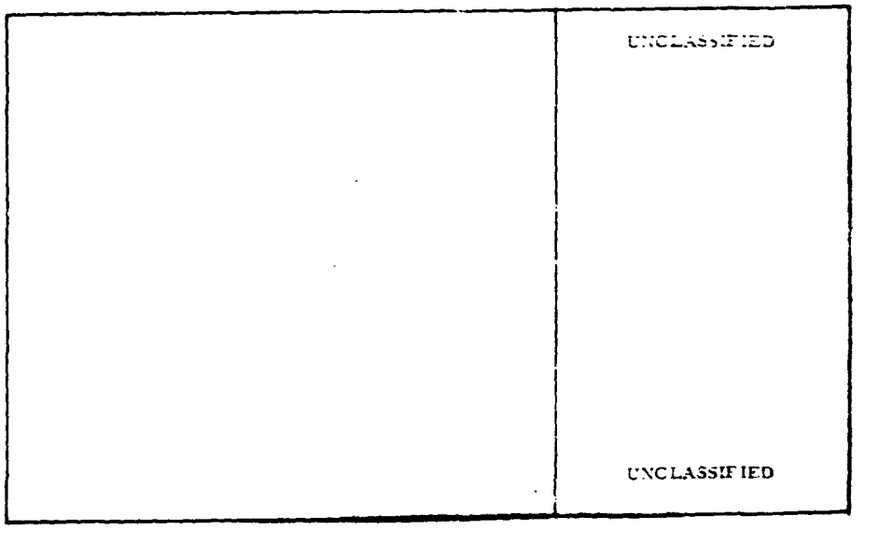
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