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THE THERMODYNAMICS OF THE POLYETHYLENE-HYDROCARBON VAPOR SYSTEM

F. J. Krieger

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PREPARED FOR:

UNITED STATES AIR FORCE PROJECT RAND

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MEMO. NO.
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F. J. Krieger

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Report on P.E.J. RAND

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PREFACE

This study was done at the request of the Scientific Advisor to the Physics Division, Research Directorate, Air Force Special Weapons Center, Kirtland Air Force Base, New Mexico.

It is a contribution to a better understanding of the complex problems involved in the physics of re-entry bodies. Polyethylene is the third of a series of ablative materials to be investigated by means of mathematical techniques similar to those used at RAND in the parametric study of certain low-molecular-weight compounds as nuclear rocket propellants.

The results of the investigation of graphite and polystyrene, the first two materials to be studied in the series, are reported in RAND Memoranda RM-3326-PR, The Thermodynamics of the Graphite-Carbon Vapor System, and RM-3708-PR, The Thermodynamics of the Polystyrene-Hydrocarbon Vapor System.

SUMMARY

↓ The purpose of this study is the thermodynamic investigation of polyethylene over a range of temperatures up to 6000⁰K and pressures up to 10⁶ atmospheres.

Two sets of equilibrium composition equations are used, one representing a pure gas phase, the other a heterogeneous system of gas and solid carbon. The gas phase of the heterogeneous chemical system, like the homogeneous gas phase, comprises 70 gaseous carbon and hydrocarbon species.

The results of the computational program are presented in both tabular and graphic form. The latter is a conventional Mollier diagram in which specific enthalpy is plotted against specific entropy, with cross plots of temperature, pressure, and molecular weight.

↙
* 10 to the 6th power

ACKNOWLEDGMENTS

This study involved considerable hand and machine computation. The efforts of the following RAND Physics Department staff members are gratefully acknowledged: Donald A. Brown, for his extensive liaison and computational work; and Elizabeth J. Force, for her meticulous graphical presentation of the tabulated results.

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I. INTRODUCTION

This study considers a chemical system that under certain conditions of temperature and pressure is a pure gas mixture and under others is a disperse system, or smoke. In this case the smoke is a gas that contains a condensed phase, solid carbon or graphite, symbolized by C_s .

In deriving the computations, the following assumptions have been made:

- (1) Thermal equilibrium is maintained between the solid particles and the gas phase.
- (2) The pressure due to the thermal motion of the solid particles can be neglected.
- (3) The gas phase obeys the ideal-gas law.
- (4) The molar volume of solid carbon is essentially constant, that is, independent of temperature and pressure.

II. COMPOSITION EQUATIONS

In this study it is assumed that the gas formed by heating polyethylene, whose molecular formula is $[C_2H_4]_x$ or, simply, CH_2 , at various pressures up to a temperature of $6000^\circ K$ is a mixture of H_2 , C_s (graphite), C (gas), and 67 other carbon and hydrocarbon chemical species for which thermochemical data are available. The presence or absence of a condensed phase makes it necessary to consider two distinct sets of chemical equations.

A. Solid carbon present. In terms of H_2 and C_s as independent components, the chemical equations for the dependent, or derived, components are given by the expression,

$$a_1 C_s + b_1 H_2 = C_{a_1} H_{2b_1}, \quad (1)$$

where a_1 has the integral values 0, 1, 2, ..., and b_1 has the half-integral values 0, 1/2, 1, 3/2,

The equations required to determine the equilibrium composition of the nonhomogeneous gas mixture are obtained from mass-balance and equilibrium considerations. The following two equations are derived from mass-balance considerations:

$$n_s = 1 - \sum_{i=1}^{69} a_i n_i, \quad (2)$$

and

$$n_{H_2} = 1 - \sum_{i=1}^{69} b_i n_i, \quad (3)$$

where n_s is the number of moles of C_s , a_1 is the coefficient of C_s on the left-hand side of Eq. (1), n_{H_2} is the number of moles of H_2 , b_1 is the coefficient of H_2 on the left-hand side of Eq. (1), and n_i is the corresponding number of moles of component i .

The equilibrium equations are obtained by considering the free energy F of the system and the partial molar free energy of chemical potential $\mu_j = \partial F / \partial n_j$ of each component. The chemical potential is a

function of the state and composition of the system. For an ideal gas

$$\mu_i = \mu_i^{\circ} + RT \ln (n_i P/n), \quad i = H_2, 1, \dots, 69, \quad (4)$$

where μ_i° is the chemical potential of component i in the standard state of unit partial pressure, R is the gas constant, T is the temperature, P is the pressure, and n is the total number of moles of gas in the mixture.

The chemical potential for graphite is given by

$$\mu_s = \mu_s^{\circ} + (P - 1)\bar{V}_s, \quad (5)$$

where μ_s° is the standard molar free energy for graphite, \bar{V}_s is the molar volume of graphite, and P is the pressure of the system.

The condition for chemical equilibrium is that for all possible reactions represented by Eq. (1),

$$\Delta F = \sum \mu_j \Delta n_j = 0, \quad j = C_s, H_2, 1, \dots, 69, \quad (6)$$

at constant temperature and pressure. Equations (4) and (5) may, therefore, be combined to give

$$\begin{aligned} RT \ln (n_i P/n) = a_1 \mu_s^{\circ} + b_1 \mu_{H_2}^{\circ} - \mu_i^{\circ} + a_1 (P - 1)\bar{V}_s \\ + b_1 RT \ln (n_{H_2} P/n). \end{aligned} \quad (7)$$

Because the equilibrium constants K_1 associated with the chemical reactions (1) are defined by the relation

$$\Delta F^{\circ} = \mu_i^{\circ} - a_1 \mu_s^{\circ} - b_1 \mu_{H_2}^{\circ} = - RT \ln K_1, \quad (8)$$

Eq. (7) may be written in the form

$$\ln (n_1 P/n) = \ln K_1 + a_1 (P - 1)\bar{V}_g/RT + b_1 \ln (n_{H_2} P/n), \quad (9)$$

or

$$n_1 = K_1 \exp \left[a_1 (P - 1)\bar{V}_g/RT \right] (P/n)^{b_1 - 1} (n_{H_2})^{b_1}. \quad (10)$$

Equations (2), (3), and (10) form a system of 71 non-linear equations in 71 unknowns which can be solved by a process of iteration.

B. Solid carbon absent. In terms of H_2 and C (gas) as independent components, the chemical equations for the dependent, or derived, components are given by the expression

$$a_j C + b_j H_2 = C_{a_j} H_{2b_j}, \quad (11)$$

where a_j has the integral values 0, 1, 2, ..., and b_j has the half-integral values 0, 1/2, 1, 3/2,

The mass-balance equations are

$$n_C = 1 - \sum a_j n_j, \quad (12)$$

and

$$n_{H_2} = 1 - \sum b_j n_j, \quad (13)$$

where n_C is the number of moles of C, a_j is the coefficient of C on the left-hand side of Eq. (11), n_{H_2} is the number of moles of H_2 , b_j is the coefficient of H_2 on the left-hand side of Eq. (11), and n_j is the corresponding number of moles of component j.

The equilibrium equations are given by the expression

$$n_j = K_j (P/n)^{a_j + b_j - 1} (n_C)^{a_j} (n_{H_2})^{b_j}, \quad (14)$$

where n is the total number of moles of gas in the equilibrium

mixture, P is the total pressure in atmospheres, and K_j is the thermodynamic equilibrium constant of component j . These values of K_j are quite different from those in Eq. (10) because of the reactions with which they are associated.

III. THERMODYNAMIC EQUATIONS

The molecular weight of the gas mixture is given by the relation

$$M = \frac{14.027}{\bar{n}}, \quad (15)$$

where 14.027 is the formula weight of the input material CH_2 and \bar{n} is the total number of moles in the gas mixture, including C_s .

The specific free energy (in calories per gram) of the gas mixture is given by the expression

$$f = \frac{1}{14.027} \left\{ \sum_i^g n_i [\mu_i^\circ + RT \ln (n_i P/n)] + n_s [\mu_s^\circ + c(P - 1)\bar{v}_s] \right\}, \quad (16)$$

which is derived from Eqs. (4) and (5). The summation is over all gaseous species. The constant $c = 0.0242172$ converts cc-atmospheres to calories.

The specific entropy (in calories per degree per gram) of the gas mixture is given by the expression

$$s = \frac{1}{14.027} \left\{ \sum_i^g n_i [S_i^\circ - R \ln (n_i P/n)] + n_s [S_s^\circ - c\alpha_v(P - 1)\bar{v}_s] \right\}, \quad (17)$$

where S_i° and S_s° are the standard molar entropy of component i and graphite, respectively, at a given temperature, and α_v is the volume coefficient of thermal expansion of graphite.

The specific enthalpy (in calories per gram) of the gas mixture is given by the expression

$$h = \frac{1}{14.027} \left\{ \sum_i^g n_i H_i^\circ + n_s [H_s^\circ + c(1 - \alpha_v T)(P - 1)\bar{v}_s] \right\}, \quad (18)$$

where H_i° and H_s° are the standard molar heat content of component i and graphite, respectively, at a given temperature.

The specific internal energy (in calories per gram) of the gas mixture is given by the expression

$$u = \frac{1}{14.027} \left\{ \sum_i^g n_i (H_i^0 - RT) + n_s \left[H_s^0 - c[1 + (P - 1)\alpha_v T] \bar{V}_s \right] \right\}. \quad (19)$$

The terms representing the increase in a thermodynamic property from one atmosphere to P atmospheres for graphite, namely,

$$\Delta F = (P - 1)\bar{V}_s, \quad (20)$$

$$\Delta S = -\alpha_v(P - 1)\bar{V}_s, \quad (21)$$

$$\Delta H = (1 - \alpha_v T)(P - 1)\bar{V}_s, \quad (22)$$

$$\Delta U = -\alpha_v T(P - 1)\bar{V}_s, \quad (23)$$

are readily derived from the differential formulas relating the various thermodynamic functions. Each of the above terms must be multiplied by the factor $c = 0.0242172$ to convert it from cc-atmospheres to calories.

The specific volume of the gas mixture (in cubic centimeters per gram) is given by the expression

$$v = \frac{1}{14.027} \left\{ nRT/P + n_s \bar{V}_s \right\}, \quad (24)$$

where the first term in the brackets is the volume of the gas phase and the second term is that of the solid phase.

IV. BASIC DATA

The pertinent thermodynamic properties (heat content, entropy, free energy, and heat of formation) for the 71 chemical species considered in this study were taken partly from JANAF Thermochemical Data⁽¹⁾ and partly from Los Alamos Scientific Laboratory Report LA-2556.⁽²⁾ In the latter report the thermodynamic functions are expressed in polynomial form. The molecular weights and heats of formation of the various components are listed in the following table. The isomeric forms of certain species are listed in the same order as they appear in Tables III and IV of the LASL report.

	<u>Component</u>	<u>Molecular Weight</u>	<u>Heat of Formation at 0°K (cal/mole)</u>	<u>Reference</u>
1.	H	1.008	51,632	1
2.	H ₂	2.016	0	1
3.	C _s (graphite)	12.011	0	1
4.	C	12.011	169,576	1
5.	CH	13.019	141,183	1
6.	CH ₂	14.027	67,015	1
7.	CH ₃	15.035	32,805	1
8.	CH ₄	16.043	-15,991	1
9.	C ₂	24.022	197,000	1
10.	C ₂ H	25.030	116,700	2
11.	C ₂ H ₂	26.038	54,325	1
12.	C ₂ H ₃	27.046	66,900	2
13.	C ₂ H ₄	28.054	14,520	1
14.	C ₂ H ₆	30.070	-16,517	2
15.	C ₃	36.033	188,104	1
16.	C ₃ H	37.041	127,100	2
17.	C ₃ H ₂	38.049	106,700	2
18.	C ₃ H ₃	39.057	77,300	2
19.	C ₃ H ₄	40.065	46,017	2
20.	C ₃ H ₄	40.065	47,700	2
21.	C ₃ H ₅	41.073	34,900	2
22.	C ₃ H ₆	42.081	8,468	2

	<u>Component</u>	<u>Molecular Weight</u>	<u>Heat of Formation at 0°K (cal/mole)</u>	<u>Reference</u>
23.	C ₃ H ₆	42.081	17,800	2
24.	C ₃ H ₈	44.097	-19,482	2
25.	C ₄	48.044	240,500	1
26.	C ₄ H	49.052	154,000	2
27.	C ₄ H ₂	50.060	111,300	2
28.	C ₄ H ₃	51.068	102,500	2
29.	C ₄ H ₄	52.076	75,300	2
30.	C ₄ H ₄	52.076	71,300	2
31.	C ₄ H ₅	53.084	67,800	2
32.	C ₄ H ₅	53.084	67,400	2
33.	C ₄ H ₆	54.092	38,090	2
34.	C ₄ H ₆	54.092	42,740	2
35.	C ₄ H ₆	54.092	29,780	2
36.	C ₄ H ₆	54.092	42,000	2
37.	C ₄ H ₈	56.108	3,480	2
38.	C ₄ H ₈	56.108	4,960	2
39.	C ₄ H ₈	56.108	980	2
40.	C ₄ H ₈	56.108	2,240	2
41.	C ₄ H ₈	56.108	12,500	2
42.	C ₄ H ₁₀	58.124	-23,670	2
43.	C ₄ H ₁₀	58.124	-25,300	2
44.	C ₅	60.055	240,298	1
45.	C ₅ H	61.063	185,400	2
46.	C ₅ H ₂	62.071	165,000	2
47.	C ₅ H ₃	63.079	135,600	2
48.	C ₅ H ₄	64.087	103,600	2
49.	C ₅ H ₄	64.087	108,300	2
50.	C ₅ H ₄	64.087	102,300	2
51.	C ₅ H ₆	66.103	25,200	2
52.	C ₆	72.066	287,000	2
53.	C ₆ H	73.074	211,300	2
54.	C ₆ H ₂	74.082	168,600	2
55.	C ₆ H ₃	75.090	158,300	2

	<u>Component</u>	<u>Molecular Weight</u>	<u>Heat of Formation at 0°K (cal/mole)</u>	<u>Reference</u>
56.	C ₆ H ₄	76.098	132,000	2
57.	C ₆ H ₄	76.098	132,800	2
58.	C ₆ H ₄	76.098	124,000	2
59.	C ₆ H ₆	78.114	24,000	2
60.	C ₇	84.077	287,000	2
61.	C ₇ H	85.085	240,000	2
62.	C ₇ H ₂	86.093	220,000	2
63.	C ₈	96.088	339,000	2
64.	C ₈ H	97.096	267,000	2
65.	C ₈ H ₂	98.104	225,000	2
66.	C ₉	108.099	334,000	2
67.	C ₉ H	109.107	291,000	2
68.	C ₉ H ₂	110.115	271,000	2
69.	C ₁₀	120.110	393,000	2
70.	C ₁₀ H	121.118	324,000	2
71.	C ₁₀ H ₂	122.126	282,000	2

The molar volume of graphite ($\bar{V}_g = 5.5524$ cc) was derived from a mean density of 2.1632 gm/cc based on measurements of 49 samples at the Los Alamos Scientific Laboratory. (3)

The volume coefficient of thermal expansion for graphite is given by the expression

$$\alpha_v = \frac{1}{v} \left[\frac{\partial v}{\partial T} \right]_p = (18.80 + 0.001875T) \times 10^{-6} \text{ cc/cc-deg} \quad (25)$$

for $T > 773^\circ\text{K}$. This expression was derived from data on the linear coefficient of expansion of lampblack obtained at the National Carbon Research Laboratories. (4)

Two values of the gas constant were used: $R = 1.98726$ cal/deg-mole and $R = 82.0597$ cc-atm/deg-mole. Their ratio gives the conversion factor $c = 0.0242172$.

V. COMPUTATIONAL PROCEDURE

The two sets of equilibrium composition equations--the one involving solid carbon and the other gaseous species only--represent two mutually exclusive contiguous regions. It is expedient to determine the border line between the two regions, that is, the conditions of temperature and pressure under which solid carbon just vanishes.

This can be done by making use of the fact that under certain conditions the value of n_g in Eq. (2) changes sign. Thus, for a specified pressure, a temperature interval can be found in which the change of sign occurs. If this interval is divided into, say, three equally spaced temperatures, the sublimation temperature of graphite (that is, the temperature at which graphite disappears) at any desired pressure may be determined by interpolation. Thus, at 10^{-3} atm the sublimation temperature is 2912°K , at one atm it is 3365°K , while at 10^3 atm it is 3799°K . It is interesting to note that in the graphite-carbon vapor system⁽⁵⁾ the corresponding temperatures are 3151°K , 4127°K , and 5908°K , respectively, while in the polystyrene-hydrocarbon vapor system⁽⁶⁾ they are 2990°K , 3524°K , and 4128°K , respectively. The comparison is shown graphically in Fig. 3.

VI. RESULTS

The results of this study are presented numerically in Tables 1 and 2 and graphically in Figs. 1 and 2. Figure 1 is a conventional Mollier diagram for polyethylene; specific enthalpy is plotted against specific entropy, with cross plots of temperature, pressure, and molecular weight. The temperatures range from 6000°K to 500°K; the pressures from 10^6 atm to 10^{-8} atm. The dotted line demarcates the pure gas phase (above) from the smoke (below). The cross plots of constant molecular weight represent chemical composition and reflect the increase in concentration of the larger molecules (C_3 through C_{10}) with increase in temperature and pressure, particularly in the vicinity of the gas-smoke borderline. Figure 2 is a plot of volume against temperature with cross plots of constant pressure.

All the computations required to obtain the results in Tables 1 and 2 were made on the RAND JOHNNIAC computer. In the tables the numbers are represented in "floating decimal" notation; the first two digits, minus 50, indicate a power of 10, and the next five digits indicate the decimal form of the number. Thus 5512345 represents 0.12345×10^5 and 4512345 represents 0.12345×10^{-5} .

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Table 1

SUMMARY OF COMPUTED VALUES OF VOLUME, MOLECULAR WEIGHT, MOLES OF GAS,
AND MOLES OF SOLID CARBON FOR POLYETHYLENE AT VARIOUS
TEMPERATURES AND PRESSURES

Tempera- ture, T (^o K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
546000	55999999	50292308	52168437	50832769	00000000
546000	54999999	51378804	52129976	51107919	00000000
546000	53999999	52475382	52103570	51135433	00000000
546000	52999999	53710441	51693031	51202400	00000000
546000	51999999	54985737	51499482	51280830	00000000
546000	50999999	56104506	51471125	51297733	00000000
546000	49999999	57105220	51467928	51299768	00000000
546000	48999999	58105294	51467602	51299976	00000000
546000	47999999	59105301	51467570	51299997	00000000
546000	46999999	60105302	51467566	51299999	00000000
546000	45999999	61105302	51467566	51300000	00000000
546000	44999999	62105302	51467566	51300000	00000000
546000	43999999	63105302	51467566	51300000	00000000
546000	42999999	64105302	51467566	51300000	00000000
545500	55999999	50252536	52178717	50784868	00000000
545500	54999999	51331299	52136229	51102965	00000000
545500	53999999	52398547	52113243	51123865	00000000
545500	52999999	53538641	51837901	51167406	00000000
545500	51999999	54821729	51549242	51255388	00000000
545500	50999999	55945452	51477367	51293840	00000000
545500	49999999	56963161	51468590	51299344	00000000
545500	48999999	57965058	51467669	51299934	00000000
545500	47999999	58965249	51467576	51299993	00000000
545500	46999999	59965268	51467567	51299999	00000000
545500	45999999	60965270	51467566	51300000	00000000
545500	44999999	61965270	51467566	51300000	00000000
545500	44100000	62965270	51467566	51300000	00000000
545500	43100000	63965270	51467566	51300000	00000000
545000	55999999	50213556	52192126	50730092	00000000
545000	54999999	51287128	52142897	50981616	00000000
545000	53999999	52336958	52121765	51115197	00000000
545000	52999999	53416474	51985171	51142381	00000000
545000	51999999	54606921	51676033	51207489	00000000
545000	50999999	55820747	51499908	51280591	00000000
545000	49999999	56870738	51471175	51297702	00000000
545000	48999999	57876832	51467932	51299765	00000000
545000	47999999	58877450	51467603	51299976	00000000
545000	46999999	59877512	51467570	51299997	00000000

Table 1--continued

Temperature, T (°K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
545000	45000000	60877518	51467566	51299999	00000000
545000	45100000	61877518	51467566	51299999	00000000
545000	44100000	62877518	51467566	51300000	00000000
545000	43100000	63877518	51467566	51300000	00000000
544500	55000000	50175668	52210208	50667291	00000000
544500	54000000	51244678	52150907	50929508	00000000
544500	53000000	52285806	52120202	51108566	00000000
544500	52000000	53330208	52111802	51125462	00000000
544500	51000000	54430620	51857527	51163574	00000000
544500	50000000	55627775	51588217	51238466	00000000
544500	49000000	56762260	51484438	51289551	00000000
544500	48100000	57786709	51469329	51298872	00000000
544500	48100000	58789468	51467743	51299886	00000000
544500	47100000	59789736	51467584	51299988	00000000
544500	46100000	60789763	51467568	51299998	00000000
544500	44999999	61789766	51467566	51299999	00000000
544500	44100000	62789766	51467566	51300000	00000000
544500	43100000	63789766	51467566	51300000	00000000
544000	55999999	50139817	52234761	50597499	00000000
544000	54999999	51202371	52162196	50864815	00000000
544000	53999999	52241341	52136006	51103134	00000000
544000	52999999	53267395	52122754	51114268	00000000
544000	51999999	54314712	52104297	51134489	00000000
544000	50999999	55421229	51779240	51180008	00000000
544000	49999999	56585018	51561074	51250002	00000000
544000	48999999	57682735	51480770	51291760	00000000
544000	47999999	58700064	51468869	51299166	00000000
544000	46999999	59701820	51467696	51299917	00000000
544000	45999999	60701995	51467579	51299991	00000000
544000	44999999	61702013	51467567	51299999	00000000
544000	43999999	62702014	51467566	51300000	00000000
544000	42999999	63702014	51467566	51300000	00000000
543900	55999999	50133012	52240604	50582990	00000000
543900	54999999	51193782	52165150	50849344	00000000
543900	53999999	52232953	52137380	51102103	00000000
543900	52999999	53256782	52124631	51112547	00000000
543900	51999999	54296967	52107766	51130160	00000000
543900	50999999	55388639	51823470	51170340	00000000
543900	49999999	56539882	51592782	51236629	00000000
543900	48999999	57654989	51488607	51287080	00000000
543900	48100000	58681427	51469650	51298668	00000000

Table 1--continued

Temperature, T (°K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
543900	47100000	59684163	51467772	51299868	00000000
543900	46100000	60684434	51467587	51299986	00000000
543900	44999999	61684461	51467568	51299998	00000000
543900	44100000	62684464	51467566	51299999	00000000
543900	43100000	63684464	51467566	51300000	00000000
543800	55999999	50126362	52246772	50568418	00000000
543800	54999999	51185144	52168423	50832842	00000000
543800	54313384	51667185	52149138	50940534	44960000
543800	54251188	51846760	52145284	50956372	48911088
543800	54158489	52138278	52140559	50985485	49124533
543800	54106909	52209455	52139253	51100730	44420000
543800	53999999	52224672	52138791	51101065	00000000
543800	52999999	53246677	52126410	51110963	00000000
543800	51999999	54280711	52111084	51126273	00000000
543800	50999999	55358780	51869131	51161391	00000000
543800	50100000	56495173	51629732	51222745	00000000
543800	49100000	57622239	51501136	51279903	00000000
543800	48100000	58662038	51471009	51297807	00000000
543800	47100000	59666436	51467902	51299784	00000000
543800	46100000	60666866	51467599	51299978	00000000
543800	45100000	61666909	51467569	51299997	00000000
543800	44100000	62666913	51467566	51299999	00000000
543800	43100000	63666914	51467566	51300000	00000000
543500	55999999	50107414	52267382	50524603	00000000
543500	55195131	50732504	52200937	50698076	45100000
543500	54999999	51168007	52143147	50782339	50197558
543500	53999999	52200676	51990761	50971494	50444285
543500	52999999	53213894	51972740	51104386	50398139
543500	51999999	54237546	52111630	51116013	49964224
543500	51676334	54361754	52117387	51119492	44650000
543500	50999999	55284228	52101048	51138814	00000000
543500	50100000	56377166	51761491	51184204	00000000
543500	49100000	57498556	51576080	51243490	00000000
543500	48100000	58589349	51487332	51287832	00000000
543500	47100000	59611936	51469344	51298863	00000000
543500	46100000	60614037	51467738	51299890	00000000
543500	44999999	61614240	51467583	51299989	00000000
543500	44100000	62614260	51467568	51299998	00000000
543500	43100000	63614262	51467566	51299999	00000000

Table 1--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular weight, M	Moles of Gas, n	Moles of Solid, n _s
543000	55999999	49798050	52308475	50454720	00000000
543000	55436407	50207091	52272393	50514952	44760000
543000	54999999	51145849	52114590	50716561	50507540
543000	53999999	52168164	51812696	50940464	50785518
543000	52999999	53175906	51760561	51100038	50843904
543000	51999999	54180184	51751485	51102647	50840091
543000	50999999	55190824	51743023	51108728	50800546
543000	49999999	56222910	51722256	51127011	50671989
543000	48999999	57298818	51695268	51170263	50314859
543000	48367907	57931850	51718070	51195343	44650000
543000	48100000	58390541	51630352	51222526	00000000
543000	47100000	59464065	51530484	51264418	00000000
543000	46100000	60518367	51474911	51295360	00000000
543000	44999999	61525871	51468135	51299635	00000000
543000	44100000	62526449	51467621	51299965	00000000
543000	43100000	63526505	51467571	51299996	00000000
542500	55999999	49592039	52346513	50404804	00000000
542500	55572213	50109392	52327736	50427996	44610000
542500	54999999	51119632	52111851	50656155	50597917
542500	53999999	52134851	51794421	50898572	50867115
542500	52999999	53144813	51720132	50987559	50960277
542500	51999999	54146648	51709990	51100244	50973219
542500	50999999	55148074	51706034	51101242	50974306
542500	49999999	56152083	51696853	51103985	50973046
542500	48999999	57164578	51669970	51112529	50968376
542500	47999999	58200593	51603247	51137155	50953696
542500	46999999	59262391	51518359	51179408	50911949
542500	46100000	60304350	51508376	51208098	50678189
542500	45306810	61114608	51583420	51240427	44880000
542500	45100000	61370262	51554064	51253165	00000000
542500	44100000	62423602	51484296	51289636	00000000
542500	43100000	63437952	51468428	51299448	00000000
542000	55999999	49456805	52359276	50390423	00000000
542000	55619794	49762303	52347363	50403812	44330000
542000	54999999	50921164	52119826	50591320	50579289
542000	53999999	51974649	51872824	50805911	50801169
542000	52999999	53113209	51728215	50964324	50961890
542000	51999999	54116608	51704707	50996292	50994178
542000	50999999	55117053	51701979	51100039	50997806
542000	49999999	56117297	51701104	51100251	50998185
542000	49100000	57117949	51699142	51100809	50998223

Table 1--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
542000	48100000	58119997	51693096	51102559	50998217
542000	47100000	59126446	51674733	51108071	50998180
542000	46100000	60146028	51624495	51124807	50998054
542000	45100000	61190647	51533944	51162943	50997621
542000	44100000	62226134	51479052	51193273	50995343
542000	43100000	63234583	51470860	51200494	50974062
541500	55999999	49339978	52362050	50387431	00000000
541500	55657904	49532824	52351136	50399473	44670000
541500	54999999	50678472	52131680	50533163	50532065
541500	53999999	51592518	52108591	50646097	50645619
541500	52999999	52751754	51822471	50852835	50852633
541500	51999999	53857446	51718112	50976685	50976631
541500	51100000	54875384	51703103	50997522	50997488
541500	50100000	55877326	51701523	50999776	50999727
541500	49100000	56877573	51701344	51100006	50999953
541500	48100000	57877759	51701262	51100027	50999976
541500	47100000	58878286	51701050	51100087	50999978
541500	46100000	59879949	51700387	51100277	50999979
541500	45100000	60885206	51698298	51100876	50999979
541500	44100000	61901821	51691777	51102769	50999979
541500	43100000	62954107	51672029	51108727	50999980
541000	55999999	49224994	52364718	50384597	00000000
541000	55697737	49333118	52353053	50397304	44320000
541000	54999999	50493830	52139302	50503476	50503467
541000	53999999	51327240	52133865	50523924	50523920
541000	52999999	52340792	52121210	50578623	50578620
541000	51999999	53424850	51966402	50725733	50725732
541000	51100000	54540621	51758989	50924057	50924056
541000	50100000	55579471	51708061	50990520	50990521
541000	49100000	56584443	51702032	50999026	50999027
541000	48100000	57584955	51701418	50999902	50999902
541000	47100000	58585006	51701356	50999989	50999990
541000	46100000	59585011	51701350	50999998	50999999
541000	45100000	60585012	51701349	51100000	50999999
541000	44100000	61585014	51701348	51100000	50999999
541000	43100000	62585018	51701346	51100001	51100000
535000	55999999	48885915	52463134	50302870	00000000
535000	55742806	49124791	52442617	50316911	44780000
535000	54999999	50344112	52140294	50499914	50499914

Table 1--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular weight, M	Moles of Gas, n	Moles of Solid, n _s
535000	53999999	51166036	52140235	50500123	50500123
535000	52999999	52148372	52140137	50500473	50500473
535000	51999999	53146897	52139843	50501523	50501523
535000	51100000	54147634	52138929	50504825	50504825
535000	50100000	55150717	52136116	50515255	50515255
535000	49100000	56160306	52127973	50548042	50548042
535000	48100000	57188952	52108571	50645979	50645979
535000	47100000	58247828	51827787	50847258	50847258
535000	46100000	59285238	51719219	50975154	50975153
535000	45100000	60291727	51703221	50997338	50997338
535000	44100000	61292427	51701538	50999731	50999731
535000	43100000	62292498	51701368	50999972	50999973

Table 2

SUMMARY OF COMPUTED VALUES OF DENSITY, SPECIFIC ENTHALPY,
SPECIFIC ENERGY, AND SPECIFIC ENTROPY FOR POLYETHYLENE
AT VARIOUS TEMPERATURES AND PRESSURES

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
546000	55399999	51342104	54776896	54706107	51405727
546000	54999999	50263988	54883793	54792057	51454941
546000	53999999	49210356	55107745	54962328	51526450
546000	52999999	48140757	55166353	55149148	51677530
546000	51999999	47101446	55240820	55216948	51882442
546000	50999999	45956875	55257127	55231819	52100484
546000	49999999	44950332	55259094	55233613	52110569
546000	48999999	43949720	55259296	55233797	52120387
546000	47999999	42949654	55259317	55233816	52130176
546000	46999999	41949647	55259319	55233817	52139963
546000	45999999	40949647	55259319	55233818	52149749
546000	44999999	39949647	55259319	55233818	52159536
546000	43999999	38949647	55259319	55233818	52169322
546000	42999999	37949647	55259319	55233818	52179109
545500	55399999	51395982	54699044	54637887	51392179
545500	54999999	50301841	54794081	54713849	51439339
545500	53999999	49250911	54925147	54828630	51499990
545500	52999999	48185652	55128299	55115255	51611441
545500	51999999	47121694	55210073	55190173	51828654
545500	50999999	46105769	55247750	55224854	51988474
545500	49999999	45103824	55253164	55229839	52109537
545500	48999999	44103620	55253743	55230372	52119420
545500	47999999	43103600	55253801	55230426	52129217
545500	46999999	42103598	55253807	55230431	52139004
545500	45999999	41103597	55253808	55230432	52148791
545500	44999999	40103597	55253808	55230432	52158577
545500	44100000	39103597	55253808	55230432	52168364
545500	43100000	38103597	55253808	55230432	52178150
545000	55999999	51468259	54620352	54568635	51377176
545000	54999999	50348275	54709321	54639787	51423186
545000	53999999	49296772	54801084	54719482	51476375
545000	52999999	48240110	55100914	54908283	51559383
545000	51999999	47164766	55157818	55143120	51728867
545000	50999999	46121840	55228811	55208935	51952110
545000	49999999	45114837	55246015	55224926	52108170
545000	48999999	44114046	55248075	55226841	52118339
545000	47999999	43113966	55248286	55227036	52128165
545000	46999999	42113958	55248307	55227056	52137955

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
545000	45999999	41113957	55248309	55227058	52147742
545000	45100000	40113957	55248310	55227059	52157528
545000	44100000	39113957	55248309	55227058	52167315
545000	43100000	38113957	55248309	55227058	52177101
544500	55999999	51569255	54540515	54497974	51360351
544500	54999999	50408666	54626890	54567631	51405818
544500	53999999	49349887	54696789	54627575	51454428
544500	52999999	48302766	54815258	54735272	51518645
544500	51999999	47232223	55112355	55101926	51633406
544500	50999999	46159272	55180471	55165269	51849542
544500	49999999	45131188	55232136	55213676	52105221
544500	49100000	44127077	55241687	55222633	52116991
544500	48100000	43126667	55242712	55223593	52126991
544500	47100000	42126624	55242815	55223690	52136799
544500	46100000	41126620	55242826	55223700	52146587
544500	44999999	40126619	55242827	55223701	52156374
544500	44100000	39126619	55242827	55223701	52166161
544500	43100000	38126619	55242827	55223701	52175947
544000	55999999	51715216	54459982	54426122	51341380
544000	54999999	50494141	54543525	54494517	51386175
544000	53999999	49414351	54605775	54547329	51433015
544000	52999999	48373978	54673450	54608694	51485340
544000	51999999	47317750	54827123	54750909	51563875
544000	50999999	46237400	55120009	55109808	51707553
544000	49999999	45170934	55185071	55170903	51940140
544000	48999999	44146469	55228784	55212251	52113914
544000	47999999	43142844	55236515	55219561	52125527
544000	46999999	42142486	55237282	55220286	52135495
544000	45999999	41142451	55237359	55220358	52145300
544000	44999999	40142447	55237366	55220366	52155088
544000	43999999	39142447	55237367	55220366	52164875
544000	42999999	38142447	55237367	55220366	52174661
543900	55999999	51751810	54443874	54411662	51337302
543900	54999999	50516043	54526382	54479454	51381834
543900	53999999	49429270	54588646	54532231	51428677
543900	52999999	48389434	54649645	54587459	51479313
543900	51999999	47336737	54781733	54709815	51552384
543900	50999999	46257307	55110588	55101176	51683702
543900	49999999	45185225	55170376	55157302	51902931
543900	48999999	44152674	55222671	55206809	52112365
543900	48100000	43146750	55234911	55218409	52125121

Table 2--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
543900	47100000	42146163	55236143	55219575	52135206
543900	46100000	41146106	55236265	55219690	52145022
543900	44999999	40146100	55236277	55219701	52154812
543900	44100000	39146099	55236278	55219702	52164599
543900	43100000	38146099	55236278	55219702	52174385
543800	55999999	51791376	54427789	54397188	51333123
543800	54999999	50540117	54509010	54464173	51377322
543800	54313384	50149883	54544920	54494286	51401401
543800	54251188	50118097	54548718	54497209	51405374
543800	54158489	49723179	54558935	54505851	51414403
543800	54106909	49477428	54570318	54516039	51422958
543800	53999999	49445091	54571752	54517542	51424291
543800	52999999	48405386	54627054	54567.16	51473447
543800	51999999	47356238	54740199	54672218	51541598
543800	50999999	46278722	55101980	54932915	51661347
543800	50100000	45201949	55155606	55143614	51864567
543800	49100000	44160709	55213788	55198719	52110056
543800	48100000	43151048	55232925	55216893	52124605
543800	47100000	42150051	55234971	55218851	52134902
543800	46100000	41149955	55235169	55219019	52144738
543800	45100000	40149945	55235188	55219038	52154529
543800	44100000	39149944	55235190	55219039	52164316
543800	43100000	38149944	55235191	55219040	52174103
543500	55999999	51930970	54379573	54353560	51319906
543500	55195131	51136518	54430760	54396145	51348603
543500	54999999	50595211	54418747	54378060	51352433
543500	53999999	49498314	54430316	54381718	51385647
543500	52999999	48467520	54473698	54421899	51431096
543500	51999999	47420969	54611454	54553927	51506104
543500	51676334	47276430	54654635	54595383	51524962
543500	50999999	46351830	54804166	54735334	51602349
543500	50100000	45265134	55117184	55108051	51759436
543500	49100000	44200578	55171453	55159379	51984198
543500	48100000	43169678	55218883	55204611	52120718
543500	47100000	42163415	55230758	55215939	52133749
543500	46100000	41162856	55231822	55216951	52143819
543500	44999999	40162802	55231923	55217048	52153634
543500	44100000	39162797	55231934	55217058	52163423
543500	43100000	38162796	55231935	55217059	52173210

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
543000	5599999	52125305	54297408	54278081	51294555
543000	55436407	51482878	54313767	54291880	51305691
543000	5499999	50685637	54279158	54243837	51309619
543000	5399999	49594655	54294458	54253733	51344072
543000	5299999	48568484	54304304	54261704	51379493
543000	5199999	47554987	54321504	54277868	51418290
543000	5099999	46524040	54375170	54328957	51470480
543000	4999999	45448610	54540115	54486132	51563390
543000	4899999	44334651	54942763	54870398	51745394
543000	48367907	44107313	55120114	55111811	51857370
543000	48100000	43256054	55143777	55134319	51974833
543000	47100000	42215486	55186761	55175523	52119765
543000	46100000	41192913	55221539	55208986	52140578
543000	4499999	40190160	55226156	55213421	52151850
543000	44100000	39189951	55226498	55213749	52161746
543000	43100000	38189931	55226531	55213780	52171543
542500	5599999	52168907	54213416	54199079	51263962
542500	55572213	51914142	54217059	54201900	51268711
542500	5499999	50835892	54184950	54155978	51275418
542500	5399999	49741557	54209629	54176972	51313292
542500	5299999	48690541	54221728	54186658	51349603
542500	5199999	47681901	54225335	54189821	51383597
542500	5099999	46675337	54232248	54196389	51419210
542500	4999999	45657535	54253738	54216907	51461198
542500	4899999	44607613	54321063	54281207	51523187
542500	4799999	43498520	54515430	54466852	51641028
542500	4699999	42381110	54852748	54789204	51827571
542500	46100000	41328568	55112897	55105526	52100145
542500	45306810	40872533	55153550	55145035	52120104
542500	45100000	40270078	55167612	55158645	52129644
542500	44100000	39236070	55209536	55199277	52155266
542500	43100000	38228335	55220583	55209977	52169362
542000	5599999	52218911	54141638	54130575	51232044
542000	55619794	52131181	54141807	54130365	51234820
542000	5499999	51108558	54112366	53900584	51243107
542000	5399999	50102600	54138025	54114422	51281332
542000	5299999	48883321	54161630	54134214	51322845
542000	5199999	47857573	54166550	54138311	51357495
542000	5099999	46854312	54167503	54139156	51390562
542000	4999999	45852534	54168907	54140501	51423930
542000	49100000	44847821	54173193	54144629	51458851

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
542000	48100000	43833350	54186729	54157669	51498737
542000	47100000	42790849	54229353	54198731	51554237
542000	46100000	41684798	54358789	54323425	51656464
542000	45100000	40524527	54653758	54607588	51850368
542000	44100000	39442215	54888863	54834099	52102688
542000	43100000	38426286	54950322	54893512	52112210
541500	55999999	52294136	53815055	53732722	51197691
541500	55657904	52187679	53813649	53728757	51199932
541500	54999999	51147389	53506853	53342546	51207729
541500	53999999	50168771	53627726	53484235	51238016
541500	52999999	49133022	53945536	53763482	51283925
541500	51999999	48116625	54113949	53931849	51327196
541500	51100000	47114235	54117221	53960225	51361698
541500	50100000	46113982	54117586	53963404	51394533
541500	49100000	45113950	54117668	53964156	51427207
541500	48100000	44113926	54117816	53965598	51459933
541500	47100000	43113858	54118276	53970063	51492877
541500	46100000	42113642	54119727	53984177	51526520
541500	45100000	41112968	54124317	54102880	51562372
541500	44100000	40110886	54138825	54116985	51605202
541500	43100000	39104809	54184479	54161373	51669954
541000	55999999	52444455	53323681	53269193	51158161
541000	55697737	52300193	53325384	53269096	51160325
541000	54999999	51202498	51838779	53111204	51167637
541000	53999999	50305585	51694721	52861959	51187211
541000	52999999	49293433	52715522	52109782	51213351
541000	51999999	48235376	53296124	53193237	51256803
541000	51100000	47184972	53599746	53468822	51314287
541000	50100000	46172571	53701523	53561191	51356008
541000	49100000	45171102	53714548	53573012	51389810
541000	48100000	44170953	53715889	53574229	51422553
541000	47100000	43170938	53716024	53574351	51455187
541000	46100000	42170936	53716039	53574365	51487810
541000	45100000	41170936	53716046	53574372	51520432
541000	44100000	40170936	53716065	53574390	51553056
541000	43100000	39170934	53716123	53574448	51585684
535000	55999999	53112877	-52506700	-52721244	51107212
535000	55742806	52801334	-52469631	-52694115	51109259
535000	54999999	51290602	-53337890	-53421224	51120893

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
535000	53191999	50602077	-53380514	-53420136	51137307
535000	52797999	49673978	-53384335	-53420267	51153725
535000	51399999	48680748	-53383326	-53418900	51170354
535000	51100000	47677118	-53378824	-53414589	51187667
535000	50100000	46663492	-53364467	-53400966	51207146
535000	49100000	45623806	-53319319	-53358140	51233420
535000	48100000	44529232	-53184455	-53230214	51279598
535000	47100000	43403504	52927169	52326997	51359219
535000	46100000	42350583	53268834	53199757	51424614
535000	45100000	41342785	53299383	53228735	51463017
535000	44100000	40341964	53302679	53231861	51496264
535000	43100000	39341832	53303011	53232176	51528949

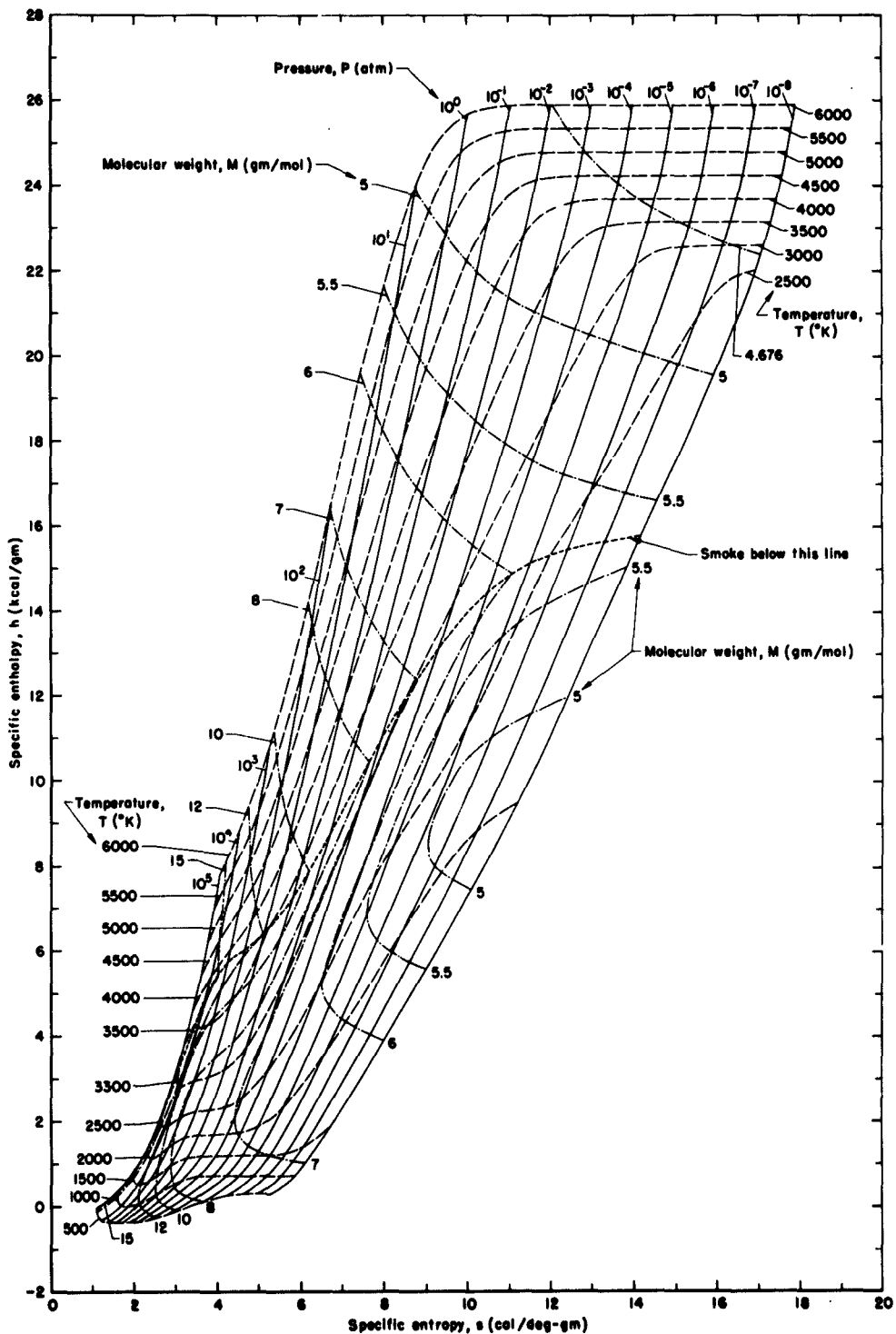


Fig. 1—Specific enthalpy versus specific entropy for polyethylene with cross plots of temperature, pressure, and molecular weight

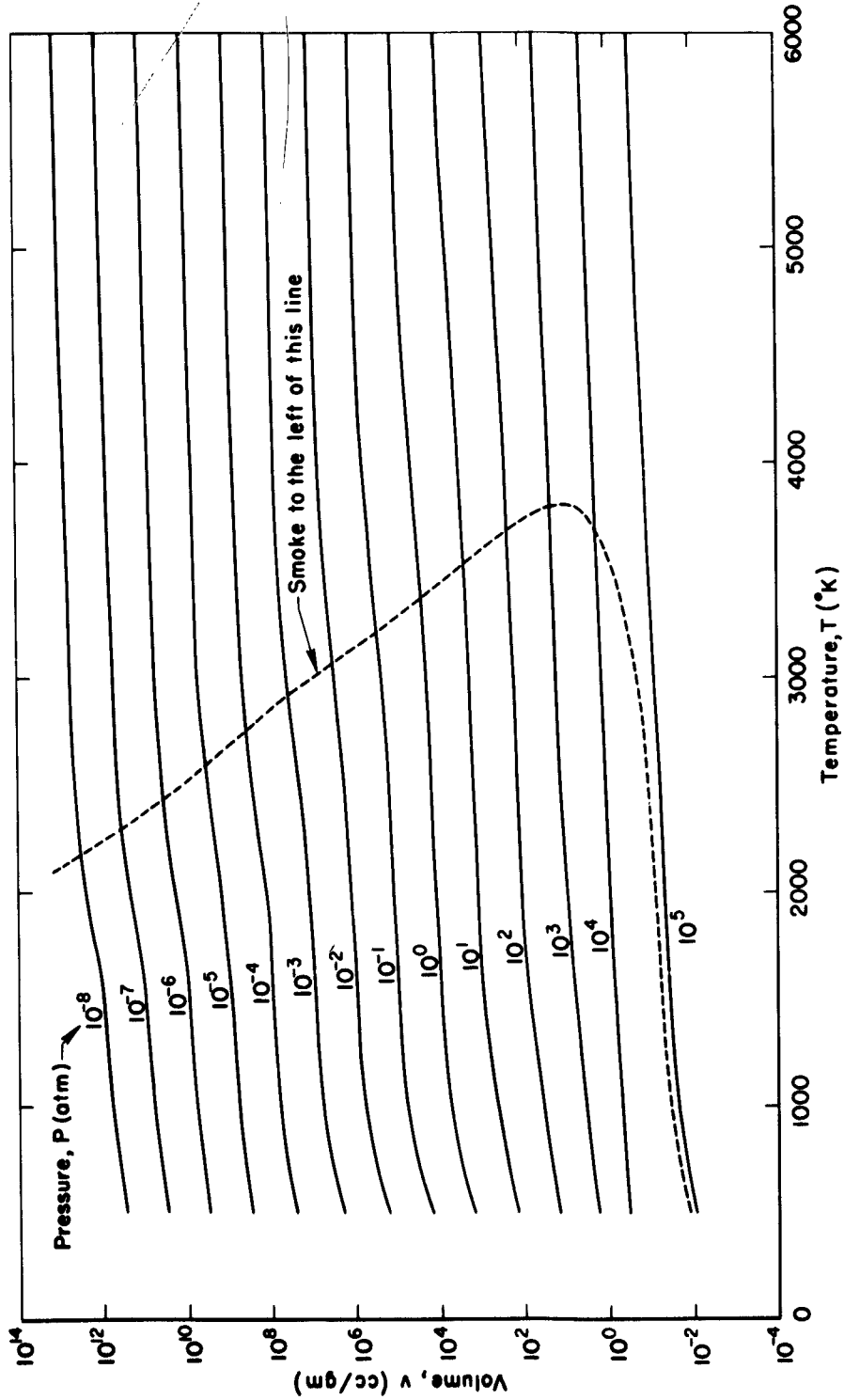


Fig. 2—Volume versus temperature for polyethylene with cross plots of constant pressure

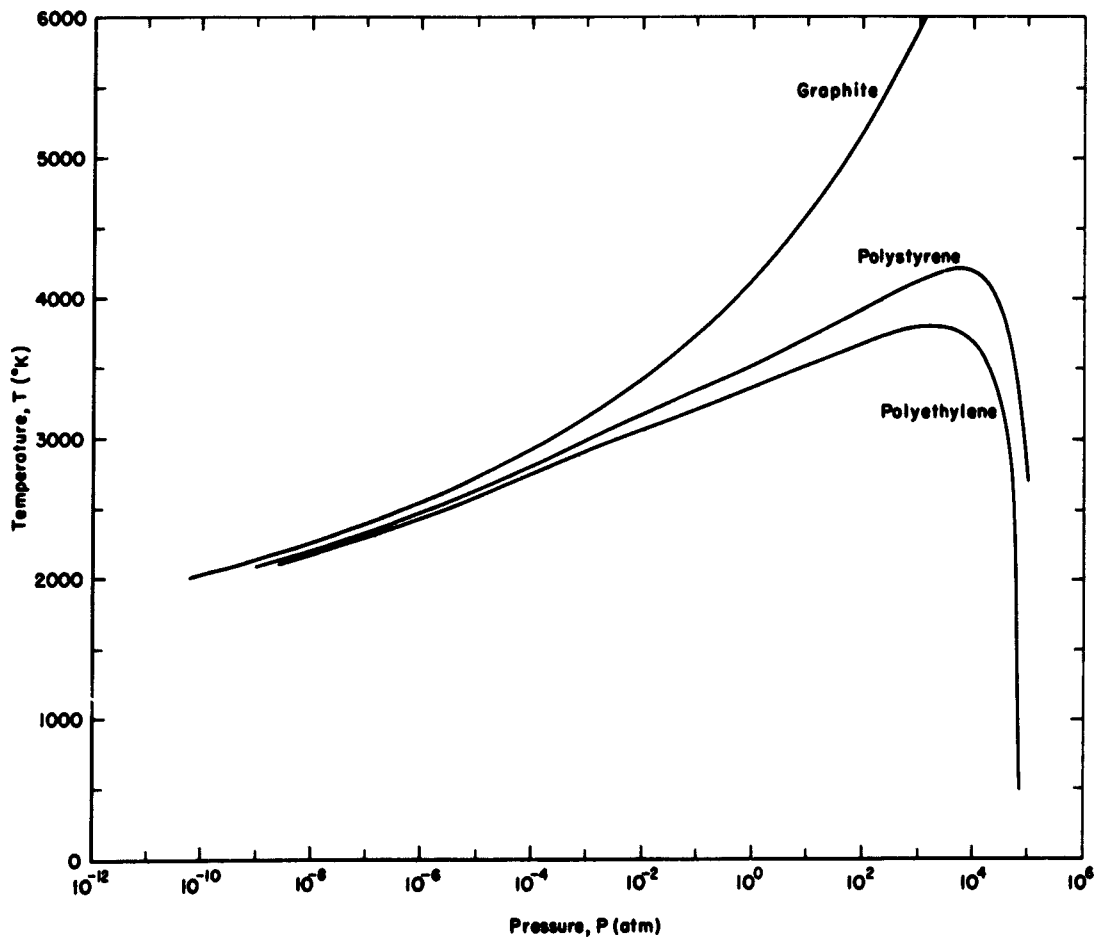


Fig. 3—Sublimation temperature for graphite, polystyrene, and polyethylene at various pressures