**MODIFICATION OF
THE GRAY EQUATION OF STATE
IN THE LIQUID-VAPOR REGION**

David A. Young

April 15, 1974

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MODIFICATION OF THE GRAY EQUATION OF STATE IN THE LIQUID-VAPOR REGION*

ABSTRACT

A modification of the GRAY three-phase equation of state is described. This modification permits accurate calculation of the pressure in the mixed phase liquid-vapor region. A listing of the computer code modification is given along with a listing of two-phase region parameters for sixteen metals. Plots of the modified equation of state are also presented.

INTRODUCTION

When a porous solid metal is rapidly heated, it may enter a mixed phase liquid-vapor state at low pressure. In order for accurate predictions of such processes to be made, a three phase equation of state with an adequate representation of the equilibrium between liquid and vapor is needed.

THEORY

At present the GRAY¹ three-phase equation of state (EOS) uses a modified van der Waals theory for the liquid-vapor region, which gives rise to unphysical maxima and minima (van der Waals loops) in isotherms drawn in the pressure-volume plane (Fig. 1). What are needed are the experimentally observed horizontal tie lines which connect the high density liquid with the low density vapor. The locus of tie line end points forms a dome-shaped curve in p-V space, as shown in Fig. 1. The top of the dome is the critical point. The liquid and vapor states coalesce above the critical temperature T_c , and hence no changes in GRAY are needed above this temperature. The problem, then, is to modify GRAY in the two phase region so that a realistic equation of state results.

CALCULATIONS

We begin with a computation of the critical point using GRAY pressure and energy isotherms, $P(V,T)$

and $E(V,T)$. This is done by an iteration process which locates the lowest isotherm which has no van der Waals loops (the critical isotherm), and also the volume at which $(\partial P/\partial V)_T = 0$ (critical volume). Now we have the four critical constants V_c , T_c , $P_c = P(V_c, T_c)$, and $E_c = E(V_c, T_c)$.

The next task is to select a set of subcritical temperatures for which energies and densities at the tie-line end points and pressures will be computed. We select an arbitrary number of equally spaced temperatures between T_c and T_{mo} , the melting point parameter used in GRAY. These isotherms are used as base lines for interpolation so that the pressure can be computed for any volume and temperature within the two phase region.

For a more accurate interpolation a larger set of temperatures is required, but this in turn would be more time consuming in the computation of the equation of state. We have chosen the minimum number of temperatures for each element compatible with the desired smoothness and accuracy of the equation of state. The lowest acceptable tie line pressure is taken to be roughly 1 bar (10^{-6} Mbar), since pressures below this are generally unimportant for the physical processes of interest, and they may be computed with sufficient accuracy by extrapolation from the 1 bar level.

Once the set of tie line temperatures is chosen, the corresponding pressures and equilibrium liquid and vapor densities are computed by the Maxwell construction. That is, a constant pressure tie line is drawn through the van der Waals loop so that the p-V area above the line is equal to that below. Alternatively, we seek a pressure p_e such that

$$\int_{V_{\min}}^{V_{\max}} (p - p_e) dV = 0$$

when the integral is taken from the liquid volume $V_{\min}$ to the vapor volume $V_{\max}$. This calculation is done by an iteration procedure in which a given estimate of p_e is used in the evaluation of the above integral, and the sign of that integral is used to determine what the next estimate of p_e should be. Once $V_{\min}$ and $V_{\max}$ at

*Work performed under the auspices of the U.S. Atomic Energy Commission.

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1. E.B. Royce, "GRAY, A Three-Phase Equation of State for Metals", Lawrence Livermore Laboratory Rpt. UCRL-51121 (1971).

temperature T are obtained, then the energies $E(V_{\min}, T)$ and $E(V_{\max}, T)$ are computed, and the calculation proceeds to the next temperature.

This preliminary calculation is done once for each material, and the computed critical point and tie line data are then stored. Listings of the critical point and tie line calculations are shown in Appendix A. The critical point and tie line data are shown in Table I for the sixteen metals in the GRAY report.¹ The data needed for the equation of state calculation can either be computed directly and stored, or read in and stored. Of course, any desired variation in the calculation described above or any data for a new material will require a fresh calculation.

Hydrodynamic calculations require pressure as a function of volume and energy, $P(V, E)$. The pressure will be calculated directly from GRAY everywhere except within the boundary of the liquid-vapor region. The boundary is constructed from line segments in the E - V plane which join the stored tie line end points together. The boundaries joining the $E = 0$ axis to the lowest liquid and vapor tie line and points are linear in density rather than volume. The solid-vapor sublimation curve is disregarded and the liquid-vapor boundary

is extrapolated to a volume $1.04V_0$ at $z = 0$. This is done to prevent the appearance of liquid under tension in the model.

The first task of the modification in GRAY then consists of determining whether the (E, V) point of interest is within the two-phase boundary, and if so, determining between which two tie lines the point lies. Once this is done, the temperature is estimated by interpolation, assuming that the energy varies linearly with temperature. Finally the pressure is determined by interpolation using the proportionality between $\ln p$ and $1/T$ predicted by the Clausius-Clapeyron equation. This coding, which may be inserted into the GRAY subroutine, is listed in Appendix B.

Plots of p - V isotherms for the sixteen GRAY metals are shown in Appendix C. Here the tie lines predicted by interpolation procedures are clearly shown, and some roughness due to the approximations used in these procedures also appears.

ACKNOWLEDGEMENT

We acknowledge the support of Mr. Don Kohler of DNA, the technical monitor for the DNA-sponsored portion of this project.

Fig. 1. A schematic diagram of GRAY isotherms in the p - V plane. The subcritical ($T < T_c$) isotherms exhibit nonphysical van der Waals loops, which are to be replaced by constant pressure tie lines (dashed lines). The locus of the tie line end points forms the dome-shaped coexistence curve (dotted curve), with the critical point at the top.

Table I

Here the critical point and tie line parameters are listed for each of the sixteen metals of the GRAY report. The first line of numbers after the name of the metal lists the four critical point parameters, which are defined as follows: TC is the critical temperature (degrees K), VC is the critical volume (cm^3/g), PC is the critical pressure (Mbar), and EC is the critical energy ($\text{Mbar}\cdot\text{cm}^3/\text{g}$). The tie line parameters follow the critical point data and are defined as follows: TEMP is the tie line temperature (degrees K), VMX is the volume of the vapor end of the tie line (cm^3/g),

VMN is the volume of the liquid end of the tie line (cm^3/g), EVMX is the energy at VMX and TEMP ($\text{Mbar}\cdot\text{cm}^3/\text{g}$), EVMN is the energy at VMN and TEMP ($\text{Mbar}\cdot\text{cm}^3/\text{g}$), and PRES is the tie line pressure (Mbar). The index JAA is the number of equally spaced subcritical temperatures (including T_{mo}) for which tie line data are to be computed. Here $JAA = JAB - 1$, where JAB is the index used in the tie line generation code in Appendix A. The index JMAX is the total number of tie lines used, including the critical point.

BERYLLIUM

JAA=10 JMAX=10

TC	VC	PC	EC	TEMP	VMX	VMN	EVMX	EVMN	PRES
1.1028E+04	1.8863E+00	2.0928E-02	4.1628E-01	1.0917E+04	4.1867E+00	1.1828E+00	4.7096E-01	3.2280E-01	1.4235E-02
				9.9065E+03	6.6667E+00	1.0204E+00	4.7516E-01	2.8216E-01	9.2249E-03
				8.8957E+03	1.1111E+01	9.4340E-01	4.7190E-01	2.5155E-01	5.6057E-03
				7.8849E+03	1.6667E+01	8.9286E-01	4.6077E-01	2.2599E-01	3.1083E-03
				6.8740E+03	3.3333E+01	8.5470E-01	4.5037E-01	2.0337E-01	1.5338E-03
				5.8632E+03	5.0000E+01	8.3333E-01	4.3480E-01	1.8378E-01	6.0738E-04
				4.8524E+03	1.6667E+02	8.0000E-01	4.2108E-01	1.6128E-01	2.3285E-04
				3.8416E+03	5.0000E+02	7.3529E-01	4.0509E-01	1.2966E-01	4.9149E-05
				2.8308E+03	5.0000E+03	6.7114E-01	3.8911E-01	9.5140E-02	3.9372E-06

MAGNESIUM

JAA=10 JMAX=9

TC	VC	PC	EC	TEMP	VMX	VMN	EVMX	EVMN	PRES
7.4169E+03	1.9569E+00	4.8860E-03	9.9126E-02	6.7902E+03	4.1867E+00	1.1111E+00	1.1254E-01	7.4549E-02	3.2589E-03
				6.1635E+03	7.1429E+00	9.7087E-01	1.1397E-01	6.4128E-02	2.0652E-03
				5.5368E+03	1.1111E+01	9.0090E-01	1.1230E-01	5.6596E-02	1.2210E-03
				4.9101E+03	2.0000E+01	8.5470E-01	1.1017E-01	5.0315E-02	6.5951E-04
				4.2834E+03	3.3333E+01	8.1567E-01	1.0686E-01	4.4784E-02	3.1074E-04
				3.6567E+03	1.0000E+02	7.9365E-01	1.0375E-01	3.9861E-02	1.1466E-04
				3.0301E+03	2.0000E+02	7.8125E-01	9.9799E-02	3.5441E-02	4.4717E-05
				2.4034E+03	1.0000E+03	7.4627E-01	9.5965E-02	2.9469E-02	7.9731E-06

ALUMINUM

JAA=10 JMAX=9

TC	VC	PC	EC		
1.1533E+04	1.2118E+00	1.0468E-02	1.4590E-01		
TEMP	VMX	VMN	EVMX	EVMN	PRES
1.0502E+04	3.0303E+00	6.9930E-01	1.6646E-01	1.0529E-01	6.6685E-03
9.4704E+03	5.2632E+00	6.0606E-01	1.6642E-01	8.7614E-02	3.9305E-03
8.4391E+03	9.0909E+00	5.5556E-01	1.6307E-01	7.4444E-02	2.1766E-03
7.4078E+03	1.6667E+01	5.2356E-01	1.5824E-01	6.3819E-02	1.0529E-03
6.3765E+03	3.3333E+01	5.0251E-01	1.5255E-01	5.4898E-02	4.2583E-04
5.3452E+03	1.1111E+02	4.8780E-01	1.4669E-01	4.7095E-02	1.3457E-04
4.3139E+03	3.3333E+02	4.7847E-01	1.4028E-01	4.0142E-02	3.6220E-05
3.2826E+03	2.0000E+03	4.6948E-01	1.3405E-01	3.3670E-02	4.1429E-06

TITANIUM

JAA=10 JMAX=9

TC	VC	PC	EC		
1.4466E+04	7.5718E-01	1.17E0E-02	1.2300E-01		
TEMP	VMX	VMN	EVMX	EVMN	PRES
1.3246E+04	1.9231E+00	4.3103E-01	1.3790E-01	9.1128E-02	7.5217E-03
1.2025E+04	3.3333E+00	3.7037E-01	1.3715E-01	7.6923E-02	4.5300E-03
1.0805E+04	5.8224E+00	3.4014E-01	1.3419E-01	6.6851E-02	2.5253E-03
9.5839E+03	1.1111E+01	3.2259E-01	1.3015E-01	5.8992E-02	1.2674E-03
8.3632E+03	2.5000E+01	3.1250E-01	1.2561E-01	5.2637E-02	5.4393E-04
7.1426E+03	5.0000E+01	3.0303E-01	1.2057E-01	4.6203E-02	1.8974E-04
5.9219E+03	1.6667E+02	2.8902E-01	1.1572E-01	3.8716E-02	5.5024E-05
4.7013E+03	1.0000E+03	2.7322E-01	1.1098E-01	3.0642E-02	7.8376E-06

STAINLESS

JAA=10 JMAX=10

TC	VC	FC	EC		
1.4721E+04	4.5299E-01	1.7495E-02	1.0011E-01		
TEMP	VMX	VMN	VMX	VMN	PRES
1.3487E+04	1.0526E+00	2.6954E-01	1.1037E-01	7.6220E-02	1.1674E-02
1.2253E+04	1.7857E+00	2.3256E-01	1.0963E-01	6.4620E-02	7.3730E-03
1.1019E+04	3.0303E+00	2.1231E-01	1.0702E-01	5.5742E-02	4.3342E-03
9.7846E+03	5.2632E+00	1.9920E-01	1.0347E-01	4.8453E-02	2.3168E-03
8.5505E+03	1.0000E+01	1.9011E-01	9.9534E-02	4.2270E-02	1.0726E-03
7.3164E+03	2.5000E+01	1.8382E-01	9.5435E-02	3.6925E-02	4.0490E-04
6.0823E+03	5.0000E+01	1.7889E-01	9.1204E-02	3.2155E-02	1.0810E-04
4.8482E+03	2.5000E+02	1.7513E-01	8.7175E-02	2.7830E-02	2.4321E-05
3.6141E+03	2.5000E+03	1.6584E-01	8.3289E-02	2.2099E-02	1.9346E-06

NICKEL

JAA=10 JMAX=10

TC	VC	FC	EC		
1.4817E+04	3.9012E-01	1.9262E-02	9.7229E-02		
TEMP	VMX	VMN	VMX	VMN	PRES
1.3568E+04	9.2593E-01	2.3041E-01	1.0730E-01	7.3639E-02	1.2734E-02
1.2319E+04	1.5373E+00	1.9841E-01	1.0643E-01	6.2207E-02	7.9557E-03
1.1071E+04	2.7027E+00	1.8116E-01	1.0373E-01	5.3549E-02	4.6163E-03
9.8220E+03	5.0000E+00	1.7007E-01	1.0031E-01	4.6497E-02	2.4225E-03
8.5733E+03	1.0000E+01	1.6260E-01	9.6389E-02	4.0550E-02	1.1013E-03
7.3247E+03	2.0000E+01	1.5743E-01	9.2205E-02	3.5427E-02	4.0236E-04
6.0760E+03	5.0000E+01	1.5408E-01	8.8108E-02	3.0983E-02	1.0354E-04
4.8273E+03	2.5000E+02	1.5033E-01	8.4170E-02	2.6456E-02	2.1691E-05
3.5787E+03	3.3333E+03	1.4144E-01	8.0410E-02	2.0263E-02	1.4851E-06

MONEL

JAA=10 JMAX=10

TC	VC	PC	EC		
1.3177E+04	4.0685E-01	1.6063E-02	8.1996E-02		
TEMP	VMX	VMN	VMX	EVMN	PRES
1.2087E+04	9.4340E-01	2.4510E-01	9.0365E-02	6.2863E-02	1.0835E-02
1.0996E+04	1.5625E+00	2.1136E-01	8.9700E-02	5.3560E-02	6.9355E-03
9.9051E+03	2.6316E+00	1.9342E-01	8.7677E-02	4.6385E-02	4.1463E-03
8.8144E+03	4.5455E+00	1.8149E-01	8.4876E-02	4.0483E-02	2.2606E-03
7.7237E+03	9.0909E+00	1.7301E-01	8.1807E-02	3.5438E-02	1.0817E-03
6.6329E+03	2.0000E+01	1.6722E-01	7.8464E-02	3.1084E-02	4.2715E-04
5.5422E+03	5.0000E+01	1.6260E-01	7.5055E-02	2.7183E-02	1.2593E-04
4.4515E+03	2.0000E+02	1.5949E-01	7.1738E-02	2.3731E-02	2.8717E-05
3.3607E+03	1.6667E+03	1.5175E-01	6.8561E-02	1.9257E-02	2.7584E-06

COPPER

JAA=10 JMAX=10

TC	VC	PC	EC		
1.2256E+04	3.6489E-01	1.5711E-02	6.0804E-02		
TEMP	VMX	VMN	VMX	EVMN	PRES
1.1210E+04	8.5470E-01	2.1978E-01	6.9981E-02	4.5527E-02	1.0405E-02
1.0163E+04	1.4493E+00	1.9157E-01	7.0855E-02	3.8991E-02	6.5348E-03
9.1164E+03	2.5200E+00	1.7658E-01	7.0279E-02	3.4199E-02	3.8239E-03
8.0698E+03	4.3478E+00	1.6722E-01	6.8797E-02	3.0286E-02	2.0287E-03
7.0232E+03	8.3333E+00	1.6377E-01	6.6907E-02	2.6917E-02	9.3392E-04
5.9765E+03	2.0000E+01	1.5625E-01	6.4776E-02	2.3914E-02	3.4743E-04
4.9299E+03	5.0000E+01	1.5291E-01	6.2403E-02	2.1166E-02	9.1616E-05
3.9833E+03	2.5000E+02	1.4948E-01	6.0011E-02	1.8309E-02	1.8076E-05
2.8366E+03	2.5000E+03	1.4045E-01	5.7614E-02	1.4044E-02	1.1381E-06

NIOSIUM

JAA=10 JMAX=10

TC	VC	PC	EC		
2.4572E+04	4.3271E-01	1.8231E-02	1.2547E-01		
TEMP	VMX	VMN	EVMX	EVMN	PRES
2.2468E+04	1.0526E+00	2.5000E-01	1.3280E-01	9.5856E-02	1.1918E-02
2.0364E+04	1.8182E+00	2.1231E-01	1.2961E-01	7.9690E-02	7.3063E-03
1.8260E+04	3.2256E+00	1.9157E-01	1.2298E-01	6.7025E-02	4.1205E-03
1.6155E+04	5.8824E+00	1.7857E-01	1.1668E-01	5.6743E-02	2.0749E-03
1.4051E+04	1.2500E+01	1.6949E-01	1.1036E-01	4.8132E-02	8.9018E-04
1.1947E+04	3.3333E+01	1.6313E-01	1.0415E-01	4.0867E-02	2.9821E-04
9.8427E+03	1.1111E+02	1.5549E-01	9.8197E-02	3.4934E-02	7.1443E-05
7.7384E+03	5.0000E+02	1.5337E-01	9.2703E-02	2.8429E-02	1.2106E-05
5.6342E+03	1.0000E+04	1.4368E-01	8.7787E-02	2.0787E-02	4.8219E-07

TANTALUM

JAA=11 JMAX=11

TC	VC	PC	EC		
2.5647E+04	2.2426E-01	1.8859E-02	6.9179E-02		
TEMP	VMX	VMN	EVMX	EVMN	PRES
2.3710E+04	5.0761E-01	1.3298E-01	7.3904E-02	5.4391E-02	1.3026E-02
2.1773E+04	8.3333E-01	1.1338E-01	7.1117E-02	4.6206E-02	8.5704E-03
1.9836E+04	1.3514E+00	1.0235E-01	6.8402E-02	3.9681E-02	5.3058E-03
1.7899E+04	2.3256E+00	9.5657E-02	6.5427E-02	3.4242E-02	3.0368E-03
1.5962E+04	4.1667E+00	8.9528E-02	6.2296E-02	2.9644E-02	1.5652E-03
1.4025E+04	8.3333E+00	8.6207E-02	5.9191E-02	2.5718E-02	6.9689E-04
1.2088E+04	2.0000E+01	8.3222E-02	5.6184E-02	2.2440E-02	2.5058E-04
1.0151E+04	5.0000E+01	8.2169E-02	5.3311E-02	1.9519E-02	6.4971E-05
8.2140E+03	2.5000E+02	7.9051E-02	5.0669E-02	1.6144E-02	1.3360E-05
6.2770E+03	2.5000E+03	7.4738E-02	4.8263E-02	1.2348E-02	1.0494E-06

TUNGSTEN

JAA=11 JMAX=11

TC	VC	PC	EC		
2.6037E+04	1.7646E-01	2.3899E-02	7.0744E-02		
TEMP	VMX	VMN	EVHX	EVHN	PRES
2.4081E+04	4.0984E-01	1.0331E-01	7.5240E-02	5.5210E-02	1.6294E-02
2.2125E+04	6.8493E-01	8.7873E-02	7.3553E-02	4.6823E-02	1.0563E-02
2.0169E+04	1.1364E+00	7.9365E-02	7.0964E-02	4.0270E-02	6.4337E-03
1.8213E+04	1.9608E+00	7.3855E-02	6.8027E-02	3.4908E-02	3.6170E-03
1.6257E+04	3.5714E+00	7.0126E-02	6.4945E-02	3.0457E-02	1.8276E-03
1.4301E+04	7.6923E+00	6.8634E-02	6.1899E-02	2.7022E-02	7.9780E-04
1.2344E+04	1.6667E+01	6.7114E-02	5.8886E-02	2.3577E-02	2.8077E-04
1.0388E+04	5.0000E+01	6.5020E-02	5.6056E-02	1.9861E-02	7.0619E-05
8.4322E+03	2.5000E+02	6.2539E-02	5.3429E-02	1.5990E-02	1.3554E-05
6.4761E+03	2.5000E+03	6.0096E-02	5.1038E-02	1.2214E-02	1.0055E-06

GOLD

JAA=11 JMAX=10

TC	VC	PC	EC		
1.8797E+04	1.7282E-01	1.6429E-02	3.3677E-02		
TEMP	VMX	VMN	EVHX	EVHN	PRES
1.7267E+04	4.0486E-01	1.0277E-01	3.7348E-02	2.5207E-02	1.1008E-02
1.5737E+04	6.8493E-01	8.8731E-02	3.7975E-02	2.1248E-02	6.9990E-03
1.4208E+04	1.1494E+00	8.1037E-02	3.7184E-02	1.8254E-02	4.1583E-03
1.2678E+04	2.0408E+00	7.6161E-02	3.6171E-02	1.5828E-02	2.2551E-03
1.1148E+04	4.0000E+00	7.2833E-02	3.4970E-02	1.3777E-02	1.0759E-03
9.6185E+03	9.0909E+00	7.0423E-02	3.3659E-02	1.1986E-02	4.2498E-04
8.0888E+03	2.5000E+01	6.8537E-02	3.2295E-02	1.0385E-02	1.2517E-04
6.5591E+03	1.1111E+02	6.7249E-02	3.0943E-02	8.9317E-03	2.3185E-05
5.8294E+03	5.0000E+02	6.6050E-02	2.9630E-02	7.4815E-03	2.5477E-06

LEAD

JAA=11 JMAX=9

TC	VC	FC	EC		
7.0133E+03	2.7138E-01	3.7027E-03	1.1552E-02		
TEMP	VMX	VMN	VMX	VMN	PRES
6.4448E+03	6.4103E-01	1.6103E-01	1.3131E-02	8.5541E-03	2.4717E-03
5.8763E+03	1.0870E+00	1.3928E-01	1.3193E-02	7.2017E-03	1.5674E-03
5.3078E+03	1.8182E+00	1.2771E-01	1.2987E-02	6.2033E-03	9.2995E-04
4.7394E+03	3.2258E+00	1.2034E-01	1.2665E-02	5.3950E-03	5.0447E-04
4.1709E+03	6.2500E+00	1.1547E-01	1.2269E-02	4.7161E-03	2.4131E-04
3.6024E+03	1.4286E+01	1.1186E-01	1.1933E-02	4.1171E-03	9.5812E-05
3.0339E+03	3.3333E+01	1.0929E-01	1.1368E-02	3.5811E-03	2.8653E-05
2.4654E+03	1.4286E+02	1.0823E-01	1.0911E-02	3.0920E-03	6.2510E-06

THORIUM

JAA=11 JMAX=10

TC	VC	PC	EC		
2.0701E+04	3.5715E-01	7.4418E-03	4.3707E-02		
TEMP	VMX	VMN	VMX	VMN	PRES
1.9036E+04	8.0645E-01	2.1142E-01	4.5197E-02	3.4366E-02	5.1267E-03
1.7372E+04	1.3158E+00	1.7953E-01	4.3403E-02	2.8897E-02	3.3484E-03
1.5707E+04	2.1739E+00	1.6129E-01	4.1249E-02	2.4444E-02	2.0434E-03
1.4042E+04	3.7037E+00	1.4903E-01	3.8951E-02	2.0687E-02	1.1401E-03
1.2378E+04	7.1429E+00	1.4025E-01	3.6678E-02	1.7486E-02	5.6252E-04
1.0713E+04	1.4286E+01	1.3369E-01	3.4426E-02	1.4745E-02	2.3266E-04
9.0485E+03	3.3333E+01	1.2887E-01	3.2299E-02	1.2402E-02	7.3324E-05
7.3839E+03	1.4286E+02	1.2500E-01	3.0341E-02	1.0399E-02	1.7313E-05
5.7193E+03	1.0000E+03	1.1848E-01	2.8551E-02	8.3972E-03	2.0229E-06

MULBERRY

JAA=11 JMAX=10

TC	VC	PC	EC		
2.0338E+04	2.1427E-01	1.2667E-02	4.0268E-02		
TEMP	VMX	VMN	VMX	VMN	PRES
1.8618E+04	4.9751E-01	1.2610E-01	4.2211E-02	3.0854E-02	8.5247E-03
1.6898E+04	8.4036E-01	1.0741E-01	4.0686E-02	2.5544E-02	5.4092E-03
1.5179E+04	1.4286E+00	9.6712E-02	3.8695E-02	2.1261E-02	3.1799E-03
1.3459E+04	2.8641E+00	8.9767E-02	3.6546E-02	1.7704E-02	1.6865E-03
1.1739E+04	5.0000E+00	8.4746E-02	3.4361E-02	1.4676E-02	7.7338E-04
1.0019E+04	1.2500E+01	8.1103E-02	3.2246E-02	1.2097E-02	2.8511E-04
8.2992E+03	3.3333E+01	7.8431E-02	3.0201E-02	9.8874E-03	7.4596E-05
6.5794E+03	1.6667E+02	7.6336E-02	2.8320E-02	7.9763E-03	1.3267E-05
4.8596E+03	1.6667E+03	7.4405E-02	2.6619E-02	6.2721E-03	9.4074E-07

URANIUM

JAA=11 JMAX=10

TC	VC	PC	EC		
1.8759E+04	1.8316E-01	1.2831E-02	3.4251E-02		
TEMP	VMX	VMN	VMX	VMN	PRES
1.7209E+04	4.3290E-01	1.0741E-01	3.6630E-02	2.6058E-02	8.5609E-03
1.5659E+04	7.3529E-01	9.1743E-02	3.5691E-02	2.1675E-02	5.3918E-03
1.4109E+04	1.2658E+00	8.2988E-02	3.4291E-02	1.8220E-02	3.1525E-03
1.2560E+04	2.2727E+00	7.7399E-02	3.2685E-02	1.5384E-02	1.6685E-03
1.1010E+04	4.5455E+00	7.3475E-02	3.1020E-02	1.2989E-02	7.6812E-04
9.4597E+03	1.0000E+01	7.0621E-02	2.9345E-02	1.0940E-02	2.8741E-04
7.9097E+03	3.3333E+01	6.8540E-02	2.7745E-02	9.1714E-03	7.7622E-05
6.3598E+03	1.4286E+02	6.7069E-02	2.6224E-02	7.6437E-03	1.4276E-05
4.8099E+03	1.2500E+03	6.5147E-02	2.4833E-02	6.1259E-03	1.2119E-06

APPENDIX A

The following listing contains the critical point and tie line calculations required for the computation of the equation of state in the liquid-vapor region. This was introduced as a subroutine in the WONDY hydrodynamic code at Livermore. COMMON statements are needed to join common variables in the GRAY EOS subroutine and in this subroutine. Also, in cases where several different materials may enter the two-phase region, the critical point and tie line parameter (Table I), including JAA and JMAX, must be subscripted

according to the material layer being described. The index JAA must be given a value, as required by the first statement in the listing.

Attached to this listing are two subprograms for pressure (PT) and energy (ET) according to the GRAY EOS. These subprograms contain only the liquid and vapor portions of GRAY, since the solid EOS is not needed in the two-phase construction. These subprograms also need COMMON statements joining them with the GRAY subroutine.

MAIN SUBROUTINE

```

C      CALCULATION OF CRITICAL POINT
      JAB=JAA+1
      AJAA=JAA
      NK=9
      NK1=NK-1
      NK2=NK-2
      NK3=NK-3
      DELT=T-2.0*TM0
      DELV=3.0*V0S/20.
      VIN=V0S
      VCEST=4.5*V0S
      IR=1
      IT=1
112  IT=IT+1
      V=VIN
      P1=PT(V,T)
      JVC=(VCEST-V)/DELV
      DO 110 J=1,JVC
      V=V+DELV
      P2=PT(V,T)
      IF((P2-P1)/DELV) ,111,111
110  P1=P2
      IR=IR+1
      IF(IR-2) ,123
      DELV=0.7*DELV
      GO TO 112
123  DELT=.5*DELT
      T=T-DELT
      IR=1
      GO TO 112
111  IF(IT-100) ,115,115
      T=T+DELT*.5
      VIN=V-2.*DELV
      GO TO 112
115  TC=T
      VC=V
      ECC=ET(V,T)
      PC=P2
      WRITE(3,FMT88)TC,VC,PC,ECC
      WRITE(3,FMT9)
C      COEXISTENCE CALCULATION
      DO 100 J=2,JAB
      AJ=J-1
      T=TC-AJ*(TC-TM0)/AJAA
      DELRHO=0.0125*RHO0*AP0
      RHO=.0
      P1=.0
      K1=1
      DO 20 K=1,100
      RHO=RHO+DELRHO
      V=1.0/RHO
      P2=PT(V,T)
      IF((P2-LE.P1).AND.(K1.EQ.2))GO TO 20
      IF(P2.GT.P1)GO TO 12
      PMAX=P1
      K1=2
      GO TO 20
12  IF(K1.EQ.1)GO TO 20
      PMIN=P2
      GO TO 16
20  P1=P2
16  PEQ=.5*(PMAX+PMIN)
      IF(PEQ.GT.0)GO TO 22
      PEQ=.5*PMAX
22  DO 25 KIT=1,50
      DO 300 K=1,NK2
      DO 400 L=1,9
      AL=L
      V=(10.**((NK-K))/AL
      RHO=1./V
      P1=PT(V,T)
      IF(P1-GE.PEQ)GO TO 41
400  CONTINUE
300  CONTINUE
      K=NK1
      DO 45 L=10,2500
      AL=L
      V=100.0/AL
      RHO=1./V
      P1=PT(V,T)
      IF(P1-GE.PEQ)GO TO 41
45  CONTINUE
41  RHOMIN=RHO
      SUM2=.0
      IN=1
      IF(K.GT.NK3)GO TO 53
      DO 55 KK=K,NK3
      DELRHO=1.0/(10.0**((NK-KK)))
      DO 60 LL=L,10
      AL=LL
      RHO=AL*DELRHO
      V=1.0/RHO
      P1=PT(V,T)
      F=P1-PEQ
      SUM2=SUM2+F*DELRHO/RHO**2
      IF(F.LE.0.)IN=2

```

MAIN SUBROUTINE (continued)

```

60 CONTINUE
55 L=1
53 DO 65 LL=L,2500
  DELRHO=.01
  AL=LL
  RHO=AL/100.
  V=1.0/RHO
  P1=PT(V,T)
  F=(P1-PEQ)
  SUM2=SUM2+F*DELRHO/RHO**2
  IF (IN.EQ.2)GO TO 64
  IF (F.GE.0)GO TO 65
  IN=2
64 IF (F.GE.0)GO TO 62
65 CONTINUE
62 RHOMAX=RHO
  IF (KIT.GE.2)GO TO 68
  PEQ1=PEQ
  IF (SUM2.LT.0)GO TO 72
  PEQ2=PEQ1+.1*(PMAX-PEQ1)
71 PEQ=PEQ2
  SUM1=SUM2
  GO TO 25
72 IF (PMIN.LE.0)PMIN=0.
  PEQ2=PEQ1-.1*(PEQ1-PMIN)
  GO TO 71

```

```

68 IF (ABS(F*(SUM1-SUM2)-1.0E-6)69,69,
  PEQ3=(SUM2*PEQ1/SUM1-PEQ2)/(SUM2/SUM1-1.)
  IF (PEQ3.LT.0)PEQ3=.5*PEQ2
  PEQ=PEQ3
  PEQ1=PEQ2
  PEQ2=PEQ3
  SUM1=SUM2
25 CONTINUE
69 VHM(J)=VH=1./RHOMAX
  VHX(J)=VX=1./RHOMIN
  PRES(J)=PEQ
  TEMP(J)=T
  EVHM(J)=EM=ET(VM,T)
  EVHX(J)=EX=ET(VX,T)
  IF (PEQ-1.E-5)9,9,
100 WRITE (3,FMT88)T,RHOMIN,RHOMAX,EM,EX,PEQ
  J=JAB
9 JMAX=J
  WRITE (3,FMT88)T,RHOMIN,RHOMAX,EM,EX,PEQ
  VHX(1)=VHM(1)=VC
  EVMX(1)=EVHM(1)=ECC
  PRES(1)=PC
  TEMP(1)=TC
FMT9 FORMAT(///)
*MT88 FORMAT(6E15.6)

```

PRESSURE SUBPROGRAM

```

FUNCTION PT(V,T)
  XM=9.38
  TSQ=T*T
  IF (V.GT.VJ) GO TO 2
  X=(VBS-V)/VBS
  XSQ=X*X
  IF (X.GT.0) GO TO 12
  TM=TM0*(1.+(G0M2-8./3.)*X+((G0M2-5./3.)*(G0M-4./3.))
  1-AM)*XSQ)/(1.0-X)**2
  GO TO 13
12 TM=TM0*(1.+(G0M2-2./3.)*X+((G0M-1./3.)*(G0M2+1./3.))
  1-AM)*XSQ)
13 SX=S*X
  EQ=(C*X)**2*(1.+SX/3.+(SX*SX)*(1.-G0M/S)/6.)
  1/(2.* (1.-SX))+EQ0*(1.+G0M*X)+EQH
  AX=AM*X
  GM=G0M-AX
  D=-2.*GM+2./3.
  TG=XM*TM
  VBSMX=VBS*(1.-X)
  IF (T.GT.TG) GO TO 15
  E=EQ+TM*(DSP-.5*AP)+(GP2-.5*AP/TM)*TSQ+3.*RP*T
  PC=(.5*(GAMMAE-G0M+AX)*GP*TSQ-TM*(DSP-.5*AP*
  1(1.+TSQ/TM**2))*(D+G0M-AX))/VBSMX
  GO TO 16
15 E=EQ+TM*(DSP-.5*AP*(1.-XM**2))+3.0*RP*T
  1-XM*AP*T+GP2*T**2
  PC=(.5*(GAMMAE-G0M+AX)*GP*TSQ-TM*(DSP-.5*AP*
  1(1.0-XM**2+2.0*XM*T/TM))*(D+G0M-AX))/VBSMX
16 P1=(C**2)*X*(1.-(1.+5*G0M)*X+.5*AM*XSQ)/
  1(VBSMX*(1.-SX)**2)+(G0M-AX)*(E-EQH)/VBSMX
  PT=P1+PC+PCC
  RETURN
2 Z=VB/V
  ZSQ=Z*Z
  FP=(Z*(TH-ZJ)/(ZJ*(TH-Z)))**3
  ZFAC=Z*(1.+Z+ZSQ-Z*ZSQ)/(1.-Z)**3
  PT=(RP*T*ZFAC/VB)-AYP*ZSQ/(VB*VB)+FP*(C1+C2*T
  1+C3*TSQ)
  RETURN
END

```

ENERGY SUBPROGRAM

```

FUNCTION ET(V,T)
  XM=9.38
  TSQ=T*T
  IF (V.GT.VJ) GO TO 2
  X=(VBS-V)/VBS
  XSQ=X*X
  IF (X.GT.0) GO TO 12
  TM=TM0*(1.+(G0M2-8./3.)*X+((G0M2-5./3.)*(G0M-4./3.))-AM)*XSQ)/(1.-X)**2
  GO TO 13
12 TM=TM0*(1.+(G0M2-2./3.)*X+((G0M-1./3.)*(G0M2+1./3.))
  1-AM)*XSQ)
13 SX=S*X
  EQ=(C*X)**2*(1.+SX/3.+SX*SX*(1.-G0M/S)/6.)
  1/(2.* (1.-SX))+EQ0*(1.+G0M*X)+EQH
  TG=XM*TM
  IF (T.GT.TG) GO TO 15
  ET=EQ+TM*(DSP-.5*AP)+(GP2-.5*AP/TM)*TSQ+3.*RP*T
  RETURN
15 ET=EQ+TM*(DSP-.5*AP*(1.0-XM**2))+3.0*RP*T
  1-XM*AP*T+GP2*TSQ
  RETURN
2 Z=VB/V
  ZJC=ZJ**3
  FE=(.5*VB)*(TH-ZJ)**3*(2.*Z-2.+TH)/
  1(ZJC*(TH-ZJ)**2)-(TH-ZJ)*(2.*ZJ-2.+TH)/ZJC
  ET=.5*RPD2*T-(C3*FE-GP2)*TSQ-AYP*Z/VB+C1*FE+D1
  RETURN
END

```


APPENDIX B

The following listing is to be inserted into the GRAY EOS subroutine so that the two phase liquid-vapor equilibrium may be computed. This coding makes use of the critical point and tie line calculations of Appendix A to determine whether an energy-volume point lies inside the two-phase region, and if so, to compute P(V,E). In the GRAY subroutine used in the WONDY hydrodynamic code, this insert comes just before the computation of the pressure according to the various parts of GRAY. A complete listing of GRAY as used in WONDY may be found in the report "Thermo-

Mechanical Response of Porous Carbon" (A.C. Holt, A.S. Kusubov, D.A. Young and W.H. Gust, LLL Rpt. UCRL-51330 (1973)). The insert goes between the statements (p. 67 of the above report) "IF(CARBON.EQ.1) GO TO 100" and "IF(E.LE.EM2) GO TO MELT". The two statements lying between these statements in the report are included in the insert in modified form. Once again, if several materials are being considered, the tie line parameters must be subscripted according to the material layer.

```

IF(V.LE.1.04*VPS) GO TO 124
EV=VMAX(2)
IF(E.GE.1.2*EV) GO TO 125
VXM1=VMM1-VMM(1)
EXM1=EVM1-EVM(1)
EEQM1=EVM1+(EV-EVM(2))*(V-VMM1)/(VMAX(2)-VMM(2))
DO 130 J=2,JMAX
VX=VMAX(J)
EX=EVMX(J)
VM=VMM(J)
EV=EVM(J)
EEQ=EV+(EX-EV)*(V-VM)/(VX-VM)
IF(E.LT.EEQ) GO TO 131
EBH=EV+(EVM1-EV)*(V-VM)/(VMM1-VM)
IF(E.GE.EBH) GO TO 125
EBL=EX+(EX-EXM1)*(V-VX)/(VX-VXM1)
IF(E=EBL) 133,125,125
131 EEQM1=EEQ
VXM1=VX
VMM1=VM
EXM1=EX
EVM1=EV

```

```

130 CONTINUE
J=JMAX
EBL=EX+VX/V
IF(E.GE.EBL) GO TO 125
SLEN=EV/(0.96/VPS-1.0/VM)
EBH=EV+SLEN*(1.0/V-1.0/VM)
IF(E.GE.EBH) GO TO 124
TEM1=TEMP(J-1)
TE=TEMP(J)
T=(E/EEQM1)*(TE-300.)*300.
ST=BHVAPOR
GO TO 134
133 ST=BHVAPOR
ERAT=(EEQM1-E)/(E-EEQ)
TE=TEMP(J)
TEM1=TEMP(J-1)
T=(TE+ERAT+TEM1)/(1.+ERAT)
134 PQ=PRES(J)
SLPR=LOGF(PRES(J-1)/PQ)/(1./TEM1-1./TE)
PS=PQ*EXP(SLPR*(1.0/T-1.0/TE))
GO TO RTN
125 IF(X.LT.XJ) GO TO VAPR
124 IF(E.LE.EMI) GO TO SOLID

```

APPENDIX C

A log-log plot of pressure-density isotherms is shown here for each of the sixteen metals in the GRAY report (Ref. 1). The liquid-vapor region is emphasized. The temperatures of the adjacent isotherms are 2000°K apart and the highest and lowest isotherms are labelled

in degrees Kelvin. Zigzags in the high density isotherms represent melting. Mismatching of isotherms at the two-phase boundary may be seen near the critical point in some of the plots.

Beryllium

Aluminum

Titanium

Nickel

Monel

Niobium

Thorium

Mulberry

Uranium