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N 63 16290

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TECHNICAL NOTE

D-1664

FORMULATION AND DIGITAL CODING OF APPROXIMATE HYDROGEN
PROPERTIES FOR APPLICATION TO HEAT-TRANSFER
AND FLUID-FLOW COMPUTATIONS

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WASHINGTON

May 1963

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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SUMMARY

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A digital computer program coded in FORTRAN language is described that permits calculation of real fluid state relations, thermodynamic properties, and transport properties of molecular hydrogen in any fixed ortho-para combination. The program is oriented toward application in numerical integration of heat-transfer and fluid-flow calculations, and results cover the temperature range from melting to dissociation for pressures up to 340 atmospheres (approx. 5000 lb/sq in. abs).

Properties are obtained by combinations of analytical and empirical formulations with tabulations of published data. No unpublished data are used or presented; however, unsubstantiated extrapolations are used to maintain the continuous range of results. Typical maximum errors with respect to published properties are about 1 percent in density, the larger of 1 percent or 3 calories per gram in enthalpy, and 5 percent in specific heats.

Any two state variables (p, T, v), or enthalpy and either pressure or specific volume may be specified as independent variables. Iterative solutions are used in calculating variables normally formulated as independent variables. Computation speed increased with accuracy in the trial value of the dependent variable. Results, however, are independent of the trial values since only single-valued continuous formulations are used.

The FORTRAN coding results in a total storage requirement of about 2100 words and uses subroutines for the calculation of logarithms, exponentials, and square roots. Included in the total are 50 erasable words, 31 words used in returning results, and a table of constants using 215 words. The list of constants contains data that specify the dimensional set and the para-ortho composition, which can be prepared conveniently by an additional subroutine.

INTRODUCTION

Many analyses have indicated that molecular hydrogen has characteristics that make it attractive as a working fluid for nuclear-rocket propulsion applica-

tions. Hydrogen used in such systems will probably be carried as a liquid in the paramodification because of boil-off problems typical of normal or ortho-hydrogen. Commercially available liquid hydrogen, however, may contain up to 5 or 10 percent unconverted ortho-hydrogen, and, in addition, many ground tests of systems or system components may utilize pressurized hydrogen in the normal composition.

Many design and analysis problems in the field of nuclear-rocket propulsion, many of which are conveniently solved with the aid of electronic digital computers, involve the flow and heat transfer of the working fluid. In this regard, a "library" of hydrogen properties that can be prepared to approximate any fixed para-ortho composition has been developed at the Lewis Research Center and is described herein. Where possible, the resulting properties are compared with the published experimental data.

In anticipation of heat-transfer and fluid-flow computations (by techniques that may be numerical), a series of useful parameters has been selected and is described in detail.

For fluid in the vapor state, saturation conditions intended for use with two-phase heat-transfer correlations of the Martinelli form (refs. 1 and 2) are also included.

A digital computer program for achieving this end may have many criteria of "efficiency" including storage requirements, execution speed, accuracy of results, and versatility. Versatility could include such factors as the ease of preparation, loading, calling, and updating. For use in numerical integration, an additional requirement is imposed, namely, that results must be unique, precise, single-valued, and continuous over the range of interest. Thus, computed properties must have a precision that is unjustified by the accuracy of the resulting data.

In order to attain the desired continuity and versatility with a minimal storage requirement, the accuracy of the computed properties has been compromised. The errors with respect to published hydrogen properties are presented herein to illustrate the validity of the techniques used, specifically, a series of analytical and empirical data fits that are differentiated, integrated, and combined with tabulations of data.

The mechanics of the program are presented in detail, and estimations of execution speed and storage requirements are shown.

No original data are presented herein, inasmuch as most of the source material originated at the National Bureau of Standards Cryogenic Engineering Laboratory. Properties in the cryogenic range, temperatures below 100° K, have been compared with those shown by Roder and Goodwin (ref. 3), Goodwin, Roder, and Younglove (ref. 4), Goodwin, et al. (refs. 5 and 6), two progress reports (refs. 7 and 8), and a compendium edited by Johnson (ref. 9). Transport properties are computed as recommended by Rogers, Zeigler, and McWilliams (ref. 10). At higher temperatures, the techniques of Woolley, Scott, and Brickwedde (ref. 11) are used.

ANALYSIS

The analytical techniques used herein to formulate properties of various combinations of para- and ortho-hydrogen are presented in two parts: (1) the general relations used over the range of the library are shown, and (2) the various state equations used within the temperature range of interest are shown and discussed briefly. The definitions of symbols and the detailed algebra are delegated to appendixes A and B, respectively. The external characteristics of the computer program and an error analysis of the computed properties are considered in the RESULTS section, while the FORTRAN language coding is shown in appendixes C and D.

General Relations

Equations of state for a real fluid are commonly expressed with pressure p as the dependent variable and thus with temperature T and specific volume v as the independent variables. Two forms are

$$p = \varphi(v, T) \quad (1a)$$

$$p = \frac{ZRT}{v} = \rho ZRT \quad (1b)$$

where the compressibility factor Z is generally a dimensionless function of v and T . Naturally, the variables must have a dimensionally consistent set of units, but herein units will be specified only as constants are shown.

Partial derivatives of the state parameters are used in computation of thermodynamic and transport properties of the fluid and also are useful in solving the state equation for the normally independent temperature or specific volume by iterative procedures such as Newton's method. Successive trial values are then

$$v = v + \frac{\Delta p}{(\partial p / \partial v)_T} \quad (\text{to solve for } v) \quad (2)$$

$$T = T + \frac{\Delta p}{(\partial p / \partial T)_v} \quad (\text{to solve for } T) \quad (3)$$

where Δp is the difference between the desired and computed pressures. The partial derivatives are obtained by differentiation of the state equation, or, if given in terms of the compressibility factor Z ,

$$\left(\frac{\partial p}{\partial T}\right)_v = \left(\frac{\partial p}{\partial T}\right)_\rho = \frac{RT}{v} \left(\frac{\partial Z}{\partial T}\right)_v + \frac{RZ}{v} \quad (4a)$$

$$\left(\frac{\partial p}{\partial T}\right)_v = p \left[\frac{1}{T} + \frac{(\partial Z / \partial T)_v}{Z} \right] \quad (4b)$$

$$\left(\frac{\partial p}{\partial v}\right)_T = \frac{RT}{v} \left(\frac{\partial Z}{\partial v}\right)_T - \frac{RTZ}{v^2} \quad (5a)$$

$$\left(\frac{\partial p}{\partial v}\right)_T = p \left[\frac{(\partial Z / \partial v)_T}{Z} - \rho \right] \quad (5b)$$

Equations (4b) and (5b) are obtained by substitution of equation (1b).

The state equations used herein are fitted to para-hydrogen properties at low temperatures and are largely independent of the composition at higher temperatures. The difference between para- and ortho-hydrogen state relations is assumed herein to be small, so that errors in computation of p/v relations for ortho-hydrogen compositions up to 15 percent are insignificant to errors in the para-hydrogen state equation itself. The composition is important to the thermodynamic properties, however, and is considered.

Enthalpy H_0 and specific heat at constant pressure $c_{p,0}$ for both para- and ortho-hydrogen in the ideal state ($pv = RT$ or $Z = 1$) are calculated as a function of temperature by Woolley, et al. (ref. 11). The tables (ref. 11) are used directly in computation and are interpolated semilogarithmically for intermediate temperatures. Specific heat at constant volume $c_{v,0}$ for gas in the ideal state is

$$\frac{c_{v,0}}{R} = \frac{c_{p,0}}{R} - 1 \quad (6)$$

The enthalpy and specific heat at constant volume for the real fluid can be determined by integration of the equation of state along a constant temperature path from the ideal to the real state. Enthalpy, from reference 12 or from most thermodynamics texts, is given as

$$dH = c_v dT + \left[T \left(\frac{\partial p}{\partial T}\right)_v - p \right] dv$$

which is expressed in reference 11 as

$$\frac{H_{T,\rho} - H_{T,0}}{RT} = \int_0^\rho \frac{T}{\rho} \left(\frac{\partial Z}{\partial T}\right)_\rho d\rho - (Z - 1) \quad (7)$$

The change in specific heat at constant volume at constant temperature can also be determined from (refs. 11 and 12):

$$\left(\frac{\partial c_v}{\partial v}\right)_T = T \left(\frac{\partial^2 p}{\partial T^2}\right)_v \quad (8)$$

and

$$\left. \begin{aligned} \int_0^{\rho} dc_v &= T \int_0^{\rho} \left(\frac{\partial^2 p}{\partial T^2} \right)_v dv \\ \frac{c_{v,\rho} - c_{v,0}}{R} &= -2 \int_0^{\rho} \frac{T}{\rho} \left(\frac{\partial Z}{\partial T} \right)_\rho d\rho - \int_0^{\rho} \frac{T^2}{\rho} \left(\frac{\partial^2 Z}{\partial T^2} \right)_\rho d\rho \end{aligned} \right\} \quad (9)$$

The equations of state used herein can be integrated in closed form, so that no numerical or stepwise computations are required in solution of equations (7) and (9).

The real fluid specific heat at constant pressure c_p can also be obtained by similar techniques. A substantial reduction in algebra is attained, however, through the use of c_v and the partial derivatives, as shown in most thermodynamic texts:

$$\begin{aligned} c_p &= c_v + T \left(\frac{\partial p}{\partial T} \right)_v \left(\frac{\partial v}{\partial T} \right)_p \\ &= c_v - T \left(\frac{\partial p}{\partial T} \right)_v^2 \left(\frac{\partial v}{\partial p} \right)_T \end{aligned} \quad (10)$$

The transport properties, absolute viscosity μ_0 , and thermal conductivity k_0 are computed from empirical equations shown in references 10 and 11. Again, the ideal-state values are given as functions of temperature, and the real fluid effects are determined from the state equation by using the partial derivatives $(\partial p / \partial T)_v$ or the density and a correlation given by Rodgers, et al. (ref. 10). These equations are shown in appendix B.

Relations for sonic velocity, or the speed of sound in the fluid, are derived in appendix B:

$$c = v \sqrt{-g \frac{c_p}{c_v} \left(\frac{\partial p}{\partial v} \right)_T} \quad (11)$$

Note that equation (11) is simply a generalization of the familiar form for the sonic velocity of an ideal gas:

$$c = \sqrt{\frac{c_p}{c_v} gRT} = \sqrt{\gamma gRT} \quad (\text{for } pv = RT)$$

For a wet vapor, the sonic velocity is

$$c_{\text{vap}} = \frac{v}{v_{fg}} H_{fg} \sqrt{\frac{g}{c_v T}} = v \left(\frac{\partial p}{\partial T} \right)_v \sqrt{\frac{g T}{c_v}} \quad (12)$$

The Clapeyron equation (ref. 12) is a key step in the derivation, as shown in appendix B.

Equations of State

Representation of hydrogen state relations from the melting point at 14° K to the onset of appreciable dissociation for any pressure up to 340 atmospheres is desired. In order to attain reasonable accuracy, three state equations are used, each for a "region" of the range of interest shown schematically in figure 1 in terms of temperature-entropy coordinates. These three regions and the vapor region are assigned code numbers for use in program logic and are referred to herein for convenience.

For all pressures at temperatures above 2000° K (3600° R), hydrogen is considered to be in the ideal state without regard to dissociation, that is, $pv = RT$ or $Z = 1$. In this region, coded 0, the thermodynamic and transport properties are functions of temperature only.

The state equation given by Woolley, et al. (ref. 11) is used for all pressures in the temperature range from 230° to 2000° K (414° to 3600° R). Thus, in region 2, the compressibility factor is of the form

$$Z = e^{B\rho + C\rho^2} \quad (B17)$$

The coefficients B and C are temperature dependent. For lack of a satisfactory substitute, the state equation is used over a larger temperature range than that recommended, namely, 273° to 600° K.

Numerical consistency needed for digital computations is forced at the regional boundaries through the use of smoothing (averaging) results within 10° K of the boundary. Minor changes in the properties themselves are discussed in the section RESULTS.

State relations for temperatures below 230° K are obtained from an empirical equation developed by the present author from the para-hydrogen data of reference 5. Where the coefficients A, B, C, and D are density dependent, the pressure is fitted as

$$p = A + BT + CT^2 + \frac{D}{T^2} \quad (B23)$$

Unfortunately, the algebraic forms of the coefficients are cumbersome, and utility of the state equation may be limited to high-speed digital computer application.

Unsaturated vapor is designated region -1 in figure 1. Vapor pressure and temperature are related by the equation for para-hydrogen from reference 7:

$$\log p = A + \frac{B}{T + C} + DT \quad (B37)$$

Saturation densities at a given temperature are determined from the intersection of the vapor pressure and the liquid or gas isobars. That is, the pressure-temperature relation is found from the vapor-pressure equation (B37), and the liquid-gas state equation (B23) is then solved for the saturation densities as functions of p and T . Subsequently, saturation enthalpies are evaluated at saturation density by using the liquid and gas relations.

Some reduction in accuracy potential results from this technique, since saturation density and enthalpy are directly available in more accurate forms than those that result from gas or liquid computations herein. The compromise is accepted because saturation conditions are uniquely continuous with conditions in the adjoining gas or liquid, so that smoothing is not required. A numerical evaluation of errors with respect to published data is included in the next section.

RESULTS

Three factors related to the utility of the hydrogen property program are discussed in this section: (1) specification of input data and output results, (2) estimates of storage requirements and execution speed, and (3) an analysis of the errors in computed results. The detail of the SUBROUTINE, in terms of the FORTRAN code are shown in appendix C. Also, a subroutine for conversion of units and preparation of constants is shown in appendix D.

External Characteristics of SUBROUTINE STATE

Consider first two factors that may influence the external programs which use the results of SUBROUTINE STATE: First, if trial values are needed, it is assumed that the external program supplies them. Second, the subroutine makes no provision for rejecting spurious input or checking the validity of results. Thus, spurious input may cause the return of incorrect output without warning.

CALLING sequence. - The logic of the hydrogen property subroutine is prepared to allow for solution with any two of the state parameters (p , T , or v) known or with enthalpy and either p or v known. The particular pair of knowns is specified by the code number J in the FORTRAN language calling command (refs. 13 and 14):

```
.  
.   
CALL STATE (J)  
.   
.
```

Roughly, this command means go to SUBROUTINE STATE, supply it with the value J , and on completion return to the next instruction. Of interest here, is the in-

terpretation of the call number J, as itemized in table I and summarized as follows:

CALL number, J	Interpretation (known values)
1	Temperature and specific volume
-1	Enthalpy and specific volume
2	Pressure and specific volume
3	Temperature and pressure
-3	Enthalpy and pressure
4	Pressure and an arbitrary temperature

The final combination is introduced in order to simplify the logic of calling programs in heat-transfer calculations. There is no change in the calculation of properties or restriction on the value of the temperature specified, but results are returned without modifying the storage occupied by so-called "bulk" properties (e.g., $T_{\text{film}} = \frac{T_{\text{wall}} + T}{2}$). The specification of this storage is considered next.

Common data list. - Input data and output results of the subroutine are communicated to and from other programs by specifying a list of "common" locations. The particular list assigned for SUBROUTINE STATE is shown in table I. The symbol D represents the data assumed as an independent variable for the particular call, T indicates that trial values are required, X that results are returned, and, finally, -1 indicates that results are returned from vapor region calculations.* Open blocks signify that the storage is neither modified nor inspected. The fluid region code number N FLUID is always used to initiate calculations and, except for J = 4 calls, is returned to indicate the region in which results are computed. Where smoothing is used internally, the region of lower temperature will be indicated. Trial values of the dependent state variable are not required if J > 0 and N FLUID = 0, but all trial values must be supplied if J < 0. Trial values for saturation specific volumes v_f and v_g are always mandatory whenever vapor calculations may be used either intentionally or inadvertently. (The computations will accept input within the limits $v_g > v_{\text{crit}}$ and $v_{\text{crit}} > v_f > v_{\text{crit}}/4$.)

Storage and speed estimates. - The following estimates of storage requirements and execution speed are based on FORTRAN II (ref. 14) and an IBM 7090 computer (ref. 13). In making the estimates, no provision for loading, writing, printing, and punching results is included.

*Results are returned by "updating," that is, by overwriting into storage. Thus, any previous values will be altered if results are returned. Conversely, if results are not returned (no X or -1), the previous values in storage will remain.

The core storage requirements of SUBROUTINE STATE are summarized in decimal numbers as follows:

Requirement	Number of words
FORTRAN program	1772
Data list shown in table I	31
Temporary (erasable) storage	50
Constant list	215
Convergence specification	1
Unit type code	1
Total	2070

The total of about 2100 words does not include the required logarithmic, exponential, or square-root subroutines, which may require a total of about 300 words. Also not included in the storage requirement is the subroutine shown in appendix D for preparing the "constant" list.

Estimates of execution speed have been obtained by setting up a calling routine that sequences the subroutine through many entries and clocks the execution time required. The estimates shown in table II are grouped according to fluid region numbers, as shown in figure 1, and within each group, the independent variables used are indicated by the call letter J. Trial values are determined internally by using N FLUID = 0 before the call or are supplied externally from a nonsystematic table as noted. Iterative solutions are converged to six significant figures.

Execution times vary from 0.3 to 13 minutes for 10,000 cases, or from 0.002 to 0.1 second per entry. As expected, the perfect gas computations are much faster than those in other regions and are independent of the dependent state variable. The longer times reflect more complicated formulations and iterative solutions; for example, with temperatures in the range of region 1 and a call of J = 3, additional calculations are required to determine the phase (liquid or gas) of the fluid. Similarly, for vapor (region -1) calculations, the state equations must be solved iteratively for both saturation boundaries; consequently, the time is about 0.08 second per entry.

Where enthalpy is used as an independent variable, the execution speed is further reduced because of the additional iterative loop that is activated, but the execution times have not been evaluated.

Errors in Computed Results

In the following paragraphs, the deviations in computed parameters from published properties are discussed. Also, the properties unsupported by published

data are enumerated. The discussion proceeds as shown in figure 2 and covers the range from dissociation to melting temperatures.

Two areas are not treated graphically as are the others, namely:

(1) At high temperatures, a perfect gas in the ideal state is assumed. A figure is used only to define the temperatures above which dissociation is appreciable.

(2) From 300° to 600° K, results are obtained from the formulations of Woolley, et al. (ref. 11) which were used to prepare the reference tabulations. Deviations are less than 0.1 percent and therefore are not shown.

Dissociation limits. - SUBROUTINE STATE will return results, based on a perfect gas without dissociation, for temperatures up to 5000° K (9000° R). Consequently, the program should be limited by other means to within the range of valid properties. The area in question, which is indicated in figure 3, has been prepared from the calculations of reference 15 and shows the temperature at which given deviations occur in specific heat at constant pressure as a function of pressure. A 2-percent deviation is assumed as a criterion, perfect-gas results are valid to 1800° K (3240° R) at atmospheric pressure, or to 2200° K (3960° R) at a pressure level of 100 atmospheres.

The state equation of Woolley, et al. (ref. 11) is used for temperatures up to 2000° K, but properties above 600° K are unsubstantiated, since the equation is recommended for use only to 600° K. The resulting properties are compared with ideal state results for lines of constant pressure as a function of temperature (fig. 4). Compressibility factor Z , enthalpy H , specific heat at constant pressure c_p , and viscosity μ are shown in figures 4(a), (b), (c), and (d), respectively. At 2000° K, deviations of up to 3 percent in compressibility factor are artificially smoothed, rather than up to 11 percent, as would be needed at 600° K. For a pressure level of 340 atmospheres, the differences at 2000° and 600° K are 1 and 3 percent in enthalpy, 0 and 1 percent in specific heat at constant pressure, and 0.5 and 3 percent in viscosity. For pressures less than the maximum considered herein, the effects and potential deviations are reduced, and, naturally, at low pressures the percentage differences between the real fluid and the ideal fluid are small. To reiterate, the state equation is extrapolated without substantiation as a means to avoid the alternative of completely artificial smoothing.

Transition of real fluid to cryogenic fluid. - The state equation of Woolley, et al. (ref. 11) is also used to lower recommended temperatures, namely, to 230° K (414° R). The state relation developed by the present author is used for both gaseous and liquid phases in the temperature range of region 1, 14° to 230° K.

The deviations of various properties from the tabulations of reference 11 are shown in figure 5 for the temperature range from 100° to 300° K. The computed properties are from regions 1 and 2 and include the effects of smoothing where applicable (fig. 1). Deviations in percent are shown for lines of constant density, so that the tabulations of the reference can be used without interpola-

tion. The figures are shown for para-hydrogen only, but normal (25 percent para, 75 percent ortho) hydrogen deviations are similar in trend and magnitude.

Pressure calculations agree with the reference data within $3/4$ percent for densities up to 100 amagats* (about one-third of critical) and within $1\frac{1}{2}$ percent to high density (the curves are terminated at 340 atm). Enthalpy deviations are less than 1 percent for all densities up to 500 amagats, and specific heat at constant pressure agrees with the data of reference 11 to within $2\frac{1}{2}$ percent. Specific heat at constant volume is also accurate to about $2\frac{1}{2}$ percent for the same range.

The remainder of the properties, namely, sonic velocity, viscosity, thermal conductivity, and the partial derivative $(\partial p/\partial T)_v$ are unsubstantiated in the temperature range of 100° to 300° K.

Cryogenic temperature range. - Deviations in the pressure calculations of SUBROUTINE STATE from the data of reference 7 are shown in figure 6(a) as a function of temperature. The comparison, of which only the envelope of maximum error is shown, is based on integral values of density from 1 to 44 moles per cubic centimeter. The maximum positive deviation of 1.7 percent occurs at 22° to 24° K and pressures of more than 300 atmospheres (4500 lb/sq in.), whereas the maximum negative deviation of 0.8 percent occurs at 24° K near the saturated-liquid boundary. A deviation of $1\frac{1}{2}$ percent occurs near the saturated-liquid line at 17° K (30.6° R) but represents an error of 0.06 atmosphere or 1 pound per square inch.

Liquid-phase calculations are not constrained by the melting pressure boundary (ref. 7), so that properties will be incorrect for pressures higher than or temperatures lower than the melting boundary.

Deviations in computed enthalpy from the data of reference 3 are shown in figure 6(b). Since the enthalpy passes through zero within the range of interest, the difference is shown in calories per gram or Btu per pound. Generally, the data fall within the shaded region that has a maximum deviation of about $2\frac{1}{4}$ calories per gram, whereas the full-scale range of the figure is more than 330 calories per gram. Somewhat larger deviations for the 15-atmosphere isobar near the critical temperature are not shown. These deviations are about -0.9, -2.7, 9, and 3.1 calories per gram at 36° , 35° , 34° , and 33° K, respectively. Otherwise, the deviations for the 15-atmosphere isobar fall within the shaded area.

The deviations of specific heat at constant pressure (fig. 6(c)) show comparison with data from references 7 and 12. For the most part, deviations fall within 4 percent. Deviations up to about 6 percent occur in the 15- and 20-atmosphere isobars near critical temperature. The value of specific heat at constant pressure in this range varies up to 35 Btu per pound per degree Rankine (or

*1 amagat \approx 0.0056 lb/cu ft.

cal/(g)(°K)). Results on the gas side of the vapor dome, not included in the reference data, should not be in error by nearly as large an amount as those on the liquid side.

Deviations in specific heat at constant volume in the cryogenic range are shown in figure 6(d). The comparison is made along lines of nearly constant density to match the raw data of reference 7. At low temperatures, the liquid specific heat at constant volume is as much as 5 percent high. The large negative deviations reflect the failure of the calculated values to increase rapidly near the critical point as the experimental values do.

Deviations in specific heat at constant volume with respect to computed results from reference 8 are shown in figure 6(e) with envelopes of maximum error for gaseous and liquid para-hydrogen. The value computed by SUBROUTINE STATE is higher than the reference data of the National Bureau of Standards by as much as 5 percent in the liquid phase. In the gas phase, results are within 3 percent except near the critical point.

Results of all parameters near the critical point have been inspected in detail to verify that no zero or infinite values occur. Specific heat at constant pressure should be infinite at the critical point (ref. 16), but herein it increases to a large finite value. The author considers this a desirable compromise where results may be converged to several significant figures and only rarely to a mathematical identity.

Other parameters in the cryogenic temperature range have not been directly checked against experimental data; however, the viscosity and thermal conductivity calculations are as recommended by Rogers, et al. (ref. 10).

Several computed properties in the vapor region reflect directly the correlation and fitting done by the National Bureau of Standards (e.g., vapor pressure and saturation specific heats). Saturation density and enthalpy reflect the accuracy of the liquid or gas calculations shown in figure 6. For example, enthalpy deviations of 1 and 2 calories per gram are shown in figure 6(b); therefore, the heat of vaporization should be evaluated within ± 1 calorie per gram, or about 1 percent.

CONCLUDING REMARKS

A computational technique is described that permits calculation of the properties of various combinations of para- and ortho-hydrogen for use primarily in heat-transfer and fluid-flow problems. Logic is prepared to permit the use of British or metric units and several combinations of enthalpy, pressure, temperature, or specific volume as the two independent variables. Properties are returned from a single entry to the computation routine, which operates at speed characterized by "several" entries per second. The various thermodynamic, state, and transport properties are computed from approximate analytical expressions and data tabulations to cover the range from melting temperatures to limits imposed by appreciable dissociation for pressures up to 340 atmospheres.

Accuracy can be characterized by $1\frac{1}{2}$ percent in state relations, about 2 calories per gram or 1 percent in enthalpy, and 5 percent in specific heats. Near the critical point, however, deviations of up to 6 percent in specific heat at constant pressure and 20 percent in specific heat at constant volume are expected.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, February 12, 1963

APPENDIX A

SYMBOLS

		British	British	Metric
c	sonic velocity	ft/sec	ft/sec	m/sec
c _p	specific heat at constant pressure	ft/°R	Btu/(lb)(°R)	cal/(g)(°K)
c _v	specific heat at constant volume	ft/°R	Btu/(lb)(°R)	cal/(g)(°K)
g	standard acceleration due to gravity	ft/sec ²	ft/sec ²	m/sec ²
H	enthalpy	ft	Btu/lb	cal/g
k	thermal conductivity	lb/(sec)(°R)	Btu/(ft)(sec)(°R)	cal/(cm)(sec)(°K)
P	pressure	lb/sq ft	lb/sq in.	atm
R	gas constant	ft/°R	cu ft/(sq in.)(°R)	(cc)(atm)/(g)(°R)
T	temperature	°R	°R	°K
v	specific volume	cu ft/lb	cu ft/lb	cc/g
x	vapor quality	-----	-----	-----
Z	compressibility factor, pv/RT	-----	-----	-----
ρ	density	lb/cu ft	lb/cu ft	g/cc
μ	viscosity	lb/(ft)(sec)	lb/(ft)(sec)	poises

Subscripts:

- crit critical
- f saturated liquid
- fg saturated vapor minus saturated liquid
- g saturated vapor

p constant pressure
ref reference
s constant entropy
sat saturation conditions
T temperature
v constant volume
vap wet vapor
 ρ density
O ideal state

APPENDIX B

DETAILS OF NUMERICAL METHOD

The analytical and empirical equations shown in this section are generally given in the form and dimensional system of the reference source. The conversion of units to a consistent set is shown in appendix D.

Viscosity and Thermal Conductivity

Viscosity for hydrogen in the ideal state is assumed independent of para-ortho composition and is computed for all temperatures from empirical equations given by Woolley, Scott, and Brickwedde (ref. 11).

$$\mu_0 = \frac{AT^{3/2}(T + B)}{(T + C)(T + D)} \quad (B1)$$

where

μ_0 absolute viscosity in the ideal state, poises

T temperature, °K

and

A = 85.558×10^{-6} poises/°K^{1/2}

B = 650.39° K

C = 1175.9° K

D = 19.55° K

Thermal conductivity in the ideal state for temperatures below 700° K (1260° R) is computed from empirical equations given by reference 11, where the effect of para-ortho composition is introduced through the use of $c_{p,0}$.

$$k_0 = \frac{\mu_0[A + BT + c_{p,0}(C + DT)]}{m(1 + E/T)} \quad (B2)$$

where

k_0 thermal conductivity in the ideal state, cal/(cm)(sec)(°K)

T temperature, °K

μ_0 absolute viscosity in the ideal state, poises (eq. (B1))

$c_{p,0}$ specific heat at constant pressure in the ideal state, cal/(mole)(°K)

m molecular weight, g/mole

and

$$A = 1.8341 \text{ cal}/(\text{mole})(^\circ\text{K})$$

$$B = -0.004458 \text{ cal}/(\text{mole})(^\circ\text{K}^2)$$

$$C = 1.1308$$

$$D = 8.973 \times 10^{-4}, \text{ } 1/^\circ\text{K}$$

$$E = 3.2^\circ \text{ K}$$

Ideal state thermal conductivity for temperatures above 1500° K is computed from correlations given by Rogers (ref. 10). The coefficients are those for a pressure level of 100 atmospheres.

$$k = \left[\frac{A_1}{A_2(2\pi)^{1/2}} e^{-\frac{1}{2} \left(\frac{T - A_3}{A_2} \right)^2} + A_4 + A_5 T \right] 10^{-7}$$

where

k thermal conductivity, cal/(cm)(sec)(°K)

T temperature, °K

and

$$A_1 = 3.6789 \times 10^8 \text{ } (^\circ\text{K})(\text{cal})/(\text{cm})(\text{sec})(^\circ\text{K})$$

$$A_2 = 1013.91^\circ \text{ K}$$

$$A_3 = 5268^\circ \text{ K}$$

$$A_4 = 4117 \text{ cal}/(\text{cm})(\text{sec})(^\circ\text{K})$$

$$A_5 = 6.982 \text{ cal}/(\text{cm})(\text{sec})(^\circ\text{K}^2)$$

Thermal conductivity for the temperature range from 700° to 1500° K is obtained by linear interpolation. The values for temperatures above about 500° K have been checked against those of reference 17 and agree within "a few percent."

The real-fluid viscosity and thermal conductivity for region 2 are obtained from the ideal-state values by Enskog-type corrections. According to reference 11,

$$\mu = \mu_0 [1 + A(B\rho X) + B(B\rho X)^2 + C(B\rho X)^3] \quad (B3)$$

where

μ absolute viscosity, poises

μ_0 absolute viscosity in the ideal state, poises

and

$$A = 0.175$$

$$B = 0.7557$$

$$C = -0.405$$

$$k = k_0 [1 + A(B\rho X) + B(B\rho X)^2 + C(B\rho X)^3], \text{ cal}/(\text{cm})(\text{sec})(^\circ\text{K}) \quad (B4)$$

where

k thermal conductivity, cal/(cm)(sec)(°K)

k_0 thermal conductivity in the ideal state, cal/(cm)(sec)(°K)

and

$$A = 0.575$$

$$B = 0.5017$$

$$C = -0.204$$

The term $(B\rho X)$ in equations (B3) and (B4) is given as

$$(B\rho X) = T \left(\frac{\partial Z}{\partial T} \right)_v (Z - 1) \quad (B5)$$

and an equivalent form is used in computation, namely,

$$(B\rho X) = \frac{v}{R} \left(\frac{\partial p}{\partial T} \right)_v - 1 \quad (B6)$$

For cryogenic temperatures, the real-fluid corrections are computed from equations given by Rogers, et al. (ref. 10):

$$\mu = \mu_0 + A_1 + A_2 e^{A_3 \rho} + A_4 \rho + A_5 \rho^2 + A_6 \rho^4 \quad (B7)$$

where

μ absolute viscosity, centipoises

μ_0 absolute viscosity in the ideal state (eq. (B1))

ρ density, g/cc

and

$$A_1 = -2.515 \times 10^{-6} \text{ centipoise}$$

$$A_2 = 3.5546 \times 10^{-18} \text{ centipoise}$$

$$A_3 = 400 \text{ cc/g}$$

$$A_4 = 4.6237 \times 10^{-4} \text{ (centipoise)(cc/g)}$$

$$A_5 = -2.6833 \times 10^{-3} \text{ (centipoise)(cc/g)}^2$$

$$A_6 = 4.0719 \text{ (centipoises)(cc/g)}^4$$

$$k = k_0 + (A_1 + A_2\rho + A_3\rho^2 + A_4\rho^3 + A_5\rho^4 + A_6\rho^5 + A_7\rho^6 + A_8\rho^7 + A_9\rho^8) \times 10^{-6} \quad (\text{B8})$$

where

k thermal conductivity, cal/(cm)(sec)(°K)

k_0 thermal conductivity in the ideal state, from eq. (A2)

and

$$A_1 = 1.84 \text{ cal/(cm)(sec)(}^\circ\text{K)}$$

$$A_2 = 1102.6 \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)]}$$

$$A_3 = 1.22648 \times 10^6 \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^2\text{]}$$

$$A_4 = -1.15024 \times 10^8 \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^3\text{]}$$

$$A_5 = 4.95228 \times 10^9 \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^4\text{]}$$

$$A_6 = -1.16927 \times 10^{11} \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^5\text{]}$$

$$A_7 = 1.56768 \times 10^{12} \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^6\text{]}$$

$$A_8 = -1.12433 \times 10^{13} \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^7\text{]}$$

$$A_9 = 3.36150 \times 10^{13} \text{ [cal/(cm)(sec)(}^\circ\text{K)][(cc/g)}^8\text{]}$$

Sonic Velocity

The speed of sound in the general fluid, $pv = ZRT$, can be derived from the definition of the propagation rate of infinitesimal disturbance from reference 12:

$$\begin{aligned} c^2 &= g \left(\frac{\partial p}{\partial \rho} \right)_s \\ &= -gv^2 \left(\frac{\partial p}{\partial v} \right)_s \end{aligned} \quad (B9)$$

where g is the standard acceleration due to gravity in consistent units. The partial derivative can be written as

$$\left(\frac{\partial p}{\partial v} \right)_s = \left(\frac{\partial p}{\partial T} \times \frac{\partial T}{\partial v} \right)_s = \left(\frac{\partial p}{\partial T} \right)_s \left(\frac{\partial T}{\partial v} \right)_s \quad (B10)$$

The ratio of specific heats can be expressed (from ref. 12) as

$$\gamma \equiv \frac{c_p}{c_v} = \frac{\left(\frac{\partial T}{\partial v} \right)_s \left(\frac{\partial p}{\partial T} \right)_s}{\left(\frac{\partial p}{\partial v} \right)_T} \quad (B11)$$

Substituting the relations (B10) and (B11) into the definition (B9) and extracting the square root yields

$$c = v \sqrt{-g \frac{c_p}{c_v} \left(\frac{\partial p}{\partial v} \right)_T} \quad (B12)$$

This relation is general for a fluid of the form $pv = ZRT$ and reduces to the familiar form for the ideal state:

$$c = \sqrt{\gamma g R T}$$

The sonic velocity for a fluid in the vapor state where $p = \phi(T)$ may be derived as follows. Making the substitution of (B10) into (B9) yields

$$c^2 = -gv^2 \left(\frac{\partial T}{\partial v} \right)_s \left(\frac{\partial p}{\partial T} \right)_s$$

Assuming here that entropy is a function of temperature and specific volume gives

$$ds = \left(\frac{\partial s}{\partial v}\right)_T dv + \left(\frac{\partial s}{\partial T}\right)_v dT$$

$$\frac{ds}{dv} = \left(\frac{\partial s}{\partial v}\right)_T + \left(\frac{\partial s}{\partial T}\right)_v \frac{dT}{dv}$$

For an isentropic process,

$$0 = \left(\frac{\partial s}{\partial v}\right)_T + \left(\frac{\partial s}{\partial T}\right)_v \frac{\partial T}{\partial v}_s$$

Substituting gives

$$c^2 = \frac{g v^2 \left(\frac{\partial s}{\partial v}\right)_p \left(\frac{\partial s}{\partial v}\right)_T}{\left(\frac{\partial s}{\partial T}\right)_v}$$

From the Clapeyron equation for the vapor,

$$\left(\frac{\partial s}{\partial v}\right)_p = \left(\frac{\partial s}{\partial v}\right)_T = \left(\frac{\partial p}{\partial T}\right)_v = \frac{H_{fg}}{T v_{fg}}$$

and

$$\left(\frac{\partial s}{\partial T}\right)_v = \frac{c_v}{T}$$

The sonic velocity in the vapor can then be expressed as either

$$c = v \frac{H_{fg}}{v_{fg}} \sqrt{\frac{g}{c_v T}}$$

or

$$c = v \left(\frac{\partial p}{\partial T}\right)_v \sqrt{\frac{g T}{c_v}} \quad (B13)$$

The partial derivative is the total derivative of the vapor pressure relation (eq. (15)) or $(dp/dT)_{\text{vap}}$. This result has been derived by Hirschfelder, Curtiss, and Bird (ref. 16) for sonic velocity at the critical point.

Equation of State, Region 0

The hydrogen properties in region 0 (fig. 1) are computed with the assump-

tion of a (calorically) perfect gas with an equation of state as

$$pv = RT \quad (B14)$$

Equation (B14) is solved for any dependent variable in closed form and therefore no trial values or partial derivatives are used. It is convenient to use the general form of the equations for specific heat at constant pressure and sonic velocity, however, and the derivatives are used as

$$\left(\frac{\partial p}{\partial v}\right)_T = -\frac{RT}{v^2} = -\frac{p}{v} = -\rho p \quad (B15)$$

$$\left(\frac{\partial p}{\partial T}\right)_v = \frac{R}{v} = \rho R \quad (B16)$$

Since $Z = 1$, all derivatives of Z are zero, and specific heats, enthalpy, sonic velocity, viscosity, and thermal conductivity are functions of temperature only.

Equation of State, Region 2

For the intermediate temperature range (fig. 1) the equation of state given by Woolley, Scott, and Brickwedde (ref. 11) is used. The correlating equation and a five-term series expansion are shown in the reference, but the $D_1 \dots D_4$ notation is introduced here for convenience:

$$\begin{aligned} \frac{pv}{RT} = Z &= e^{\rho B + \rho^2 C} \\ &\approx 1 + D_1 \rho + D_2 \rho^2 + D_3 \rho^3 + D_4 \rho^4 \end{aligned} \quad (B17)$$

where

$$D_1 = B$$

$$D_2 = \frac{B^2}{2} + C$$

$$D_3 = \frac{B^3}{6} + BC$$

$$D_4 = \frac{B^4}{24} + \frac{B^2 C}{2} + \frac{C^2}{2}$$

and

$$B = B_1 T^{-1/4} + B_2 T^{-3/4} + B_3 T^{-5/4}$$

where

$$B_1 = 0.0055478 \text{ (degrees Kelvin)}^{1/4}/\text{amagat}$$

$$B_2 = -0.036877 \text{ (degrees Kelvin)}^{3/4}/\text{amagat}$$

$$B_3 = -0.22004 \text{ (degrees Kelvin)}^{5/4}/\text{amagat}$$

$$C = C_1 T^{-3/2} + C_2 T^{-2}$$

$$C_1 = 0.004788 \text{ (degrees Kelvin)}^{3/2}/\text{amagat}^2$$

$$C_2 = -0.04053 \text{ (degrees Kelvin)}^2/\text{amagat}^2$$

The derivatives are readily obtained from either the exponential form or its series expansion. Because of the simpler algebra, the program computes partial derivatives from the exponential form, and because the derivatives of the exponential form cannot be integrated, the series form is used in deriving $\Delta H/RT$ and $\Delta c_v/R$:

$$\begin{aligned} \left(\frac{\partial Z}{\partial v}\right)_T &= e^{\rho B + \rho^2 C} (B + 2\rho C) \frac{\partial \rho}{\partial v} \\ &= -Z\rho^2 (B + 2\rho C) \end{aligned} \tag{B18}$$

$$\begin{aligned} \left(\frac{\partial Z}{\partial T}\right)_v &= e^{\rho B + \rho^2 C} (\rho B' + \rho^2 C') \\ &= Z(\rho B' + \rho^2 C') \end{aligned} \tag{B19}$$

or

$$\left(\frac{\partial Z}{\partial T}\right)_v \cong D_1' \rho + D_2' \rho^2 + D_3' \rho^3 + D_4' \rho^4$$

where

$$D_1' = B'$$

$$D_2' = D_1 B' + C'$$

$$D_3' = D_2 B' + D_1 C'$$

$$D_4' = D_3 B' + D_2 C'$$

$$B' = -\frac{1}{T} \left(\frac{B_1}{4} T^{-1/4} + \frac{3B_2}{4} T^{-3/4} + \frac{5B_3}{4} T^{-5/4} \right)$$

$$C' = -\frac{1}{T} \left(\frac{3C_1}{2} T^{-3/2} + 2C_2 T^{-2} \right)$$

The difference between the real and ideal-state enthalpy is obtained from

$$\frac{H_{T,\rho} - H_{T,0}}{RT} = \int_0^\rho \frac{T}{\rho} \left(\frac{\partial Z}{\partial T} \right)_\rho d\rho - (Z - 1) \quad (\text{B20a})$$

$$= T \left(\rho D_1' + \frac{D_2'}{2} \rho^2 + \frac{D_3'}{3} \rho^3 + \frac{D_4'}{4} \rho^4 \right) - (Z - 1) \quad (\text{B20b})$$

Then the second partial derivative of Z with respect to temperature at constant specific volume is

$$\left(\frac{\partial^2 Z}{\partial T^2} \right)_v \approx D_1'' \rho + D_2'' \rho^2 + D_3'' \rho^3 + D_4'' \rho^4 \quad (\text{B21})$$

where

$$D_1'' = B''$$

$$D_2'' = D_1 B'' + D_1' B' + C$$

$$D_3'' = D_2 B'' + D_2' B' + D_1 C'' + C' D_1'$$

$$D_4'' = D_3 B'' + D_3' B' + D_2 C'' + C' D_2'$$

$$B'' = \frac{1}{T^2} \left(\frac{5}{16} B_1 T^{-1/4} + \frac{21}{16} B_2 T^{-3/4} + \frac{45}{16} B_3 T^{-5/4} \right)$$

$$C'' = \frac{1}{T^2} \left(\frac{15}{4} C_1 T^{-3/2} + 6 C_2 T^{-2} \right)$$

The second integral term of equation (9) for determining $\Delta c_v/R$ is

$$\begin{aligned} \int_0^\rho \frac{T^2}{\rho} \left(\frac{\partial^2 Z}{\partial T^2} \right)_v d\rho &= \int_0^\rho T^2 (D_1'' + D_2'' \rho + D_3'' \rho^2 + D_4'' \rho^3) d\rho \\ &= T^2 \left(D_1'' \rho + \frac{D_2''}{2} \rho^2 + \frac{D_3''}{3} \rho^3 + \frac{D_4''}{4} \rho^4 \right) \end{aligned} \quad (\text{B22})$$

The remainder of the properties are computed as shown previously.

Equation of State, Region 1

Computations in region 1 are based on an empirical equation of state prepared from the para-hydrogen data of reference 5 or 7. The equation is formed by fitting isochores with the form

$$p = A + BT + CT^2 + \frac{D}{T^2} \quad (\text{B23})$$

The coefficients A, B, C, and D are shown in figures 7(a) to (d), respectively, as a function of density. The data points show the computed coefficients and the curves show the functions used to fit the data. The functions of density are fitted within two limitations for use in computing thermodynamic properties, namely, (1) that it should be possible to integrate in closed form and to differentiate them all, and (2) that a minimum number of terms should be used to increase the confidence in the slopes. The equations used are

$$A = A_1 \rho^{1.970} + A_2 \rho^{7.256} + \sum_{n=1}^4 \frac{a_n \rho^2}{[b_n + (\rho_n - \rho)^2]^{3/2}} \quad (\text{B24})$$

where

$$A_1 = -0.24337 \text{ atm}/(\text{mole}/\text{cc})^{1.970}$$

$$A_2 = 5.591 \times 10^{-10} \text{ atm}/(\text{mole}/\text{cc})^{7.256}$$

$$a_n = -10.67251, -0.06286125, -0.226, 0.0754 \text{ (atm)(cc)/mole}$$

$$b_n = 89.507, 5.654, 25.00, 20.00 \text{ (cc/mole)}^2$$

$$\rho_n = 16.822, 35.65, 20.00, 18.00 \text{ cc/mole}$$

$$B = \rho R \left\{ 1 + \rho \left[B_1 + \rho^{1.5} (B_2 + B_x) \right] \right\} \quad (\text{B25})$$

where

$$B_x = B_3 \rho (34.5 - \rho)^3 \quad (\rho \leq 34.5 \text{ mole/cc})$$

$$B_x = B_4 (\rho - 34.5)^{1.4} \quad (\rho > 34.5)$$

$$B_1 = 0.027 \ 919 \ 58 \text{ cc/mole}$$

$$B_2 = 0.000 \ 166 \ 83 \text{ (cc/mole)}^{2.5}$$

$$B_3 = 1 \times 10^{-6} / (30 \times 4.5^3) \text{ (cc/mole)}^{6.5}$$

$$B_4 = 64.5 \times 10^{-6} / 7.5^{1.40} \text{ (cc/mole)}^{3.90}$$

$$C = C_1 \rho^4 \left[1 - C_4 \rho^{1/2} (\rho - C_2) | \rho - 34.5 | \right] \quad (\text{B26})$$

where

$$C_1 = -1 \times 10^{-6} / 124 \text{ atm}/(\text{°K})^2 \text{ (cc/mole)}^4$$

$$C_2 = 25.5 \text{ cc/mole}$$

$$C_3 = 34.5 \text{ cc/mole}$$

$$C_4 = 1 / (17.6 \times \sqrt{43.1} \times 8.6) \text{ (cc/mole)}^{2.5}$$

$$D = \rho^2 \sum_{n=1}^5 \frac{a_n}{[b_n + (\rho_n - \rho)^2]^{3/2}} \quad (\text{B27})$$

where

$$a_n = -8917.152, 10296.158, -371.072, 8.623, 91.596 \quad (\text{atm})(\text{cc})/(\text{mole})(\text{°K}^2)$$

$$b_n = 63.604, 76.803, 39.310, 3.684, 16.827 \quad (\text{cc/mole})^2$$

$$\rho_n = 5.40, 18.00, 31.30, 35.70, 39.87 \quad \text{cc/mole}$$

The partial derivative of pressure with respect to temperature is

$$\left(\frac{\partial p}{\partial T} \right)_V = B + 2TC - \frac{2D}{T^3} \quad (\text{B28})$$

and the derivative with respect to specific volume becomes

$$\left(\frac{\partial p}{\partial v} \right)_T = \frac{\partial A}{\partial v} + \frac{\partial B}{\partial v} T + \frac{\partial C}{\partial v} T^2 + \frac{\partial D}{\partial v} \frac{1}{T^2} \quad (\text{B29})$$

$$\frac{\partial A}{\partial v} = -\rho \times \left\{ 1.970 A_1 \rho^{1.970} + 7.256 A_2 \rho^{7.256} + 2\rho^2 \sum_{n=1}^4 \frac{a_n}{[b_n + (\rho_n - \rho)^2]^{3/2}} - 3\rho^3 \sum_{n=1}^4 \frac{a_n(\rho_n - \rho)}{[b_n + (\rho_n - \rho)^2]^{5/2}} \right\} \quad (\text{B30})$$

$$\frac{\partial B}{\partial V} = -\rho^2 R \left(1 + \rho \left\{ 1 + \rho \left[2B_1 + \rho^{1.5} (3.5 B_2 + B_y) \right] \right\} \right) \quad (\text{B31})$$

where

$$B_y = B_3 \left[34.5 (34.5 - \rho)^3 - 3\rho (34.5 - \rho)^2 \right] \quad (\rho \leq 34.5 \text{ cc/mole})$$

$$B_y = B_4 \left[3.5 (3\rho - 34.5)^{1.4} + 1.4 (\rho - 34.5)^{0.4} \right] \quad (\rho > 34.5)$$

$$\begin{aligned} \frac{\partial C}{\partial V} &= -\rho \left[4C - \rho^4 C_1 (C_4 \rho^{1/2}) (\rho - C_2) |\rho - 34.5| + \rho \frac{|\rho - 34.5|}{(\rho - 34.5)} + \rho^{1/2} \right] \\ &= -\rho \left\{ 4C - \rho^{4.5} C_1 C_4 \left[|\rho - 34.5| \left(\frac{\rho - C_2}{2} + \rho \right) + \rho (\rho - C_2) \frac{|\rho - 34.5|}{(\rho - 34.5)} \right] \right\} \end{aligned} \quad (\text{B32})$$

$$\frac{\partial D}{\partial V} = -\rho \left\{ 2D - 3\rho^2 \sum_{n=1}^5 \frac{a_n (\rho_n - \rho)}{[b_n + (\rho_n - \rho)^2]^{5/2}} \right\} \quad (\text{B33})$$

Enthalpy and specific heat at constant volume are found from the ideal state values and the following real-gas corrections:

$$Z = \frac{pV}{RT} = \frac{p}{\rho RT} = \frac{A}{\rho RT} + \frac{B}{\rho R} + \frac{CT}{\rho R} + \frac{D}{\rho RT^3}$$

$$\left(\frac{\partial Z}{\partial T} \right)_V = -\frac{A}{\rho RT^2} + \frac{C}{\rho R} - \frac{3D}{\rho RT^4}$$

$$\left(\frac{\partial^2 Z}{\partial T^2} \right)_V = \frac{2A}{\rho RT^3} + \frac{12D}{\rho RT^5}$$

Substituting these corrections into equation (7), which was

$$\frac{H_{T,\rho} - H_{T,0}}{RT} = \int_0^\rho \frac{T}{\rho} \left(\frac{\partial Z}{\partial T} \right)_\rho d\rho - (Z - 1)$$

yields

$$\frac{H_{T,\rho} - H_{T,0}}{RT} = 1 - Z + \int_0^\rho \frac{1}{RT} \left(\frac{-A}{\rho^2} \right) d\rho + \int_0^\rho \frac{T}{R} \left(\frac{C}{\rho^2} \right) d\rho + \int_0^\rho \frac{3}{\rho R^3} T^3 \left(\frac{D}{\rho^2} \right) d\rho$$

$$H_{T,\rho} - H_{T,0} = RT - pv + \int_0^\rho \left(\frac{-A}{\rho^2} \right) d\rho + T^2 \int_0^\rho \left(\frac{C}{\rho^2} \right) d\rho + \frac{3}{T^2} \int_0^\rho \left(\frac{-D}{\rho^2} \right) d\rho$$

Then, substituting into equation (9) results in

$$\frac{c_{v,\rho} - c_{v,0}}{R} = \frac{-2}{RT} \left(T^2 \int_0^\rho \frac{C}{\rho^2} d\rho + \frac{3}{T^2} \int_0^\rho \frac{D}{\rho^2} d\rho \right)$$

The integrated terms, two of which are common, are obtained in closed form from equations (B24), (B26), and (B27) as

$$\int_0^\rho \left(\frac{-A}{\rho^2} \right) d\rho = \left[v \left(\frac{A_1 \rho^{1.970}}{0.970} + \frac{A_2 \rho^{7.256}}{6.256} \right) + \sum_{n=1}^4 \frac{a_n}{b_n} \frac{\rho - \rho_n}{[b_n - (\rho - \rho_n)^2]^{1/2}} + \sum_{n=1}^4 \frac{a_n}{b_n} \frac{\rho_n}{(b_n + \rho_n^2)^{1/2}} \right] \quad (\text{B34})$$

$$\int_0^\rho \frac{C}{\rho^2} d\rho = \rho^4 c_1 \left[\frac{v}{3} + c_4 \left(\frac{c_2 c_3}{4} - \frac{c_2 + c_3}{5} \rho + \frac{\rho^2}{6} \right) \right] \quad (\rho \leq 34.5)$$

$$= \rho^4 c_1 \left[\frac{v}{3} - c_4 \left(\frac{c_2 c_3}{4} - \frac{c_2 + c_3}{5} \rho + \frac{\rho^2}{6} \right) \right] - c_1 c_4 c_3^5 \left(\frac{c_2}{10} - \frac{c_3}{15} \right) \quad (\rho > 34.5)$$

(B35)

$$\int_0^\rho \frac{D}{\rho^2} d\rho = \sum_{n=1}^5 \frac{a_n}{b_n} \left\{ \frac{\rho_n - \rho}{[b_n + (\rho_n - \rho)^2]^{1/2}} + \frac{\rho_n}{(b_n + \rho_n^2)^{1/2}} \right\} \quad (\text{B36})$$

Terms in the preceding integrals and differentials are grouped to illustrate the similarity of the calculations in that the additional computations required to yield enthalpy and specific heats are less than might be expected.

Wet Vapor Properties, Region -1

The vapor-pressure relation given in reference 7 is

$$\log p = \left(A + \frac{B}{T + C} + DT \right) \quad (B37)$$

where

p pressure, atm

T temperature, °K

and

$$A = 2.000\ 620$$

$$B = -5.009\ 708 \times 10^1 \text{ } ^\circ\text{K}$$

$$C = 1.004\ 4 \text{ } ^\circ\text{K}$$

$$D = 1.748\ 495 \times 10^{-2} \text{ } 1/^\circ\text{K}$$

Solution of the vapor-pressure equation for unknown temperature is accomplished by an iterative procedure using the slope

$$\frac{dp}{dT} = p \left[\frac{-B}{(T + C)^2} + D \right] \quad (B38)$$

A trial value of temperature must be supplied.

When the vapor pressure and temperature are known, the fluid properties at the saturation conditions are found by computation in region 1 on the liquid and then on the gas side of the vapor dome. These calculations are performed with p and T as independent variables and v as the dependent variable. Again, trial values of v_f and v_g are mandatory.

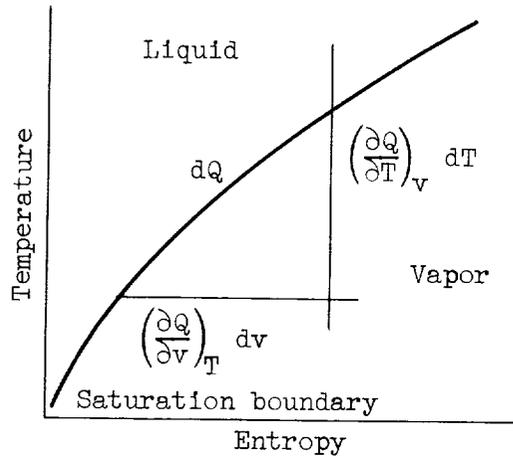
Vapor quality x is then found from

$$x = \frac{v - v_f}{v_g - v_f} = \frac{v - v_f}{v_{fg}} \quad (B39)$$

and the following properties are assumed to vary linearly with quality as

$$\left. \begin{aligned} H &= H_f + xH_{fg} \\ \mu &= \mu_f + x\mu_{fg} \\ k &= k_f + xk_{fg} \end{aligned} \right\} \quad (\text{B40})$$

Specific heat at constant volume c_v for the wet vapor is derived from conditions at the saturated liquid boundary (see sketch).



The energy change dQ is then

$$dQ = \left(\frac{\partial Q}{\partial T}\right)_v dT + \left(\frac{\partial Q}{\partial v}\right)_T dv$$

Dividing by dT and evaluating at saturation conditions yields

$$\left(\frac{dQ}{dT}\right)_{\text{sat}} = \left(\frac{\partial Q}{\partial T}\right)_v + \left(\frac{\partial Q}{\partial v}\right)_T \left(\frac{dv}{dT}\right)_{\text{sat}}$$

By definition of specific heats,

$$c_{\text{sat}} = c_v + \left(\frac{\partial Q}{\partial v}\right)_T \frac{dv_{\text{sat}}}{dT}$$

By virtue of the Clapeyron relations,

$$\left(\frac{\partial Q}{\partial v}\right)_T = \left(\frac{T \Delta s}{\Delta v}\right)_T = T \frac{dp}{dT}$$

Substituting and changing the variable from v to ρ yields the specific heat at constant volume for the vapor at saturated liquid density:

$$c_v = c_{\text{sat}} + T_p^2 \left(\frac{dp}{dT} \right) \left(\frac{dp_{\text{sat}}}{dT} \right) \quad (\text{B41})$$

where c_{sat} is computed from relations given in reference 7. The saturation-density equation of the same reference is differentiated with respect to temperature; however, the correction terms recommended are omitted. From reference 7, then

$$c_{\text{sat}} = AT(T_c - T)^{-0.1} + B + CT + DT^2 + ET^3 + FT^4 + GT^5 \quad \text{cal}/(\text{g})(\text{mole})(^\circ\text{K}) \quad (\text{B42})$$

where

T temperature, $^\circ\text{K}$

T_c critical temperature, $^\circ\text{K}$

and

$$A = 1.681\ 574\ 2 \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})/^\circ\text{K}^{0.9}$$

$$B = -3.280\ 278\ 9 \times 10^1 \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})$$

$$C = 6.816\ 987\ 1 \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})/^\circ\text{K}$$

$$D = -7.319\ 434\ 1 \times 10^{-1} \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})/^\circ\text{K}^2$$

$$E = 3.357\ 435\ 7 \times 10^{-2} \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})/^\circ\text{K}^3$$

$$F = -7.682\ 974 \times 10^{-4} \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})/^\circ\text{K}^4$$

$$G = 6.902\ 922\ 4 \times 10^{-6} \text{ cal}/(\text{g})(\text{mole})(^\circ\text{K})/^\circ\text{K}^5$$

The saturation density, used only for the slope dp_{sat}/dT in equation (B41) is also obtained from reference 7:

$$\rho_{\text{sat}} = \rho_c + A(T_c - T)^{0.38} + B(T_c - T) + C(T_c - T)^{4/3} + D(T_c - T)^{5/3} + E(T_c - T)^2 \quad \text{mole/cc} \quad (\text{B43})$$

where

$$\rho_c = 0.01559 \pm 0.00005 \text{ cc/mole (ref. 7)}$$

$$T_c = 32.976 \pm 0.015 \text{ }^\circ\text{K (ref. 7)}$$

$$A = 0.732\ 346\ 03 \times 10^{-2} \text{ mole}/(\text{cc})(^\circ\text{K})^{0.38}$$

$$B = -0.440\ 742\ 61 \times 10^{-3} \text{ mole}/(\text{cc})(^{\circ}\text{K})$$

$$C = 0.662\ 079\ 46 \times 10^{-3} \text{ mole}/(\text{cc})(^{\circ}\text{K})^{4/3}$$

$$D = 0.292\ 263\ 63 \times 10^{-3} \text{ mole}/(\text{cc})(^{\circ}\text{K})^{5/3}$$

$$E = 0.400\ 849\ 07 \times 10^{-4} \text{ mole}/(\text{cc})(^{\circ}\text{K})^2$$

Specific heat at constant volume for the vapor at densities less than saturated liquid are obtained from the relation

$$\left(\frac{\partial c_v}{\partial v}\right)_T = T \left(\frac{\partial^2 p}{\partial T^2}\right)_v$$

Isothermal integration within the vapor where the partial derivative becomes the total second derivative of the vapor pressure relation, a constant, yields

$$c_{v,v} = c_{v,v=v_{\text{sat}}} + T \left(\frac{d^2 p}{dT^2}\right) (v - v_{\text{sat}}) \quad (\text{B44})$$

Specific heat at constant pressure c_p is undefined for a wet vapor, but the storage allocated is filled with c_p of the gas at saturated vapor-density to avoid possible logical problems in external programs.

APPENDIX C

DETAILS OF SUBROUTINE STATE

The FORTRAN coding of SUBROUTINE STATE is shown in table III. The assignment of common storage is in some instances unique to the external programs used by the author, and it is anticipated that some changes would be made in applying the subroutine in other programs. The portions of these assignments that influence the internal subroutine are summarized by comments in the program and are shown in tabular form on page 9.

The assigned storage totals almost 300 words, and the subroutine requires 1772 words plus that needed for subroutines for computing logarithms, square roots, and exponentials.

Two parts of the subroutine should be given special attention if internal changes are made:

(1) Convergence logic for $J \neq 1$ (see table I) includes artificial constraint terms.

(2) Storage assignments in JUNK are overlapping and may be conflicting if the order of computation is modified.

The location of specific data tables within the major group CS is fully stated in the loading and unit conversion SUBROUTINE STATE S in appendix D.

APPENDIX D

DETAILS OF LOADING SUBROUTINE STATE S

The preparation of tables and constants, including the conversion of units from those of the references to a consistent set, and the "initialization" of some indexes is collected into a FORTRAN SUBROUTINE STATE S shown in table IV.

Three alternate techniques are suggested for preparing and initializing the list of constants:

- (1) Load the list as "data" from previously prepared cards or magnetic tape.
- (2) Load subroutine STATE S as an additional subroutine if core storage is available. About 1430 storage locations are required.
- (3) Load the subroutine in a different core load. (This will require SUBROUTINE CHAIN for the IBM 7090 computer (ref. 13), and about 200 storage locations and a tape drive unit are needed.)

Three sets of units are considered, namely a British set in pounds, feet, seconds, and degrees Rankine; a second British set in pounds per square inch and British thermal units; and a metric set in atmospheres, grams, centimeters, seconds, and degrees Kelvin. The conversions of these combinations into the desired system are shown in the coding. The first British set is requested by giving UNITS = 0, the second by UNITS < 0, and the metric set by UNITS > 0.

The contact with the computing subroutine is established by the assignments within CS, which also includes some index initialization. The ortho-hydrogen composition is specified by the word COMP in a common location.

SUBROUTINE STATE S is prepared without regard to execution speed or storage requirements and is not intended for repetitious execution.

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TABLE II. - ESTIMATES OF EXECUTION SPEED ON IBM 7090 COMPUTER.

CONVERGENCE TO SIX SIGNIFICANT FIGURES

Resulting fluid region (N FLUID)	Independent variables CALL(J)	Trial values used	Total time 10,000 entries, min	Average execution time, sec
0	V,T (1) P,V (2) P,T (3)	None required	0.3±0.2	0.002
2	V,T (1) P,T (3)	None required N FLUID = 0 (none required) Previous result (ordered sequence with steps of 10 percent or more)	1.0±0.2 1.8±0.2 1.8±0.2	0.006 .01 .01
1	V,T (1) P,T (3)	None required ^a N FLUID = 0 (none required) ^a Previous result (ordered sequence with steps of 10 percent or more) ^a	2.2±0.2 11.9±0.2 11.6±0.2	0.015 .07 .07
-1	V,T (1) V,P (2)	Random temperatures ^a Random pressures ^a	3.0±2.0 13.0±2.0	0.02 .08

^aPrevious results are used as trial values for saturation specific volumes VL and VG.

TABLE III. - SURROUTINE STATE

```

SUBROUTINE STATE (J)
C
C FLUID PROPERTY LIBRARY --- PARA-ORTHO HYDROGEN COMBINATIONS
C
C APPLICATION MUST BE EXTERNALLY LIMITED TO PREVENT USE WHERE
C WHERE DISCOCIATION OR FREEZING OCCURS OR ABOVE 5000 PSI WHERE DATA
C WILL BE EXTRAPOLATED WITHOUT WARNING
C
C THE FOLLOWING ASSIGNMENTS ORIENT -STATE- TO THE CALLING PROGRAMS
C
C -CS-, -STORE-, -CONV-, AND -UNITS- REQUIRE 215, 31, 1, AND 1 WORD
C RESPECTIVELY, AND ALL FOUR SHOULD BE IN -COMMON-
C -COMP-, REQUIRED IN -COMMON- BY -STATES-, IS NOT USED BY -STATE-
C -JUNK- IS EREASABLE AND NEED NOT BE IN -COMMON-
C -COM- AND -CORE- ARE INTERMEDIATE ASSIGNMENTS AND ARE NOT REQUIRED
C
COMMON COM
DIMENSION COM(20825), CORE(25,13), CS(400), STORE(50),
1 JUNK(50)
EQUIVALENCE (CORE,COM(100)), (CS,COM(20425)), (STORE,CORE(51)),
1 (JUNK,CORE(276)), (UNITS,COM(24)), (CONV,COM(40))
C
C ASSIGNMENT OF INPUT - OUTPUT DATA STORAGE INTO -STORE-
C IMPLICIT ASSIGNMENTS ARE C(9), CP(10), CV(11), (DP/DT)V(13)
C DIMENSIONAL SETS ARE NOTED IN THE LOADING ROUTINE -STATES-
C
EQUIVALENCE (N FLUID,STORE(5)), (P,STORE(6)), (TS,STORE(7)),
1 (V,STORE(8)), (H,STORE(12)), (XQ,STORE(14)), (VL,STORE(15)),
2 (VG,STORE(16)), (HL,STORE(17)), (HG,STORE(18)),
3 (V FILM,STORE(19)), (T FILM,STORE(26)), (VISCOS,STORE(27)),
4 (VIS L,STORE(28)), (VIS G,STORE(29)), (THERM K,STORE(30)),
5 (CP FILM,STORE(31))
C
C GROUPINGS OF CONSTANTS -- CONTACT WITH LOAD PROGRAM -STATES-
C
EQUIVALENCE (GRAV,CS), (RG,R GAS,CS(2)), (WB1,CS(3)),
1 (WB2,CS(4)), (WB3,CS(5)), (WC1,CS(6)), (WC2,CS(7)),
2 (WVS1,CS(8)), (WVS2,CS(9)), (WVS3,CS(10)), (WVS4,CS(11)),
3 (WK1,CS(12)), (WK2,CS(13)), (WK3,CS(14)), (WK4,CS(15)),
4 (WK5,CS(16)), (EKG1,CS(17)), (EKG2,CS(18)), (EKG3,CS(19)),
5 (EKG4,CS(20)), (LKG5,CS(21)), (EKG6,CS(22)),
6 (VPA,CS(23)), (VPB,CS(24)), (VPC,CS(25)), (VPD,CS(26)),
7 (T CR,CS(27)), (V CR,CS(28)), (DT FIT,CS(29)), (TFIT1,CS(30)),
8 (TFIT2,CS(31)), (TFIT3,CS(32)), (TFIT4,CS(33)), (INDX,CS(34))
DIMENSION HAR DA(1), HAR DB(1), HAR DR(1), HAR DAB(1),
1 D LIST(31)
EQUIVALENCE (HAR A1,CS(35)), (HAR A2,CS(36)), (HAR AZ0,CS(37)),
2 (HAR B1,CS(38)), (HAR B2,CS(39)), (HAR B3,CS(40)),
3 (HAR B4,CS(41)), (HAR B1A,CS(42)), (HAR B2A,CS(43)),
4 (VP LN,CS(44)), (VP CON,CS(45)),
5 (HAR C1,CS(46)), (HAR C2,CS(47)), (RHO FIT,CS(48)),
6 (HAR C4,CS(49)), (HAR C5,CS(50)), (HAR C6,CS(51)),
7 (HAR C7,CS(52)), (HAR CSM,CS(53)), (HAR DZ0,CS(54)),
8 (HAR DA,CS(55)), (HAR DR,CS(64)), (HAR DB,CS(73)),
9 (HAR DAB,CS(82))

```

TABLE III. - Continued. SUBROUTINE STATE

C

```

EQUIVALENCE (DPDT,CS(91)), (D2P DT2,CS(92)), (JJ,CS(93)),
1 (RHOS A,CS(94)), (RHOS B,CS(95)), (RHOS C,CS(96)),
2 (RHOS D,CS(97)), (RHOS E,CS(98)),
3 (CSAT A,CS(99)), (CSAT B,CS(100)), (CSAT C,CS(101)),
4 (CSAT D,CS(102)), (CSAT E,CS(103)), (CSAT H,CS(104)),
5 (C SAT G,CS(105)), (ROD VS1,CS(106)), (ROD VS2,CS(107)),
6 (ROD VS3,CS(108)), (ROD VS4,CS(109)), (ROD VS5,CS(110)),
7 (ROD VS6, CS(111)), (ROD K1,CS(112)), (ROD K2,CS(113)),
8 (ROD K3,CS(114)), (ROD K4,CS(115)), (ROD K5,CS(116)),
9 (ROD K6,CS(117)), (ROD K7,CS(118)), (ROD K8,CS(119))
EQUIVALENCE (ROD K9,CS(120)), (ROD A,CS(121)),
1 (ROD A2,CS(122)), (ROD A3,CS(123)), (ROD A4,CS(124)),
2 (ROD A5,CS(125)), (D LIST,CS(121)), (T700,CS(151)),
3 (T1500,CS(152)), (TK1500,CS(153)), (TK INT,CS(154))

```

C

C

C

EQUIVALENCING OF WORKING REGION TO TEMPORARY CORE LOCATIONS

```

DIMENSION HOLD(1), T CORE(1)
EQUIVALENCE (T CORE,JUNK(26))
EQUIVALENCE (NF,TCORE), (P1,TCORE(2)), (T1,TCORE(3)),
1 (V1,TCORE(4)), (C1,TCORE(5)), (CP1,TCORE(6)), (CV1,TCORE(7)),
2 (H1,TCORE(8)), (PTV1,TCORE(9)), (VIS,TCORE(10)),
3 (THK,HOLD,TCORE(11))

```

C

C

C

OVERLAPPING STORAGE ASSIGNMENTS

```

EQUIVALENCE (NFN1,TCORE(22)), (NDN,DVX,TCORE(23)),
2 (RGT,TCORE(24)), (TTC,TCORE(25))
EQUIVALENCE (N NEG,JUNK), (NCN,JUNK(2)), (NFN,JUNK(3)),
1 (J2,JUNK(4)), (J3,JUNK(5)), (RHO,JUNK(6)),
2 (RHO SQ,DD2, JUNK(7)), (RHO R,JUNK(8)),
3 (TX1,DP,TERM D1,RHO C2,TERM B,JUNK(9)),
4 (TX2,DV,TERM D2,TERM C,JUNK(10)),
5 (DV1,VP,C1TX2,B2TX2,TERM D3,TERM D,CR LIMT,JUNK(11)),
6 (G2TX1,B3TX1,BSQ2,D4,Z1,D2D2,DADV,VFG,JUNK(12)),
7 (WC,DD3,HFG,HAR A,JUNK(13)), (X,DWC,A INT,DT15,JUNK(14)),
8 (DX,D2C,RRT,N,TERM A1,JUNK(15)),
9 (Y1,TX4,D2,S22TV,TERM B1,HAR B,TVC,JUNK(16))
EQUIVALENCE (WB,D2D3,TERM B2,DBDV,BTVC2,JUNK(17)),
1 (TERM C1,RHODR,TERM A2,PVT,JUNK(18)), (DD4,S2TV,HAR C,JUNK(19)),
2 (BTVC,THK L,DCDV,DRS DT,DT,JUNK(20)),
3 (BRX,DWB,RHO4,RHO4C1,C INT,TTC3,JUNK(21)),
4 (D3,D2D4,RT RHO,DCV R,C SAT,TSQ,JUNK(22)),
5 (DH,RHO C3,RHO RFT,HAR D,JUNK(23)),
6 (RHO15,RHO C4,D INT,DEL VS,D2B,JUNK(24)),
7 (ABS RC3,ABS RFT,DDDV,DEL TK,JUNK(25))

```

C

C

C

INITIATE CONTACT WITH CALLING PROGRAM

```

JJ = J
IF (UNITS) 1,3,1
1 DO 2 I=6,31
2 STORE(I) = STORE(I) * D LIST(I)
3 P1 = P
NF = N FLUID

```

TABLE III. - Continued. SUBROUTINE STATE

```

      N NEG = -5
      N OUT = 100
      IF (JJ - 4) 4,5,5
4     T1 = TS
      V1 = V
      GO TO 9
5     T1 = T FILM
      V1 = V FILM
C
9     NDN = 0
7     NFN = NF
      J2 = XABSF(JJ) - 2
10    J3 = J2 - 1
      NFN1 = NFN - 1
      RGT = R GAS * T1
      TTC = T CR - T1
      NCN = 100
      IF (NFN) 100,11,170
C
C     COMPLETE CALCULATIONS FOR REGIONS OF PERFECT STATE
C
11    IF (J2) 12,13,14
12    P1 = RGT / V1
      GO TO 15
13    T1 = P1 * V1 / RG
      GO TO 15
14    V1 = RGT / P1
C
15    PTV1 = RG / V1
      PVT = - P1 / V1
      DH = 0.
      DCV R = 0.
      IF (NDN) 700,16,700
16    IF (T1 - T FIT 4) 17,700,700
17    IF (T1 - T FIT 2) 601,602,602
C
C     VAPOR REGION --- DETERMINATION OF VAPOR PRESSURE
C
100   IF (TTC) 601,601,102
102   TVC = T1 + VP C
      BTVC = VP B / TVC
      VP = 10.** (VP A + BTVC + T1 * VP D) * VP CON
      IF (NFN) 104,130,130
C
104   BTVC = BTVC / TVC
      BTVC2 = VP LN * (VP D - BTVC)
      DPDT = VP * BTVC2
      D2P DT2 = VP * (2. * VP LN * BTVC / TVC + BTVC2**2)
      IF (J2) 109,105,106
C
106   IF (JJ) 105,145,145
105   DP = P - VP
      T1 = T1 + DP/DPDT
      IF (ABSF(DP)/P - CONV) 110,110,102
C
C

```

TABLE III. - Continued. SUBROUTINE STATE

```

C      OBTAIN LIQUID-SIDE SPECIFIC VOLUME AND CHECK VALIDITY
C      RETURN TO LIQUID (+1) IF VOLUME IS LESS THAN SATURATED LIQUID
C
109 P = VP
110 J2 = 2
    V1 = VL
    NF = -2
    N NEG = 1
    GO TO 611
C
115 VL = V1
    V1 = V
    IF (DV + CONV) 601,116,116
C
C      OBTAIN GAS-SIDE SPECIFIC VOLUME AND CHECK VALIDITY
C      RETURN TO GAS (+1) IF VOLUME IS MORE THAN SATURATED VAPOR
C
116 NF = -1
    V1 = VG
    C1 = PVT
    GO TO 611
C
120 VG = V1
    V1 = V
    IF (DV - CONV) 125,125,601
125 VFG = VG - VL
    XQ = (V - VL) / VFG
    HL = HOLD(8)
    HG = H1
    HFG = HG - HL
    H1 = HL + HFG * XQ
    IF (JJ) 750,780,780
C
C      PROHIBIT ATTEMPTS TO USE V AS DEPENDENT VARIABLE IN VAPOR REGION
C      USED IN RE-STARTING NDN-VAPOR CALCS BELOW TCR
C
130 DP = (VP - P1) / P1
    IF (ABSF(DP) - CONV) 700,700,131
131 IF (DP * (V1 - V CR)) 140,700,700
140 IF (J2) 599,599,141
141 IF (JJ) 598,145,145
145 N NEG = 1
    NDN = -1
    NF = 1
    V1 = VG
    IF (VP - P1) 146,7,7
146 V1 = VL
    GO TO 7
C
C      BRANCHING TO REGIONS OF GENERAL FLUID P-T-V FORMULATION
C
170 RHO = 1./V1
    RHO SQ = RHO**2
    RHO R = RHO * RG
    IF (NFN1) 200,200,300
C

```

TABLE III. - Continued. SUBROUTINE STATE

```

C     REGION 1
C     CRYOGENIC TEMPERATURE RANGES, LIQUID AND GAS
C     STATE EQUATION OF HARRY
C
200  RHO RFT = RHO - RHO FIT
      RT RHO = SQRTF (RHO)
      ABS RFT = ABSF (RHO RFT)
      RHO 4 = RHO SQ **2
      TERM C1 = HAR C7 - RHO * HAR C6 + RHO SQ * HAR C5
      IF (RHO RFT) 201,201,202
201  TERM B1 = HAR B3 * RHO * ABS RFT**2
      TERM B2 = TERM B1 * (4.5 * ABS RFT - 3. * RHO)
      GO TO 203
202  TERM B1 = HAR B4 * ABS RFT**.40
      TERM B2 = TERM B1 * (3.5 * ABS RFT + 1.40 * RHO)
      TERM C1 = HAR CSM / RHO4 - TERM C1
C
203  RHO 15 = RHO * RT RHO
      DBDV = 1. + RHO *(HAR B1A + RHO 15 * (HAR B2A + TERM B2))
      HAR B = 1. + RHO * (HAR B1 + RHO 15 *(HAR B2 + ABS RFT * TERM B1))
C
      RHO4C1 = RHO4 * HAR C1
      RHO C2 = RHO - HAR C2
C     RHO C3 = RHO - HAR C3
C     ABS RC3 = ABSF (RHO C3)
C     RHO C4 = RT RHO * HAR C4
      HAR C = RHO4C1 * (1. - RHO C4 * RHO C2 * ABS RC3)
      DCDV = 4. * HAR C - RHO4C1 * RHO C4 * (ABS RC3 * (.5 * RHO C2 +
1      RHO) + RHO C2 * SIGNF(RHO, RHO C3))
      C INT = RHO4C1 * V1 * (.3333333 + RHO C4 * TERM C1)
C
      HAR A = 0.
      DADV = 0.
      A INT = - HAR AZO
      HAR D = 0.
      DDDV = 0.
      D INT = - HAR DZO
      N = 9
204  RHO DR = RHO - HAR DR(N)
      TERM D1 = 1. / (HAR DB (N) + RHO DR**2)
      TERM D2 = SQRTF (TERM D1)
      TERM D3 = HAR DA (N) * TERM D1 * TERM D2
      TERM D1 = TERM D1 * RHO DR * TERM D3
      TERM D2 = TERM D2 * RHO DR * HAR DAB(N)
      IF (N - 5) 205,205,206
205  HAR D = HAR D + TERM D3
      DDDV = DDDV + TERM D1
      D INT = D INT + TERM D2
      GO TO 209
206  HAR A = HAR A + TERM D3
      DADV = DADV + TERM D1
      A INT = A INT + TERM D2
209  N = N - 1
      IF (N) 207,207,204
207  DDDV = RHO SQ * (2. * HAR D - 3. * RHO * DDDV)
      HAR D = HAR D * RHO SQ

```

TABLE III. - Continued. SUBROUTINE STATE

```

TERM A1 = HAR A1 * RHO**1.970
TERM A2 = HAR A2 * RHO**7.256
DADV = RHO SQ * (2. * HAR A - 3. * RHO * DADV) + 1.970 * TERM A1
1      + 7.256 * TERM A2
HAR A = HAR A * RHO SQ + TERM A1 + TERM A2
C      1.03093 = 1. / .970
C      .15985 = 1. / 6.256
A INT = A INT / 3. + V1 * (1.03093 * TERM A1 + .15985 * TERM A2)
C
208 RRT = RHO R * T1
TERM B = HAR B * RRT
TSQ = T1 * T1
TERM C = HAR C * TSQ
TERM D = HAR D / TSQ
P1 = HAR A + TERM B + TERM C + TERM D
PVT = - RHO * (DADV + DBDV * RRT + DCDV * TSQ + DDDV / TSQ)
PTV1 = (TERM B + 2. * (TERM C - TERM D)) / T1
GO TO 305
C
210 TERM C = C INT * TSQ
TERM D = D INT / TSQ
DH = P1 * V1 - RGT + A INT - TERM C + TERM D
DCV R = - 2. * (TERM D + TERM C) / RGT
DEL VS = ROD VS1 + ROD VS2 * EXPF(RHO * ROD VS3) + RHO * (ROD VS4
1      + RHO * (ROD VS5 + RHO SQ * ROD VS6))
DEL TK = ROD K1 + RHO * (ROD K2 + RHO * (ROD K3 + RHO * (ROD K4
1      + RHO * (ROD K5 + RHO * (ROD K6 + RHO * (RODK7 + RHO *
2      (ROD K8 + RHO * ROD K9))))))
225 IF (NDN) 700,226,700
226 IF (T1 - T FIT 2) 227,227,602
227 IF (TTC) 700,700,102
C
C      REGION 3
C      MID - TEMPERATURE RANGE -- WOOLLEY-SCOTT-BRICKWEDDE
C      NBS RP-1932 COEFFICIENTS -- B AND C
C
300 TX1 = 1. / T1
TX2 = SQRTF (TX1)
301 C1TX2 = WC1 * TX2
C2TX1 = WC2 * TX1
WC = TX1 * (C1TX2 + C2TX1)
DWC = -(1.5*C1TX2 + 2.*C2TX1) * TX1
D2C = TX1 * (3.75*C1TX2 + 6.*C2TX1)
C
B2TX2 = WB2 * TX2
B3TX1 = WB3 * TX1
TX4 = SQRTF (TX2)
WB = TX4 * (WB1 + B2TX2 + B3TX1)
DWB = - TX4 * .25 * (WB1 + 3.*B2TX2 + 5.*B3TX1)
D2B = TX4 * (.3125*WB1 + 1.3125*B2TX2 + 2.8125*B3TX1)
BSQ2 = .5 * WB**2
C
C      DO = 1. (SUBSTITUTED)
C      D1 = WB (SUBSTITUTED)
C      D2 = BSQ2 + WC
D3 = WB * (BSQ2/3. + WC)

```

TABLE III. - Continued. SUBROUTINE STATE

```

D4 = BSQ2**2/6. + WC * (BSQ2 + .5*WC)
C
Z1 = RHO *(WB + RHO *(D2 + RHO *(D3 + RHO * D4)))
P1 = RHO R * T1 * (Z1 + 1.)
PTV1 = P1 * TX1 * (1. + RHO * (DWB + RHO * DWC))
PVT = - P1 * RHO SQ * (V1 + WB + RHO * (WC + WC))
305 DP = P - P1
IF (J2) 525,500,505
C
C DD1 = DWB (SUBSTITUTED)
310 DD2 = WB * DWB + DWC
DD3 = D2 * DWB + WB * DWC
DD4 = D3 * DWB + D2 * DWC
SZTV = RHO *(DWB + RHO *(.5*DD2 + RHO *(.3333333*DD3 + RHO *
1 .25*DD4)))
DH = RGT * (Z1 - SZTV)
C
C D2D1 = D2B (SUBSTITUTED)
D2D2 = WB * D2B + D2C + DWB * DWB
D2D3 = D2 * D2B + WB * D2C + DWB * (DD2 + DWC)
D2D4 = D3 * D2B + D2 * D2C + DWB * DD3 + DWC * DD2
SZ2TV = RHO *(D2B + RHO *(.5*D2D2 + RHO *(.3333333*D2D3 +
1 RHO * .25*D2D4)))
DCV R = - 2. * SZTV - SZ2TV
C ENSKOGS PRESSURE CORRECTIONS
BRX = PTV1 / RHO R - 1.
DEL VS = 1. + BRX *(EKG1 + BRX *(EKG2 + BRX * EKG3))
DEL TK = 1. + BRX *(EKG4 + BRX *(EKG5 + BRX * EKG6))
C VERIFY CHOICE OF FLUID REGION
320 IF (NDN) 700,321,700
321 IF (T1 - T FIT 4) 322,600,600
322 IF (T1 - T FIT 2) 601,700,700
C
C CHECK CONVERGENCE --- USE VARIABLE CONVERGENCE FACTOR -CONV- TO
C MAKE ADJUSTMENTS TO TRIAL VALUES
C
500 T1 = MAX1F (T1 + DP / PTV1, .25 * T1)
RGT = R GAS * T1
TTC = T CR - T1
GO TO 516
C
505 IF (MIN1F (P1, - PVT)) 506,506,510
506 P1 = P
V1 = V1 + SIGNF(.25 * V1, V1 - V CR)
N NEG = N NEG + 1
IF (N NEG) 519,599,519
510 CR LIMT = V1
IF (TTC) 512,512,511
511 CR LIMT = .25 * ABSF (V1 - V CR)
512 V1 = V1 - SIGNF (MIN1F (ABSF (DP / PVT), .25 * V1, CR LIMT), DP)
516 IF (ABSF(DP)/P - CONV) 525,525,519
519 NCN = NCN - 1
IF (NCN) 525,525,520
520 IF (J2) 521,521,170
521 IF (NFN1) 208,208,530
525 IF (NFN1) 210,210,310

```

TABLE III. - Continued. SUBROUTINE STATE

```

C
C   CONSTRAINTS RELATED TO BAD TRIAL VALUES OF TEMPERATURE
C
530 IF (TTC) 170,531,531
531 T1 = T CR
    GO TO 601
C
C   RESTART SEQUENCING --- FLUID HAS CHANGED REGIONS
C
598 V = V1
599 NF = -1
    GO TO 9
600 NF = 0
    GO TO 9
601 NF = 1
    GO TO 9
602 NF = 2
    GO TO 9
C
610 NFN = 0
    GO TO 620
611 NFN = 1
    GO TO 620
612 NFN = 2
620 DO 621 I=2,11
621 HOLD(I) = TCORE(I)
    NDN = 1
    GO TO 10
C
C   RETURN FROM SMOOTHING CALCULATIONS
C
630 IF (NFN1) 631,631,633
631 DX = (HOLD(3) - T FIT 3) / DT FIT
    GO TO 635
633 DX = (HOLD(3) - T FIT 1) / DT FIT
635 X = 1. - DX
    DO 636 I=2,11
636 T CORE(I) = T CORE(I) * DX + HOLD(I) * X
    GO TO 735
C
C   THERMODYNAMIC PROPERTIES AT IDEAL STATE --- SEMI-LOG INTERPOLATION
C   TABLE LOOK-UP OPERATIONS
C
700 X = LOGF(T1)
701 INDX = INDX - 1
702 DX = X - CS(INDX-1)
    IF (DX) 701,705,703
703 IF (CS(INDX) - X) 704,705,705
704 INDX = INDX + 1
    GO TO 702
705 DX = DX / (CS(INDX) - CS(INDX-1))
    X = 1. - DX
    Y1 = CS(INDX+19) * X + CS(INDX+20) * DX
    H1 = (CS(INDX+39) * X + CS(INDX+40) * DX) * T1 + DH
    CV1 = Y1 + R GAS * (DCV R - 1.)
    IF (J3) 728,728,710

```

TABLE III. - Continued. SUBROUTINE STATE

```

C
C   TRANSPORT PROPERTIES --- VISCOSITY AND THERMAL CONDUCTIVITY
C
710 VIS = WVS1 * T1 * SQRTF(T1) * (T1 + WVS2) / ((T1 + WVS3) * (T1
1      + WVS4))
      IF (T1 - T700) 715,715,720
715 THK = VIS * (WK1 + WK2 * T1 + Y1 * (WK3 + WK4 * T1)) / (1. + WK5 / T1)
      GO TO 725
720 DT 15 = T1500 - T1
      IF (DT 15) 723,721,721
721 THK = TK1500 - TK INT * DT 15
      GO TO 725
723 THK = ROD A * EXPF ((T1 - ROD A3)**2 * ROD A2) + ROD A4 + ROD A5
1      * T1
725 IF (NFN1) 728,727,726
726 VIS = VIS * DEL VS
      THK = THK * DEL TK
      GO TO 728
727 THK = THK + DEL TK
      VIS = VIS + DEL VS
      DV = (V - V1) / MAX1F (V, .1)
728 CP1 = CV1 - T1 * PIV1**2 / PVT
      C1 = V1 * SQRTF ( -CP1/CV1 * PVT * GRAV )
      IF (NF + 1) 115,120,730
C
C   BOUNDRY REGIONS - - - SMOOTHING CHECKS
C
730 IF (NDN) 735,731,630
731 IF (NF) 735,735,732
732 IF (NFN1) 733,733,734
733 IF (T1 - T FIT 1) 735,735,612
734 IF (T1 - T FIT 3) 735,735,610
735 IF (J3) 736,736,740
736 IF (JJ) 750,750,800
C
C   FILL IN RESULTS OF FILM PROPERTIES
C
740 CP FILM = CP1
      V FILM = V1
      VISCOS = VIS
      THERM K = THK
      GO TO 850
C
C   VERIFICATION OF ENTHALPY SOLUTIONS
C
750 DH = H - H1
      IF (ABSF(DH) / MAX1F(ABSF(H), CV1) - CONV) 751,751,752
751 IF (NF) 780,800,800
752 N OUT = N OUT - 1
      IF (N OUT) 751,755,755
C
755 IF (J2) 756,800,760
756 DT = DH / CV1
      GO TO 775
C
760 IF (NF) 761,770,770

```

TABLE III. - Concluded. SUBROUTINE STATE

```

761 NF = 1
    DH = H - HG
    VI = VG
    IF (DH) 762,762,770
762 DH = H - HL
    IF (DH) 764,764,779
764 VI = VL
    CPI = HOLD(6)
    PTV1 = HOLD(9)
    PVT = HOLD(5)
C
770 DT = DH / CPI
    DVX = (VI - V CR) * SIGNF (1., DT)
    V = VI + SIGNF (MIN1F (ABSF (DT * PTV1 / PVT), MAX1F (-TTC, DVX,
1      -.25 * DVX), .25 * V1), DT)
775 TS = T1 + DT
    GO TO 4
C
779 H1 = H
    XQ = DH / HFG
    VI = VL + XQ * VFG
    NF = -1
780 TTC3 = TTC** .3333333
    C SAT = C SAT A * TTC**(-.1) + C SAT B / T1 + C SAT C + T1 *
1 (C SAT D + T1 * (C SAT E + T1 * (C SAT H + T1 * C SAT G)))
    DRS DT = RHOS A * TTC**(-.62) + RHOS B + TTC3 * (RHOS C + TTC3 *
1 RHOS D) + TTC * RHOS E
    CV1 = C SAT - DPDT * DRS DT * VL**2 + D2P DT2 * (V1 - VL)
    C1 = V1 * DPDT * SQRTF (GRAV / CV1)
    CV1 = CV1 * T1
    PTV1 = DPDT
    VIS L = HOLD(10)
    VIS G = VIS
    VISCOS = VIS L + (VIS - VIS L) * XQ
    THK L = HOLD(11)
    THERM K = THK L + (THK - THK L) * XQ
C
C     MOVE WORKING RESULTS TO RETURN DATA AREA
C
800 DO 801 I=1,9
801 STORE (I+4) = T CORE (I)
C
C     RESTORE RETURN DATA TO CALLING DIMENSIONAL SET
C
850 IF (UNITS) 851,855,851
851 DO 852 I=6,31
852 STORE(I) = STORE(I) / D LIST(I)
855 RETURN
C
    END(1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0)

```

TABLE IV. - SUBROUTINE STATE S

SUBROUTINE STATE S

THIS IS THE LOAD ROUTINE FOR THE FLUID LIBRARY -STATE-
SET-UP ROUTINE FOR PARA-ORTHO COMBINATION AND DIMENSIONAL SET

COMMON CCM
DIMENSION COM(20825), CS(400)
EQUIVALENCE (CS,COM(20425)), (UNITS,COM(24)), (COMP,COM(34))

GROUPINGS OF CONSTANTS

DIMENSION HAR DA(1), HAR DB(1), HAR DR(1), HAR DAB(1),
1 D LIST(31)
EQUIVALENCE (GRAV,CS), (RG,R GAS,CS(2)), (WB1,CS(3)),
1 (WB2,CS(4)), (WB3,CS(5)), (WC1,CS(6)), (WC2,CS(7)),
2 (WVS1,CS(8)), (WVS2,CS(9)), (WVS3,CS(10)), (WVS4,CS(11)),
3 (WK1,CS(12)), (WK2,CS(13)), (WK3,CS(14)), (WK4,CS(15)),
4 (WK5,CS(16)), (EKG1,CS(17)), (EKG2,CS(18)), (EKG3,CS(19)),
5 (EKG4,CS(20)), (EKG5,CS(21)), (EKG6,CS(22)),
6 (VPA,CS(23)), (VPB,CS(24)), (VPC,CS(25)), (VPD,CS(26)),
7 (T CR,CS(27)), (V CR,CS(28)), (DT FIT,CS(29)), (TFIT1,CS(30)),
8 (TFIT2,CS(31)), (TFIT3,CS(32)), (TFIT4,CS(33)), (INDX,CS(34))
EQUIVALENCE (HAR A1,CS(35)), (HAR A2,CS(36)), (HAR AZO,CS(37)),
2 (HAR B1,CS(38)), (HAR B2,CS(39)), (HAR B3,CS(40)),
3 (HAR B4,CS(41)), (HAR B1A,CS(42)), (HAR B2A,CS(43)),
4 (VP LN,CS(44)), (VP CON,CS(45)),
5 (HAR C1,CS(46)), (HAR C2,CS(47)), (HAR C3,CS(48)),
6 (HAR C4,CS(49)), (HAR C5,CS(50)), (HAR C6,CS(51)),
7 (HAR C7,CS(52)), (HAR CSM,CS(53)), (HAR DZO,CS(54)),
8 (HAR DA,CS(55)), (HAR DR,CS(64)), (HAR DB,CS(73)),
9 (HAR DAB,CS(82))
EQUIVALENCE (RHOS A,CS(94)), (RHOS B,CS(95)), (RHOS C,CS(96)),
2 (RHOS D,CS(97)), (RHOS E,CS(98)),
3 (CSAT A,CS(99)), (CSAT B,CS(100)), (CSAT C,CS(101)),
4 (CSAT D,CS(102)), (CSAT E,CS(103)), (CSAT H,CS(104)),
5 (C SAT G,CS(105)), (ROD VS1,CS(106)), (ROD VS2,CS(107)),
6 (ROD VS3,CS(108)), (ROD VS4,CS(109)), (ROD VS5,CS(110)),
7 (ROD VS6,CS(111)), (ROD K1,CS(112)), (ROD K2,CS(113)),
8 (ROD K3,CS(114)), (ROD K4,CS(115)), (ROD K5,CS(116)),
9 (ROD K6,CS(117)), (ROD K7,CS(118)), (ROD K8,CS(119))
EQUIVALENCE (ROD K9,CS(120)), (ROD A,CS(121)),
1 (ROD A2,CS(122)), (ROD A3,CS(123)), (ROD A4,CS(124)),
2 (ROD A5,CS(125)), (D LIST,CS(121)), (T700,CS(151)),
3 (T1500,CS(152)), (TK1500,CS(153)), (TK INT,CS(154))

DEFINITIONS OF FLUID PROPERTY TABLE NAMES

DIMENSION T TAB(1), CP TAB(1), H TAB(1),
1 CO TAB(20), HO TAB(20)
EQUIVALENCE (T TAB,CS(155)), (CP TAB,CS(175)), (H TAB,CS(195))

CLEAR STORAGE AREA -CS- OF LOADING INFORMATION

DO 1 I=1,215
1 CS(I) = 0.

TABLE IV. - Continued. SUBROUTINE STATE S

```

GRAV = 32.17
R GAS = 766.677
C
C   TO CHANGE THE CALL - RETURN UNIT SETS MODIFY THE CORRESPONDING
C   CONVERSIONS FACTORS BELOW --- D LIST AND STORE LOCATIONS MATCH
C
DO 7 I=6,31
7 D LIST(I) = 1.
  IF (UNITS) 2,5,3
C
C   ZERO OR OPEN CODE --- UNIT SET POUNDS-FEET-SEC-RANKINE (LITERALLY)
C   NEGATIVE CODE --- BRITISH SET WITH PSI, BTU, FT/SEC, BTU/LB-R
C
2 D LIST(6) = 144.
  D LIST(10) = 778.26
  D LIST(11) = 778.26
  D LIST(12) = 778.26
  D LIST(13) = 144.
  D LIST(17) = 778.26
  D LIST(18) = 778.26
  D LIST(30) = 778.26
  D LIST(31) = 778.26
  GO TO 5
C
C   POSITIVE CODE --- METRIC UNITS WITH ATM, KELVIN, CC/GR, CAL/GR,
C   METERS/SEC, POISES
C
3 D LIST(6) = 2116.22
  D LIST(7) = 1.8
  D LIST(8) = 1. / 62.4283
  D LIST(9) = 1. / .3048
  D LIST(10) = 778.26
  D LIST(11) = 778.26
  D LIST(12) = 778.26 * 1.8
  D LIST(13) = 2116.22 / 1.8
  D LIST(15) = 1. / 62.4283
  D LIST(16) = 1. / 62.4283
  D LIST(17) = 778.26 * 1.8
  D LIST(18) = 778.26 * 1.8
  D LIST(19) = 1. / 62.4283
  D LIST(26) = 1.8
  D LIST(27) = .0672
  D LIST(28) = .0672
  D LIST(29) = .0672
  D LIST(30) = 778.26 * .0672
  D LIST(31) = 778.26
C
C   IDEAL STATE THERMODYNAMIC FUNCTIONS
C   TEMPERATURE SCALE --- DEGREES KELVIN
C
5 T TAB(1) = 10.
  T TAB(2) = 60.
  T TAB(3) = 80.
  T TAB(4) = 100.
  T TAB(5) = 120.

```

TABLE IV. - Continued. SUBROUTINE STATE S

T TAB(6) = 150.
 T TAB(7) = 200.
 T TAB(8) = 250.
 T TAB(9) = 300.
 T TAB(10) = 400.
 T TAB(11) = 500.
 T TAB(12) = 600.
 T TAB(13) = 700.
 T TAB(14) = 1000.
 T TAB(15) = 1500.
 T TAB(16) = 2000.
 T TAB(17) = 3000.
 T TAB(18) = 4000.
 T TAB(19) = 5000.

C
 C
 C

IDEAL STATE CP --- CAL / MOLE - DEG K
 PARA HYDROGEN

CP TAB(1) = 4.968
 CP TAB(2) = 5.115
 CP TAB(3) = 5.646
 CP TAB(4) = 6.455
 CP TAB(5) = 7.204
 CP TAB(6) = 7.807
 CP TAB(7) = 7.742
 CP TAB(8) = 7.380
 CP TAB(9) = 7.152
 CP TAB(10) = 7.010
 CP TAB(11) = 6.998
 CP TAB(12) = 7.010
 CP TAB(13) = 7.037
 CP TAB(14) = 7.219
 CP TAB(15) = 7.720
 CP TAB(16) = 8.195
 CP TAB(17) = 8.859
 CP TAB(18) = 9.342
 CP TAB(19) = 9.748

C

ORTHO HYDRGEN
 CO TAB (1) = 4.968
 CO TAB (2) = 4.969
 CO TAB (3) = 5.982
 CO TAB (4) = 5.039
 CO TAB (5) = 5.170
 CO TAB (6) = 5.487
 CO TAB (7) = 6.110
 CO TAB (8) = 6.565
 CO TAB (9) = 6.809
 CO TAB (10) = 6.963
 CO TAB (11) = 6.992
 CO TAB (12) = 7.009
 CO TAB (13) = 7.036
 CO TAB (14) = 7.219
 CO TAB (15) = 7.720
 CO TAB (16) = 8.195
 CO TAB (17) = 8.859
 CO TAB (18) = 9.342
 CO TAB (19) = 9.748

TABLE IV. - Continued. SUBROUTINE STATE S

```

C
C   IDEAL STATE ENTHALPY --- CAL / MOLE
C   PARA HYDROGEN
H TAB(1) = 49.6785
H TAB(2) = 299.106
H TAB(3) = 406.015
H TAB(4) = 526.837
H TAB(5) = 663.752
H TAB(6) = 890.605
H TAB(7) = 1282.70
H TAB(8) = 1 660.49
H TAB(9) = 2 023.16
H TAB(10) = 2 729.19
H TAB(11) = 3 429.24
H TAB(12) = 4 129.48
H TAB(13) = 4 831.65
H TAB(14) = 6 966.23
H TAB(15) = 10 697.20
H TAB(16) = 14 679.2
H TAB(17) = 23 230.9
H TAB(18) = 32 345.
H TAB(19) = 41 895.
C   ORTHO HYDROGEN
HO TAB (1) = 388.327
HO TAB (2) = 636.722
HO TAB (3) = 736.179
HO TAB (4) = 836.277
HO TAB (5) = 938.227
HO TAB (6) = 1 097.78
HO TAB (7) = 1 387.90
HO TAB (8) = 1 705.80
HO TAB (9) = 2 040.87
HO TAB (10) = 2 731.54
HO TAB (11) = 3 429.53
HO TAB (12) = 4 129.52
HO TAB (13) = 4 831.66
HO TAB (14) = 6 966.23
HO TAB (15) = 10 697.20
HO TAB (16) = 14 679.2
HO TAB (17) = 23 230.9
HO TAB (18) = 32 345.
HO TAB (19) = 41 895.
C
C   SET LOOP TO PREPARE EXECUTION TABULATIONS
C
COMP 1 = 1. - COMP
DO 11 I=1,19
H TAB(I) = (H TAB(I) * COMP1 + HO TAB(I) * COMP) * 778.26 / 2.0157/
1 T TAB (I)
CP TAB(I) = (CP TAB(I) * COMP1 + CO TAB(I) * COMP) * 778.26/2.0157
T TAB (I) = LOGF (T TAB(I) * 1.8)
11 CONTINUE
C
C   REGION 1 -- LIQUID-GAS LOW TEMPERATURE REGION
C
ATM = 2116.22

```

TABLE IV. - Continued. SUBROUTINE STATE S

```

T = 1.8
RHO = .125 836 72
RHO SQ = RHO * RHO
C
HAR A1 = - .24337 * ATM / RHO**1.970
HAR A2 = 5.591 E-10 * ATM / RHO**7.256
C
HAR B1 = .027 919 58 / RHO
HAR B2 = .000 166 83 / RHO **2.5
HAR B3 = 1.0 E-6 / (30. * 4.5**3) / RHO**6.5
HAR B4 = - .000 064 5 / 7.5**1.40 / RHO**3.90
HAR B1A = 2. * HAR B1
HAR B2A = 3.5 * HAR B2
C
HAR C1 = - 1. / 124.0 / 1 000 000. * ATM / T**2 / RHO**4
HAR C2 = 25.5 * RHO
HAR C3 = 34.5 * RHO
HAR C4 = 1. / (17.6 * SQRTF(43.1) * 8.6) / RHO**2.5
HAR C5 = 1. / 5.5
HAR C6 = (HAR C2 + HAR C3) / 4.5
HAR C7 = HAR C2 * HAR C3 / 3.5
HAR CSM = HAR C3 **4.5 * (HAR C2 / 63. - HAR C3 / 99.) * 8.
C
CZ = ATM * RHO * T**2
HAR DA (1) = -8917.152 * CZ
HAR DA (2) = 10296.158 * CZ
HAR DA (3) = -371.072 * CZ
HAR DA (4) = 8.623 * CZ
HAR DA (5) = 91.596 * CZ
HAR DA (6) = - 10.67251 * ATM * RHO
HAR DA (7) = - .06286125 * ATM * RHO
HAR DA (8) = -.226 * ATM * RHO
HAR DA (9) = .0754 * ATM * RHO
HAR DR (1) = 5.40 * RHO
HAR DR (2) = 18.00 * RHO
HAR DR (3) = 31.30 * RHO
HAR DR (4) = 35.70 * RHO
HAR DR (5) = 39.87 * RHO
HAR DR (6) = 16.822 * RHO
HAR DR (7) = 35.65 * RHO
HAR DR (8) = 20.00 * RHO
HAR DR (9) = 18.00 * RHO
HAR DB (1) = 63.604 * RHO SQ
HAR DB (2) = 76.803 * RHO SQ
HAR DB (3) = 39.310 * RHO SQ
HAR DB (4) = 3.684 * RHO SQ
HAR DB (5) = 16.827 * RHO SQ
HAR DB (6) = 89.507 * RHO SQ
HAR DB (7) = 5.654 * RHO SQ
HAR DB (8) = 25.00 * RHO SQ
HAR DB (9) = 20.00 * RHO SQ
C
HAR AZO = 0.
HAR DZO = 0.
DO 55 I=1,9
HAR DAB(I) = 3. * HAR DA(I) / HAR DB(I)

```

TABLE IV. - Continued. SUBROUTINE STATE S

```

IF (I - 5) 51,51,52
51 HAR DZC = HAR DZO - HAR DAB(I) * HAR DR(I) / SQRTF (HAR DB(I) +
1 HAR DR(I)**2)
GO TO 55
52 HAR AZO = HAR AZO - HAR DAB(I) * HAR DR(I) / SQRTF (HAR DB(I) +
1 HAR DR(I)**2)
55 CONTINUE

```

C
C
C

SATURATION SPECIFIC HEAT EQUATION -- FROM FIFTH PROG REPORT

```

CHT = 778.26 / 2.0157
C SAT A = 1.681 574 2 * CHT / T**.9
C SAT B = -3.280 278 9 E1 * CHT
CHT T = CHT / T
C SAT C = 6.816 987 1 * CHT T
CHT T = CHT T / T
C SAT D = -7.319 434 1 E-1 * CHT T
CHT T = CHT T / T
C SAT E = 3.357 435 7 E-2 * CHT T
CHT T = CHT T / T
C SAT H = -7.682 974 E-4 * CHT T
CHT T = CHT T / T
C SAT G = 6.902 922 4 E-6 * CHT T

```

C
C
C
C

SATURATION DENSITY EQUATION -- FROM FIFTH PROGRESS REPORT
PREPARE CONSTANTS FOR USE IN DERIVATIVE

```

RHOS A = .732 346 03 E-2 * .38 * RHO / T**.38
RHOS B = -.440 742 61 E-3 * RHO / T
RHOS C = .662 079 46 E-3 * 4./3.* RHO / T**(4./3.)
RHOS D = -.292 263 63 E-3 * 5./3.* RHO / T**(5./3.)
RHOS E = .400 849 07 E-4 * 2. * RHO / T**2

```

C
C
C
C

CONSTANTS FOR NBS RP-1932 VIRIAL EQUATION
FROM AMAGATS AND KELVIN

```

CZ = 1000. / (62.4283 * .089888)
WB1 = .0055478 * 1.8**.25 * CZ
WB2 = -.036877 * 1.8**.75 * CZ
WB3 = -.22004 * 1.8**1.25 * CZ
WC1 = .004788 * 1.8**1.5 * CZ**2
WC2 = -.04053 * (1.8 * CZ)**2

```

C
C
C

CONSTANTS FOR THERMAL CONDUCTIVITY COMPUTATION

```

WK1 = 1.8341 * 778.26 / 2.0157
WK2 = -.004458 * 778.26/ 1.8 / 2.0157
WK3 = 1.1308
WK4 = .0008973 / 1.8
WK5 = 3.2 * 1.8

```

C
C
C

CONSTANTS FOR IDEAL STATE VISCOSITY COMPUTATION

```

WVS1 = 85.558 * .0000001 * .0020886/SQRTF(1.8) * GRAV
WVS2 = 650.39 * 1.8
WVS3 = 19.55 * 1.8

```

TABLE IV. - Continued. SUBROUTINE STATE S

```

C      WVS4 = 1175.9          * 1.8
C
C      COEFFICIENTS FOR ENSKOG PRESSURE CORRECTION OF VISCOSITY AND K
C
      EKG1 = .175
      EKG2 = .7557
      EKG3 = -.405
      EKG4 = .575
      EKG5 = .5017
      EKG6 = -.204
C
C      CRYOGENIC TEMPERATURE RANGE TRANSPORT CORRECTIONS --LAMS 2527
C
      RHO = 1. / 62.4283
      RHO SQ = RHO * RHO
      CK = 778.26 * .0672
      C MU = .0672
C
      ROD VS1 = -2.515 E-6          * C MU
      ROD VS2 = 3.5546 E-18        * C MU
      ROD VS3 = 400.                * RHO
      ROD VS4 = 4.6237 E-4          * C MU * RHO
      ROD VS5 = -2.6833 E-3        * C MU * RHO SQ
      ROD VS6 = 4.0719              * C MU * RHO SQ**2
C
      ROD K1 = 1.84 E-6             * CK
      CKR = CK * RHO
      ROD K2 = 1102.6 E-6           * CKR
      CKR = CKR * RHO
      ROD K3 = 1.22648              * CKR
      CKR = CKR * RHO
      ROD K4 = -1.15024 E2          * CKR
      CKR = CKR * RHO
      ROD K5 = 4.95228 E3           * CKR
      CKR = CKR * RHO
      ROD K6 = -1.16927 E5          * CKR
      CKR = CKR * RHO
      ROD K7 = 1.56768 E6           * CKR
      CKR = CKR * RHO
      ROD K8 = -1.12433 E7          * CKR
      CKR = CKR * RHO
      ROD K9 = 3.36150 E7           * CKR
C
C      HIGH TEMPERATURE THERMAL CONDUCTIVITY FIT -- FROM ROGERS
C
      T 700 = 700.                  * T
      T1500 = 1500.                 * T
      ROD A = 3.6789 E1 / 1013.91 / SQRTF(2. * 3.14159) * CK
      ROD A2 = -.5 * (1. / 1013.91)**2 / T**2
      ROD A3 = 5268.                 * T
      ROD A4 = 4117. E-7             * CK
      ROD A5 = 6.982 E-7             * CK / T
      TK 1500 = ROD A * EXPF ((T1500 - ROD A3)**2 * ROD A2) + ROD A4
1      + ROD A5 * T 1500
      VIS 700 = WVS1 * T 700 * SQRTF(T700) * (T700 + WVS2) /
1      ((T700 + WVS3) * (T700 + WVS4))

```

TABLE IV. - Concluded. SUBROUTINE STATE S

```

TK 700 = VIS 700 * (WK1 + WK2 * T700 + CP TAB(13) * (WK3 + WK4 *
1      T700)) / (1. + WK5 / T700)
TK INT = (TK 1500 - TK 700) / (T 1500 - T 700)

C
C
C      VAPOR PRESSURE RELATIONSHIPS -- FROM FIFTH PROGRESS REPORT 7246
C
VP A = 2.000 620
VP B = -5.009 708 * 10.          * T
VP C = 1.004 4                  * T
VP D = 1.748 495 E-2           / T
VP LN = LOGF (10.)
VP CON = ATM

C
C
C      CONSTANTS DEFINING THE REGIONAL BOUNDRIES
C
T CR = 32.994 * 1.8
V CR = 65.5 / 125.8
T FIT 1 = 220. * 1.8
T FIT 2 = 240. * 1.8
T FIT 3 = 1990. * 1.8
T FIT 4 = 2010. * 1.8
DT FIT = 20.      *1.8
INDX = 157

C
CZ = COMP1 * 100.
CX = COMP * 100.
WRITE OUTPUT TAPE 6, 56, CZ, CX
56 FORMAT (47H0 FLUID PROPERTY LIBRARY WITH A COMPOSITION OF F5.1,
1 20H PERCENT PARA-, AND F5.1, 35H PERCENT ORTHO- HYDROGEN, 11/1/
261 )
RETURN

C
END(1,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0)

```

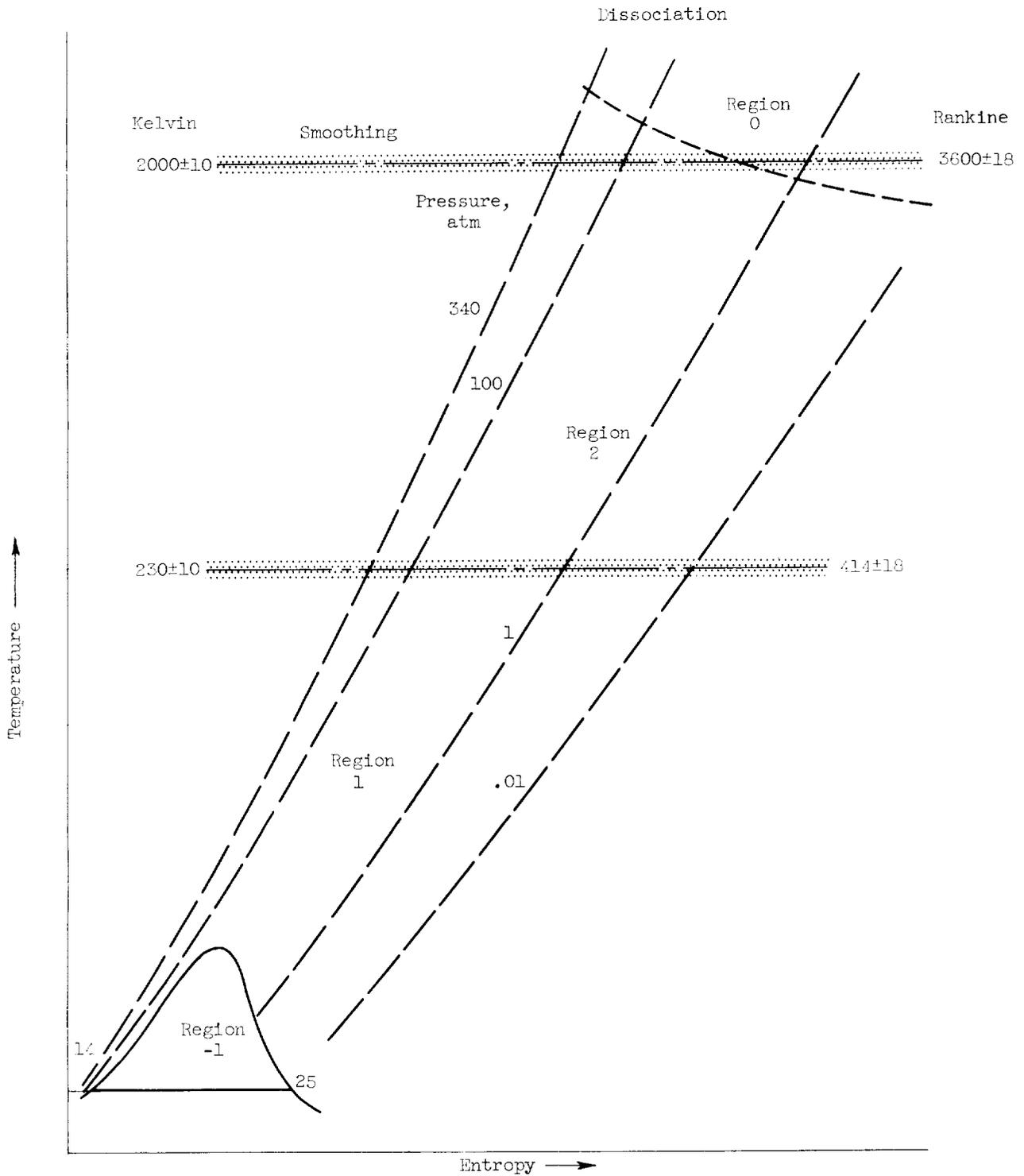


Figure 1. - Range of application of state equations.

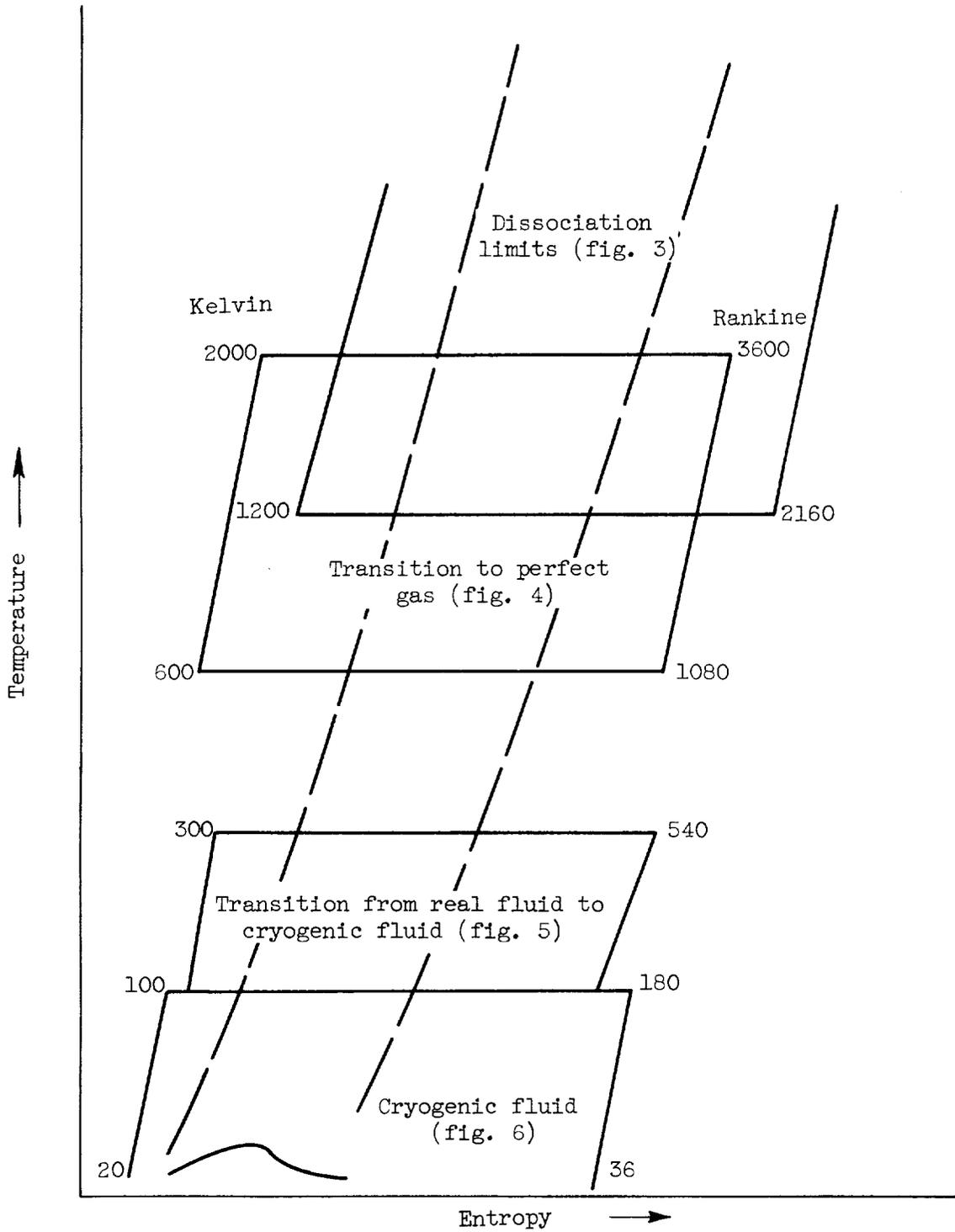


Figure 2. - Range shown in deviation figures.

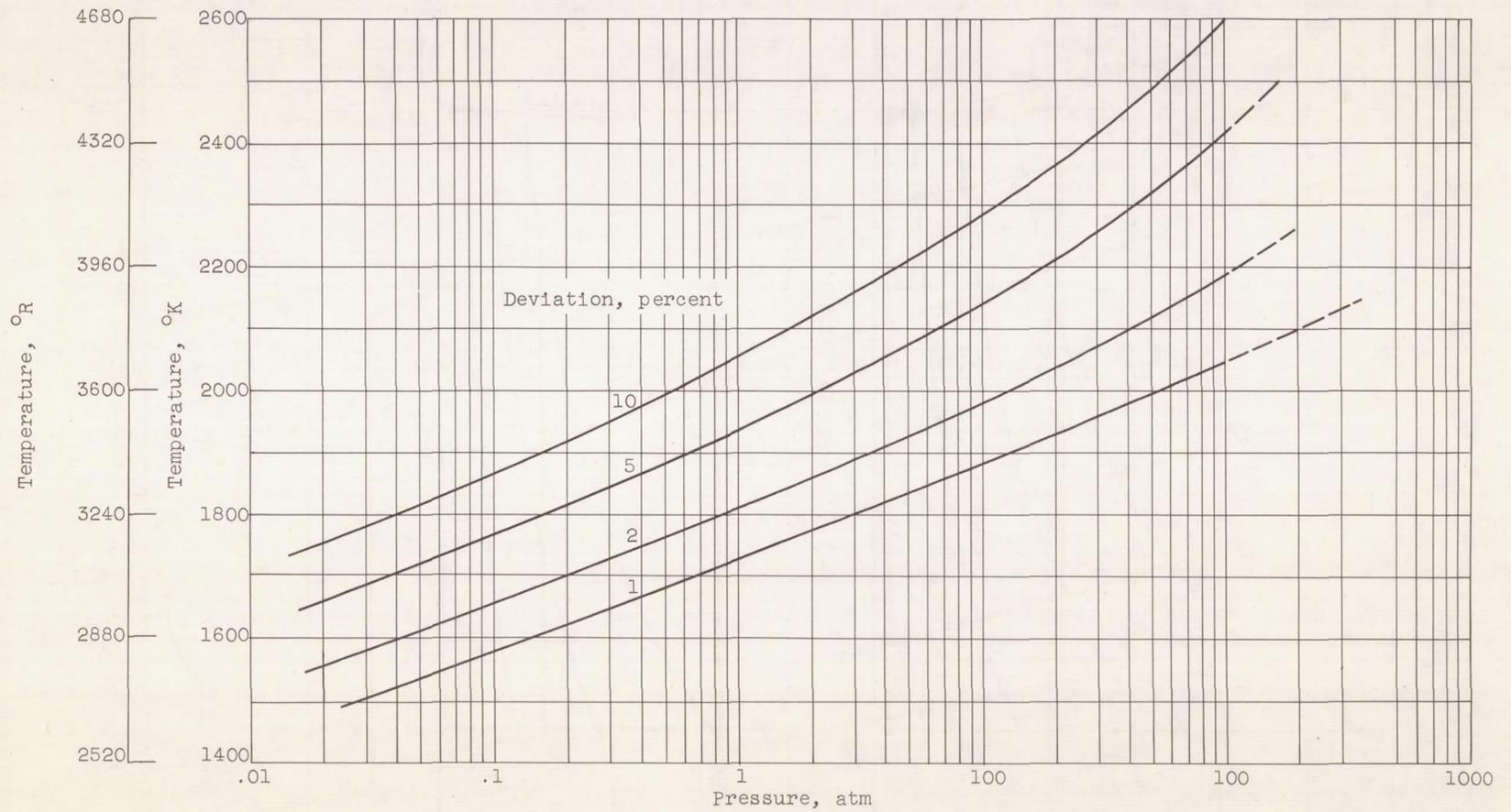
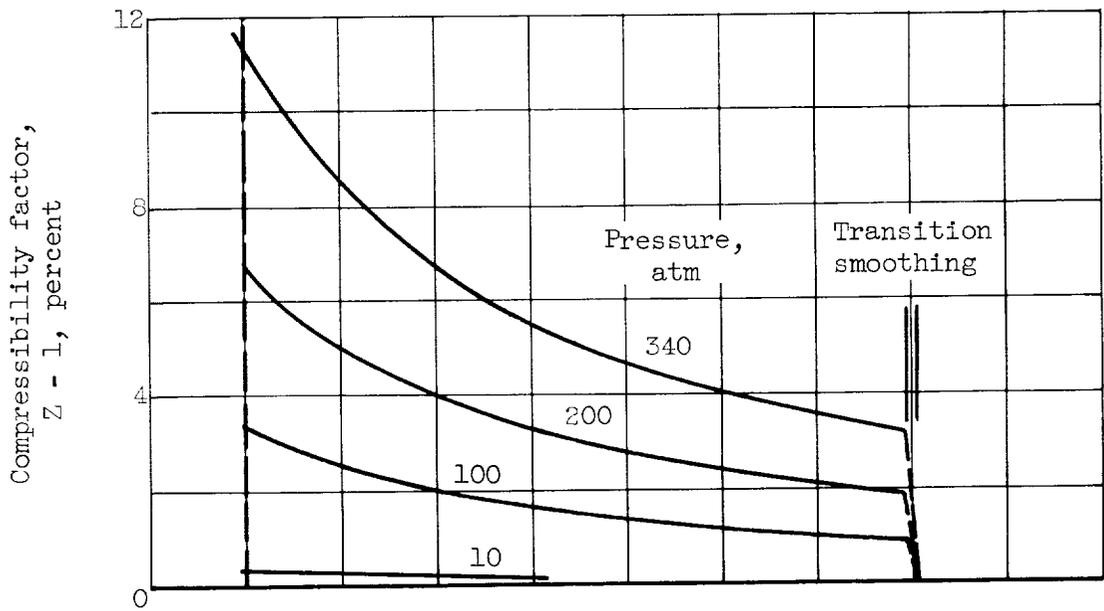
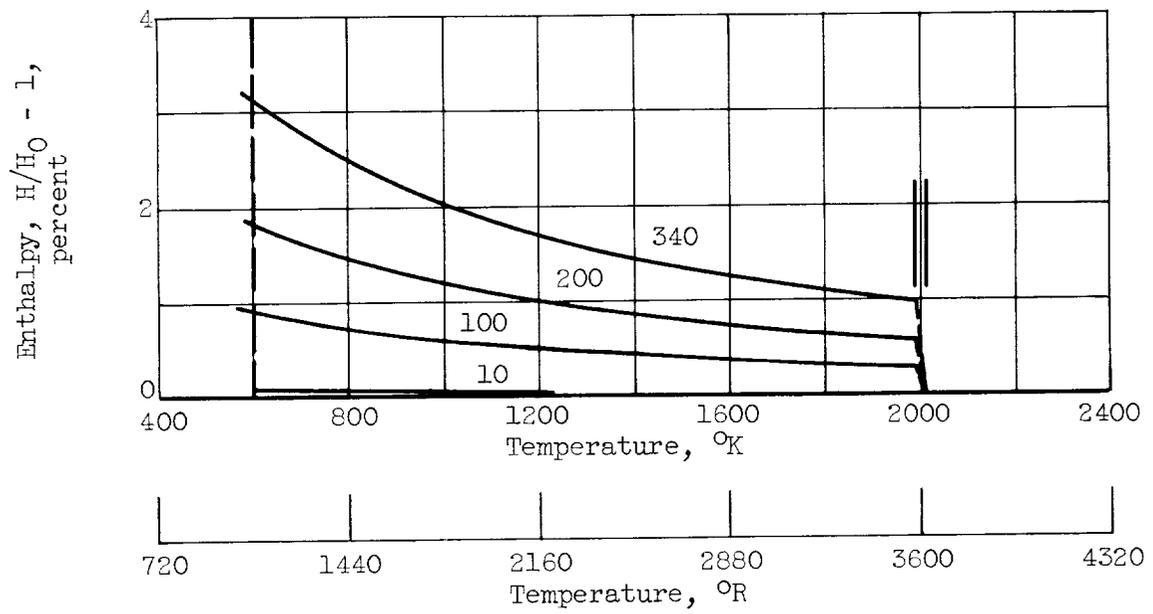


Figure 3 - Deviations in specific heat at constant pressure due to dissociation (based on equilibrium calculations of ref. 15).

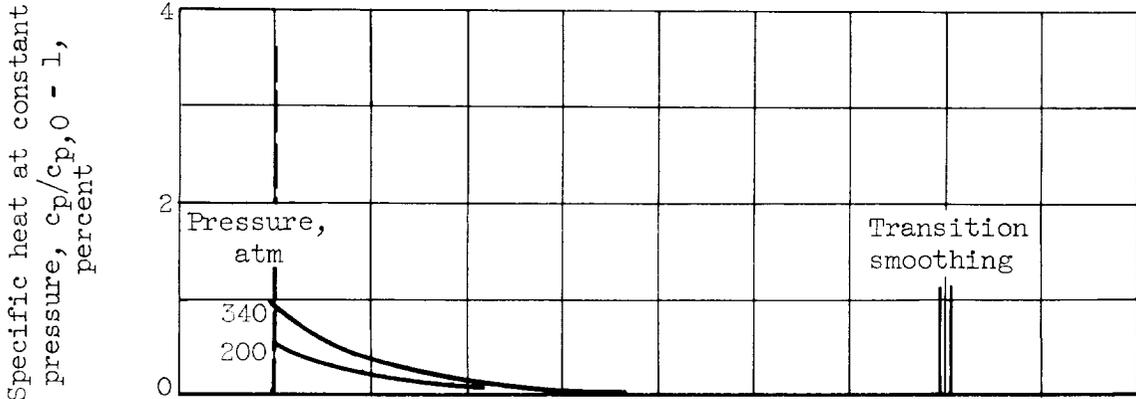


(a) Compressibility factor.

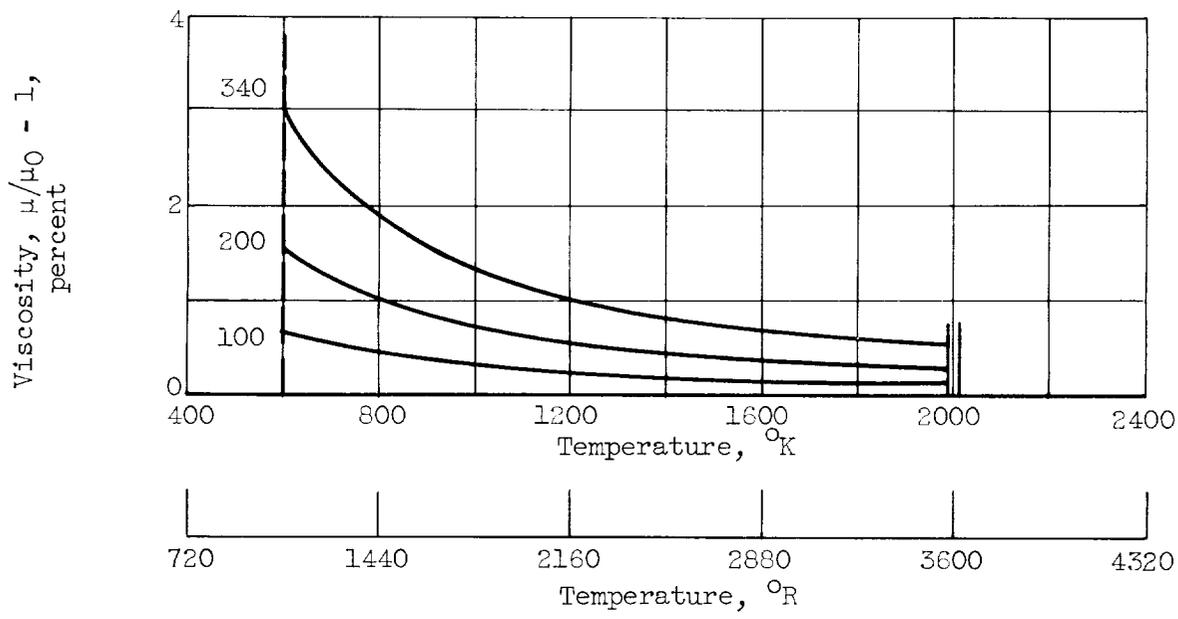


(b) Enthalpy.

Figure 4. - Real-gas properties resulting from extrapolation of state equation from reference 11.

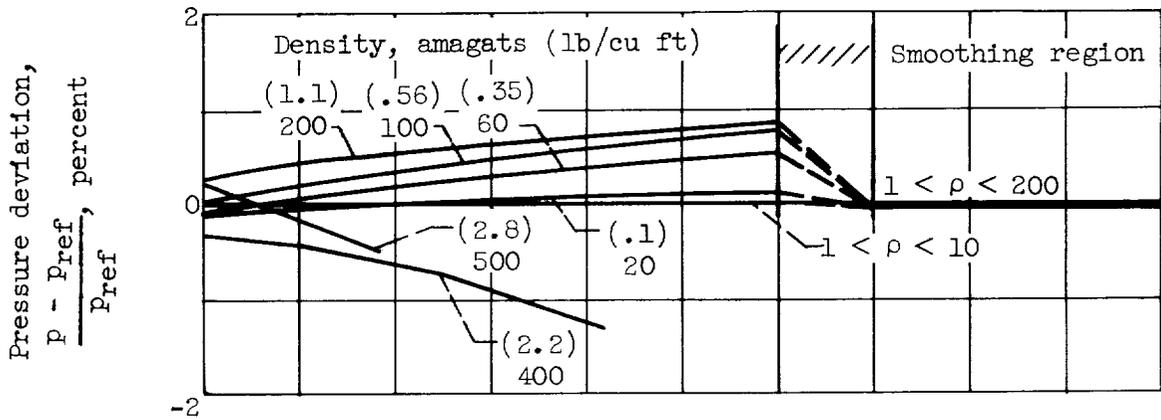


(c) Specific heat at constant pressure.

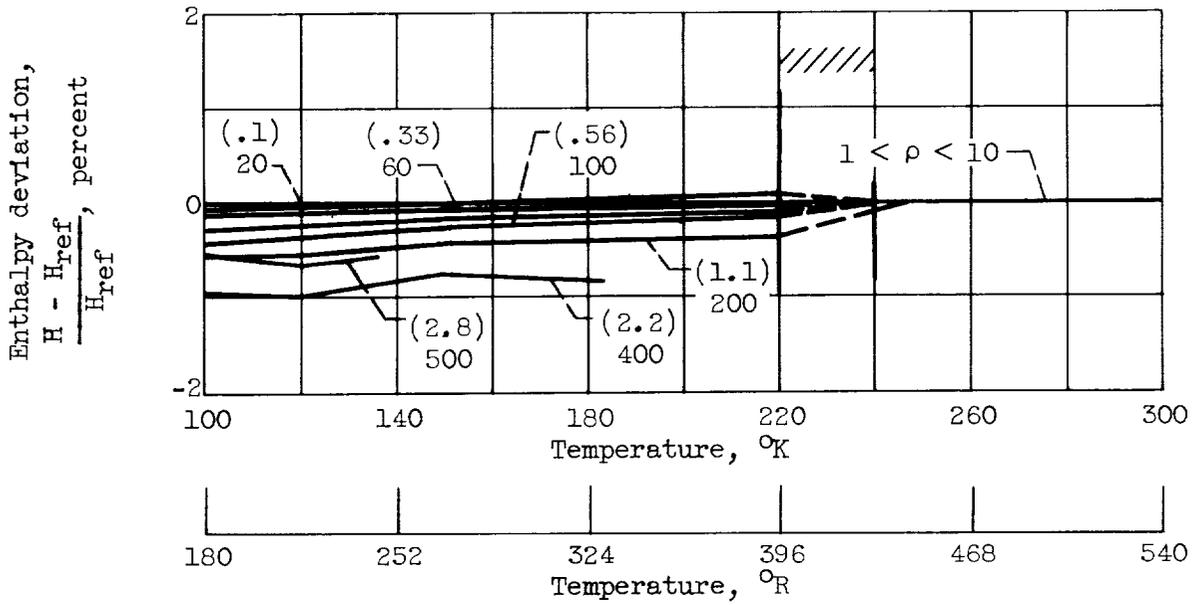


(d) Viscosity.

Figure 4. - Concluded. Real-gas properties resulting from extrapolation of state equation from reference 11.

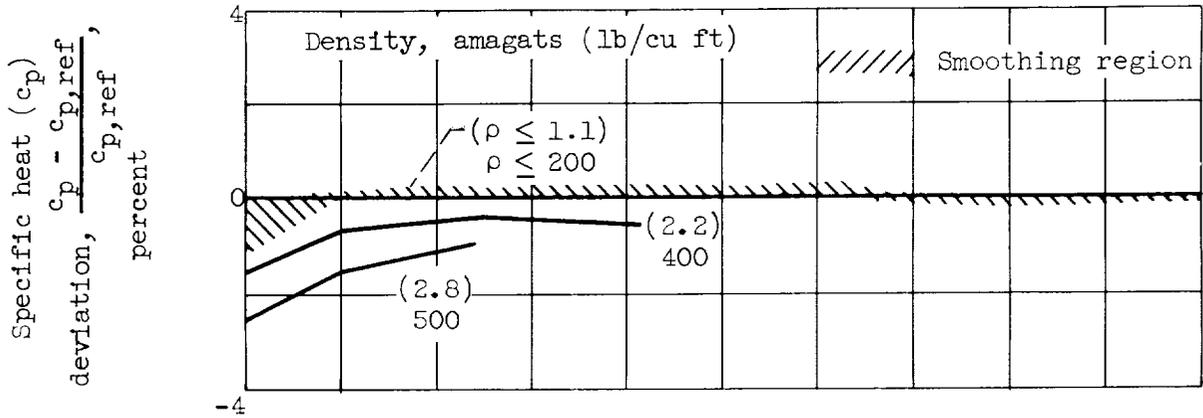


(a) Pressure.

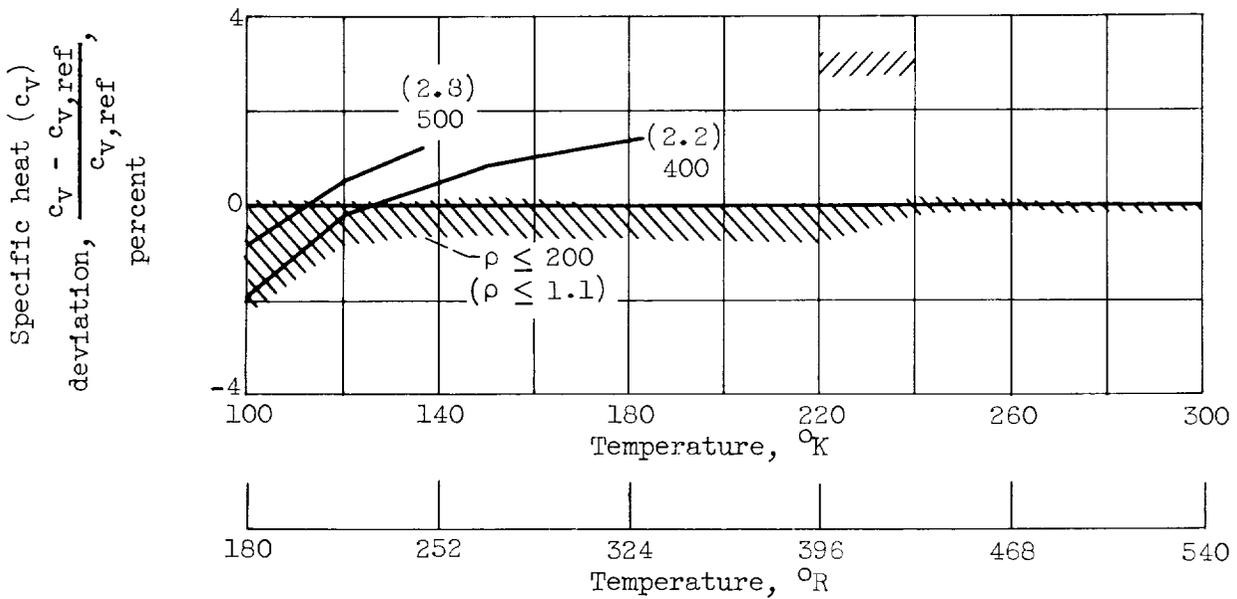


(b) Enthalpy.

Figure 5. - Deviations in computed properties from 100° to 300° K. Para-hydrogen reference data from reference 11.

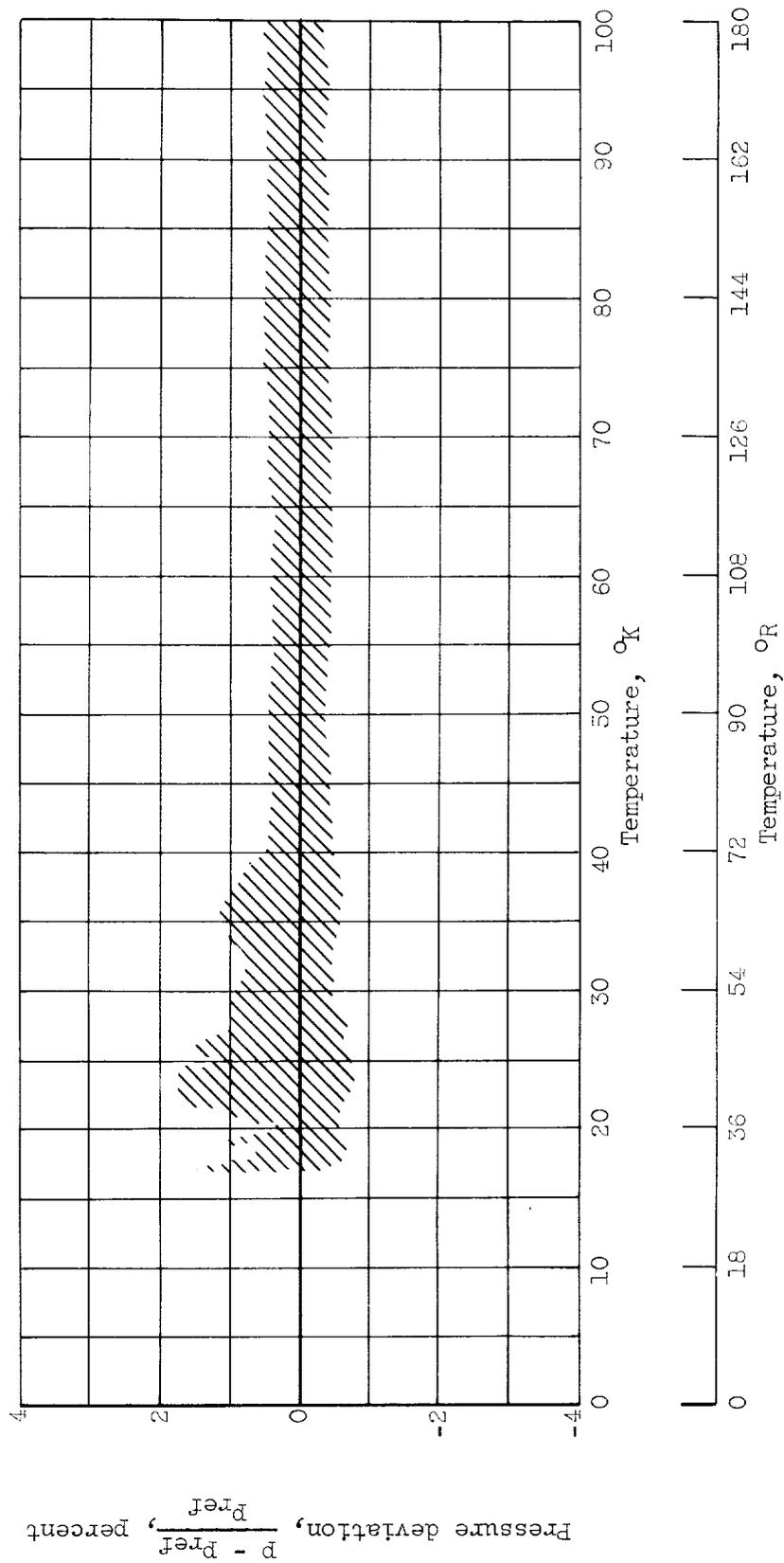


(c) Specific heat at constant pressure.



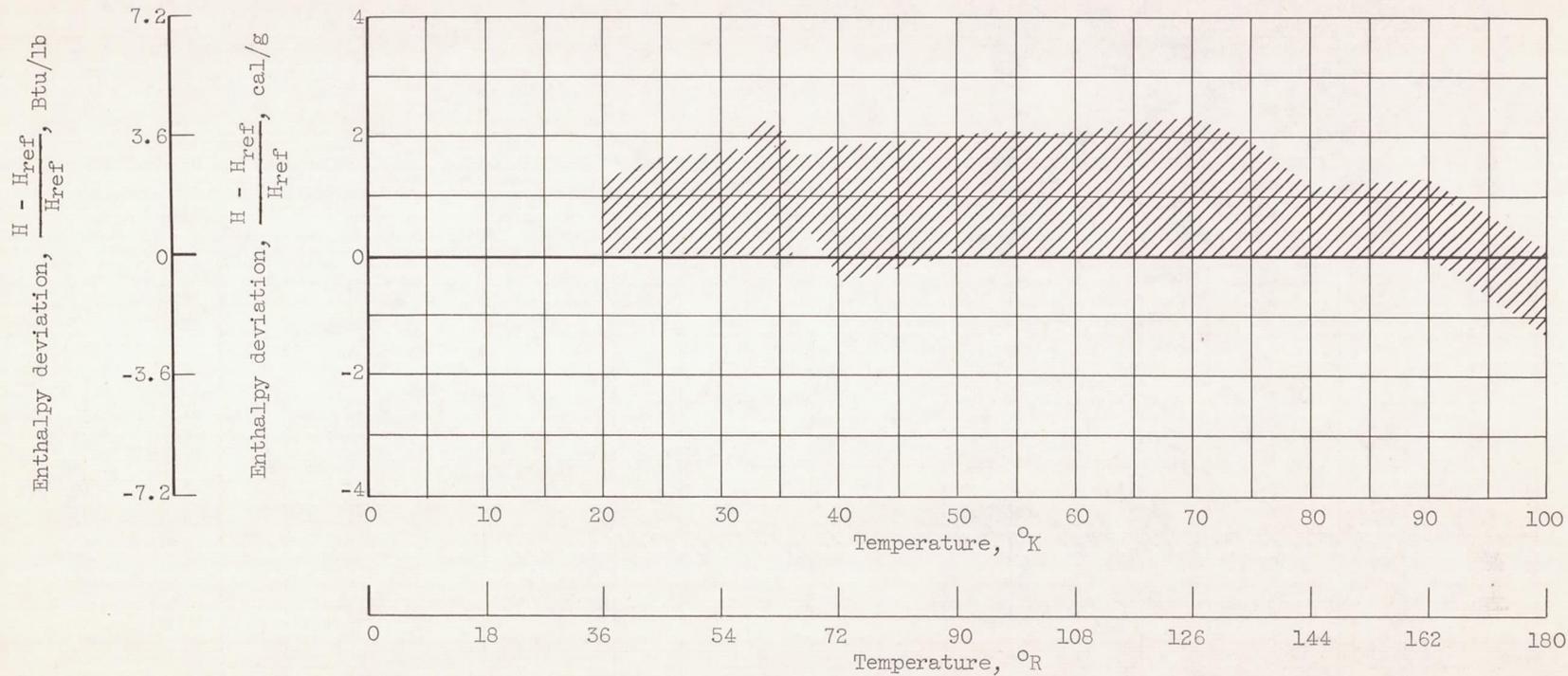
(d) Specific heat at constant volume.

Figure 5. - Concluded. Deviations in computed properties from 100° to 300° K. Para-hydrogen reference data from reference 11.



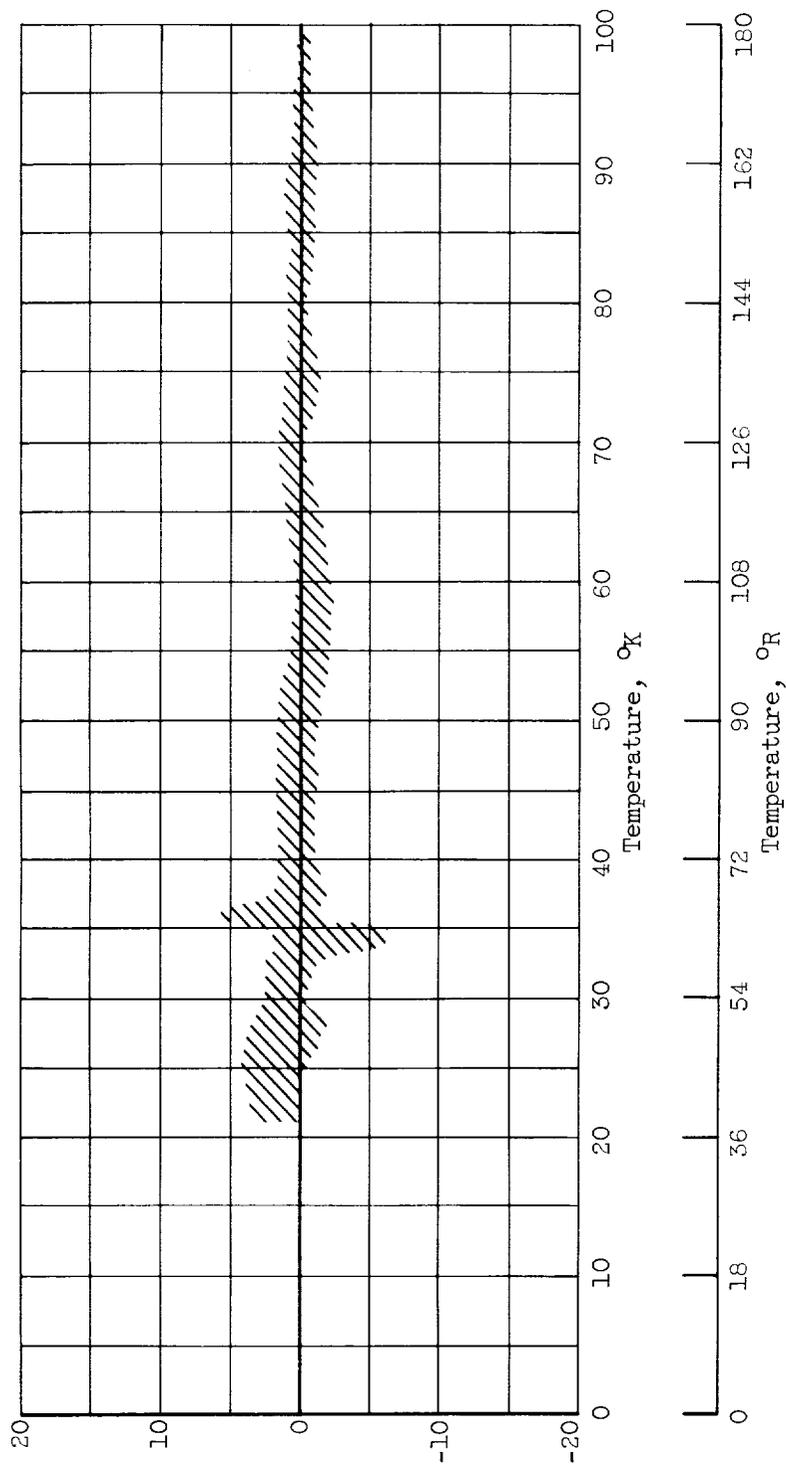
(a) Pressure from data of reference 7. Data are included for densities from 1 to 44 moles per liter; integral temperature from 17° K to 37° K by 1° K, from 38° to 50° K by 5° K, and 50° K and above by 10° K.

Figure 6. - Deviations in computed properties of para-hydrogen below 100° K.



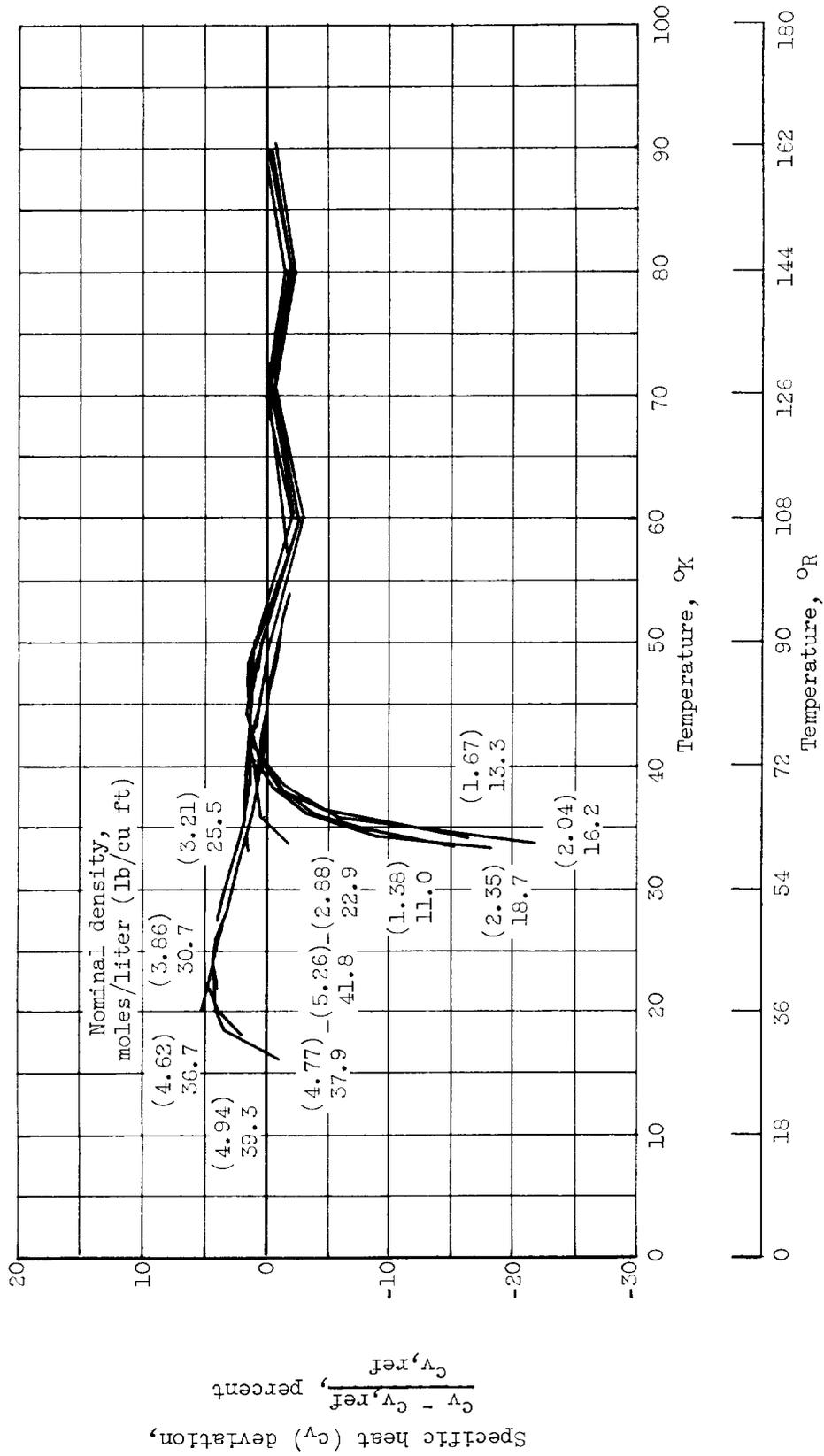
(b) Enthalpy from data of reference 3. Pressure: $p = 1, 2, 3, 5, 7, 10, 20, 30, 40, 50, 60, 80, 100, 120, 160, 200, 300, 340$ atmospheres.

Figure 6. - Continued. Deviations in computed properties of para-hydrogen below 100°K .



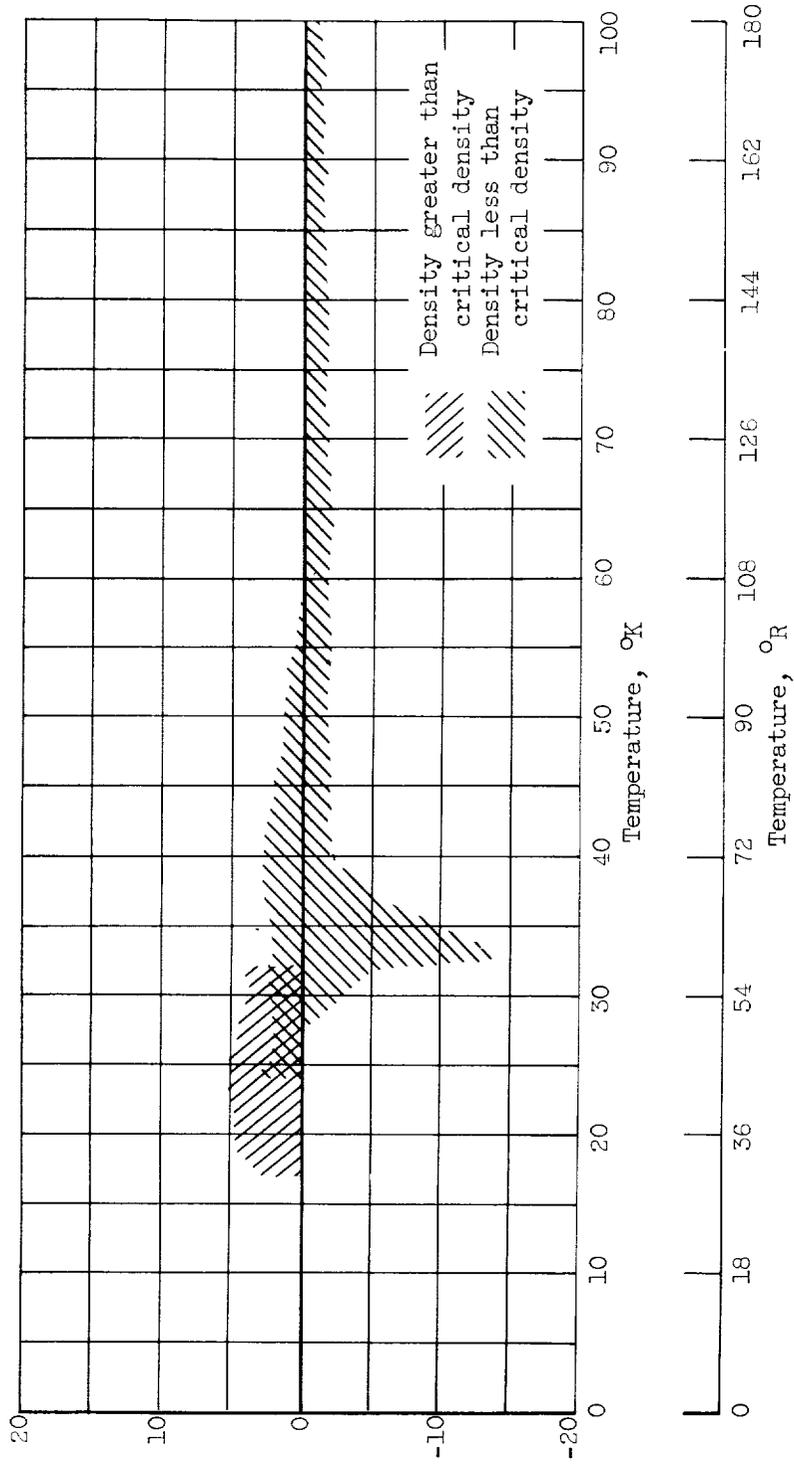
(c) Specific heat at constant pressure from data of references 2 and 7. Pressure: $p = 1$, 2, 3, 5, 7, 10, 20, 30, 40, 60, 100, 160, 200, 300, 340 atmospheres.

Figure 6. - Continued. Deviations in computed properties of para-hydrogen below 100° K.



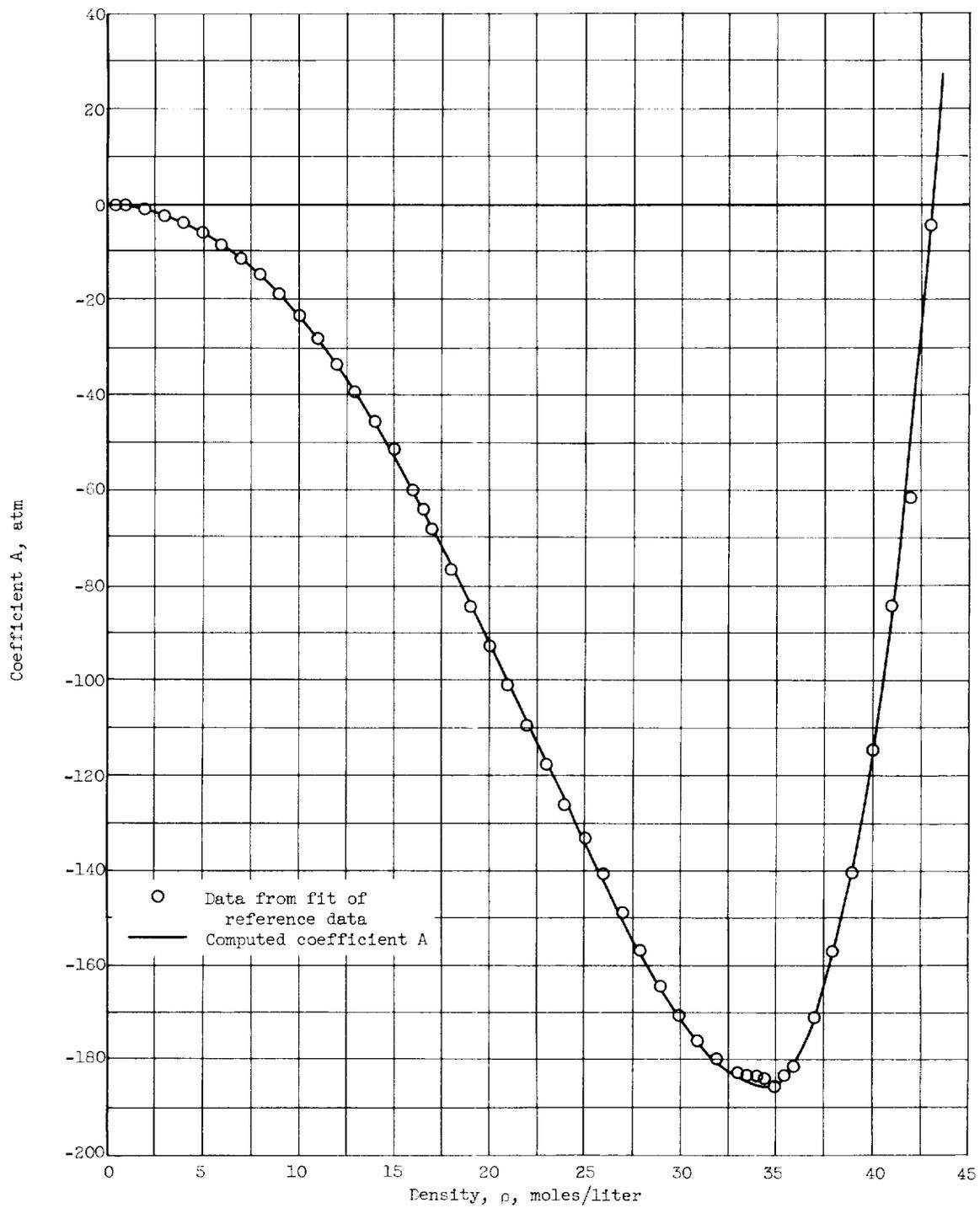
(d) Specific heat at constant volume from data of reference 7.

Figure 6. - Continued. Deviations in computed properties of para-hydrogen below 100° K.



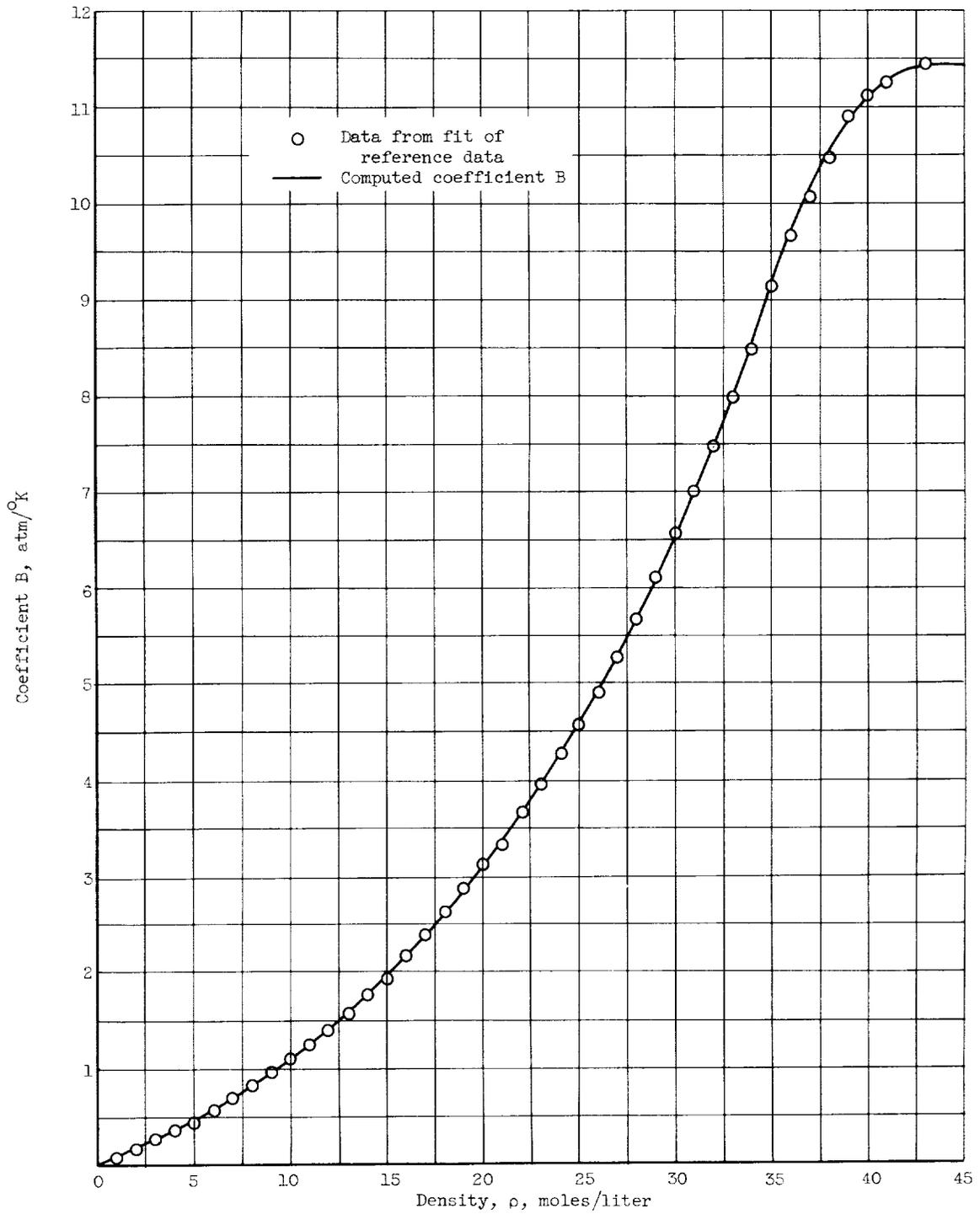
(e) Specific heat at constant volume from data of reference 8.

Figure 6. - Concluded. Deviations in computed properties of para-hydrogen below 100° K.



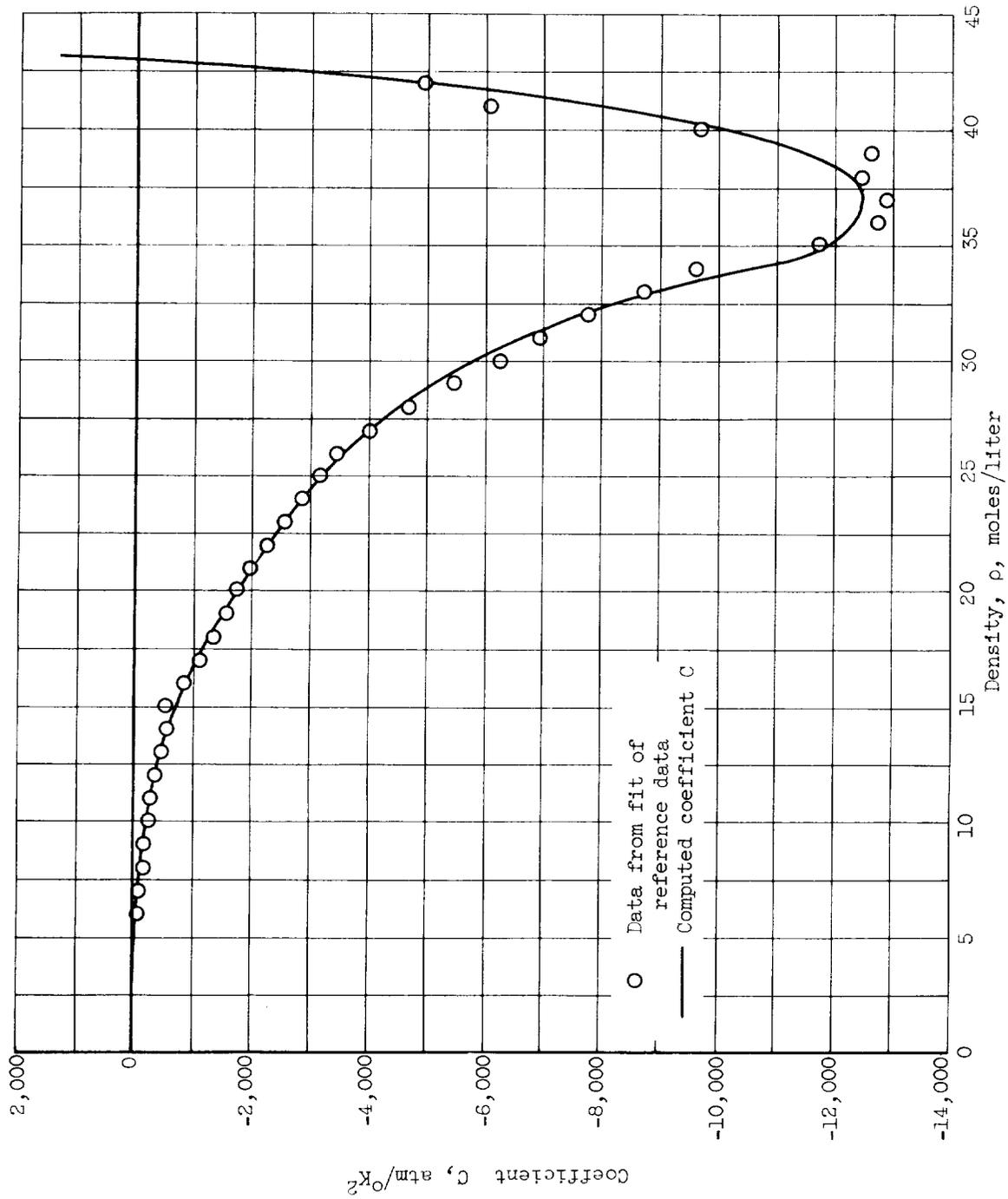
(a) Coefficient A.
$$A = A_1 \rho^{1.970} + A_2 \rho^{7.256} + \sum_{n=1}^4 \frac{\rho^2 a_n}{[b_n + (\rho - \rho_n)^2]^{3/2}}$$

Figure 7. - Coefficients of state equation for region 1. Data of reference 7 fitted by $P = A + BT + CT^2 + D/T^2$.



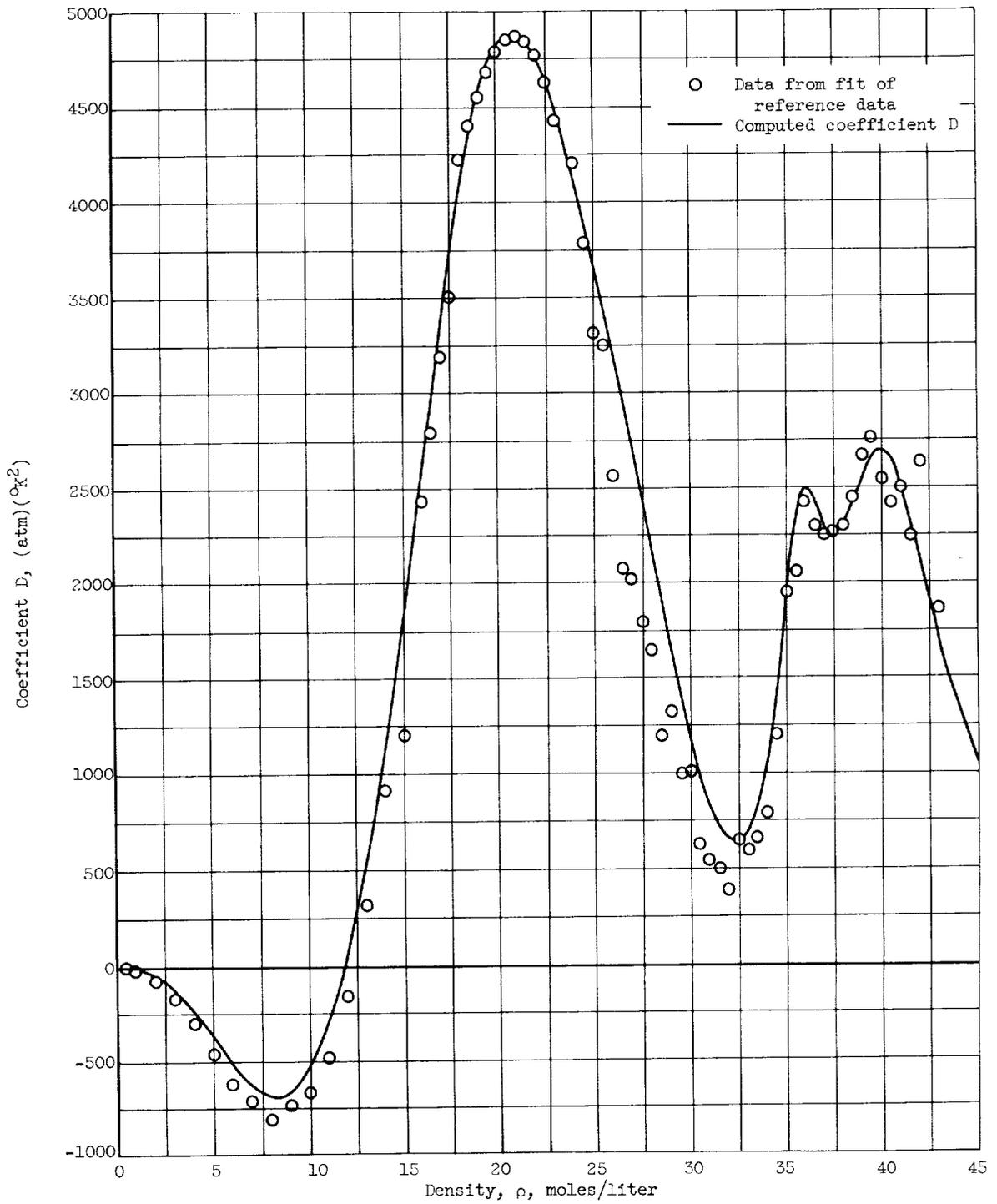
(b) Coefficient B. $B = \rho R \{ 1 + \rho [B_1 + \rho^{1.5} (B_2 + B_x)] \}$
 $\rho \leq 34.5, B_x = B_3 \rho (34.5 - \rho)^3$
 $\rho > 34.5, B_x = B_4 (\rho - 34.5)^{1.4}.$

Figure 7. - Continued. Coefficients of state equation for region 1. Data of reference 7 fitted by $P = A + BT + CT^2 + D/T^2.$



(c) Coefficient C. $C = -C_1\rho^4[1 - C_4\rho^{1/2}(\rho - C_2)]|\rho - C_3|$.

Figure 7. - Continued. Coefficients of state equation for region 1. Data of reference 7 fitted by $P = A + BT + CT^2 + D/T^2$.



(d) Coefficient D.
$$D = \rho^2 \sum_{n=1}^5 \frac{a_n}{[b_n + (\rho - \rho_n)^2]^{3/2}}$$

Figure 7. - Concluded. Coefficients of state equation for region 1. Data of reference 7 fitted by $P = A + BT + CT^2 + D/T^2$.