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An Equation of State for Sodium Over an Extended
Temperature and Density Range*

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Abstract

Coupled neutronics and hydrodynamic calculations of hypothetical core disruptive accidents of a liquid-metal fast breeder reactor require realistic equations of state of the relevant component materials over a very large range of temperature and density. This paper describes the methods used to construct a general equation of state for sodium that will be utilized in tabular form by a complex computer code under development at Los Alamos Scientific Laboratory for the assessment of reactor safety. The technique considers pressure to be the sum of a "cold pressure" determined by the cohesive energy of the solid and a thermal term that varies from resembling that in a solid at normal density to ideal gas behavior at low density. Since the predicted critical point data and vapor pressure as a function of temperature are in reasonable agreement with experiment we can have some confidence in the general shape of the isotherms; calculated vapor pressures are then supplanted by experimental values. Tabular data are presented for density from 10^{-5} to 1.2 times the normal density of the solid and for temperature from 300 K to 4000 K.

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I. Introduction

Coupled neutronics and hydrodynamic calculations of hypothetical core disruptive accidents of a liquid-metal fast breeder reactor (LMFBR) require realistic equations of state of the relevant component materials over a very large range of temperature and density. The most severe hypothetical accidents may elevate the fuel temperature to, say, 10,000 K and the coolant to well above its critical value of about 2700 K. Pressures of several tenths of a gigapascal ($1 \text{ GPa} = 10^4 \text{ bar}$) may be developed, leading to the possibility of shock compression of the materials above their normal operating density; under expansion the substances can enter the regime where behavior is essentially that of an ideal gas. This paper describes the methods used to construct a general equation of state for sodium that will be utilized in tabular form by a complex computer code under development at Los Alamos Scientific Laboratory for the assessment of reactor safety. The thermodynamic properties we derive are pressure and internal energy as functions of density and temperature, which is the formulation most useful to the code as it is being structured.

In constructing the tabular data we have used a phenomenological approach that yields, for a number of metals, reasonable agreement in predicted critical point data and vapor pressure as a function of temperature. The agreement is also fairly good in the case of sodium. It is possible therefore to have some confidence in the general shape of the pressure isotherms. Calculated vapor pressures are then supplanted by experimental values.

The range of density considered is from 10^{-5} to 1.2 times the normal density of the solid; the temperature range is from 300 K to 4000 K.

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II. Procedure

Equations of state for substances under compression usually contain an expression for a "cold curve", or pressure as a function of density at zero temperature, and to this is added thermal terms arising from lattice vibrations and electronic excitation. Use can be made of the concept of a cold curve at extended volumes also: if for a given atom the net interaction with all other atoms in the sample is one of attraction we consider the "pressure", or average interactive force per unit area of the atomic sphere, to be negative.

A formula for the cold curve that proves useful in constructing equations of state for compressed materials [1] is

$$P_c(\eta) = a\eta^{2/3} \left(\eta e^{b_r \nu} - e^{b_a \nu} \right) , \quad (1)$$

where the compression $\eta = \rho/\rho_0$, or the ratio of density to the normal zero-temperature density of the solid, and $\nu = 1 - \eta^{-1/3}$. The parameters a , b_r , and b_a are obtained from the experimental bulk modulus and solutions of the Thomas-Fermi-Dirac equation (or a suitable modification thereof), as discussed in the above reference. The corresponding energy in compression along the cold curve is given by

$$E_c(\eta) = \frac{1}{\rho_0} \int_1^\eta P_c(\eta') \frac{d\eta'}{\eta'^2} , \quad (2)$$

which can be evaluated in terms of the exponential integral.

A test of Eq. (1) in the compressive region is to compare the calculated shock Hugoniot with experimental data. In our notation, the

Hugoniot pressure, or pressure immediately behind a shock front, is given by the expression

$$P_H = \frac{P_c - \gamma_G \rho_o \eta E_c}{1 - \gamma_G (\eta - 1)/2} \quad (3)$$

where the undisturbed state is assumed to be at zero pressure and energy. In Eq. (3) the Grüneisen ratio, γ_G , relates thermal pressure P_θ to thermal energy E_θ at any compression:

$$P_\theta = \eta \rho_o \gamma_G E_\theta \quad (4)$$

At normal density the Grüneisen ratio is given by

$$\gamma_G (\eta = 1) = \frac{\alpha B_s}{\rho_o c_p} \quad (5)$$

where α is the volume coefficient of expansion, B_s is the adiabatic bulk modulus and c_p the heat capacity at constant pressure.

Substitution of accepted values for the physical properties in Eq. (5) leads at normal density to the value $\gamma_G = 1.17$. [2] Provided the temperature is less than 10^4 K or so, the Grüneisen ratio can usually be treated as a function of volume alone. In calculating the Hugoniot, we have assumed a simple dependence on compression that is commonly used in shock-wave work:

$$\gamma_G (\eta) = \frac{1.17}{\eta} \quad .$$

In Fig. 1 we compare our calculated Hugoniot curve with the smoothed experimental data of Rice. [2] The fairly good agreement substantiates the general form of Eq. (1). It is then of interest to extend the cold curve to $\eta < 1$ (as we have also shown in the figure) and here to require that the energy to expand to $\eta = 0$, as given by Eq. (2), be equal to the known heat of solidification of sodium from the vapor. This condition can easily be met, and the continuity of slope at $\eta = 1$ retained, by a simple adjustment of the parameters b_r and b_a . In Fig. 1 we have then shown the result of this calculation. The total energy of separation is taken as 26.04 kcal/mol.

The thermal contribution to pressure should approach that of an ideal gas of monatomic sodium vapor at low density (although we may in further work want to allow for possible ionization), and we therefore attempt to describe total pressure in the regime $\eta < 1$ with the expression

$$P(\eta, T) = P_c(\eta) + RT \left[\eta \rho_0 + b(T) \eta^2 + c(T) \eta^3 \right] , \quad (6)$$

where R is the gas constant divided by atomic weight, and $b(T)$ and $c(T)$ are determined by joining smoothly to the given isotherm for the solid¹ at $\eta = 1$. The thermal energy of the solid at normal density is written as

$$E_\theta = 3RD_e(x)T ,$$

¹Actually, of course, even at normal solid density the material is more properly described as a liquid at sufficiently high temperature. We have not differentiated at this density between thermal properties of a solid and of a liquid.

where $x = \theta_D/T$ and $D_e(x)$ is the Debye energy function for the Debye temperature θ_D . We can therefore write for the pressure in a solid

$$P(\eta, T) = P_c(\eta) + \eta \rho_o \gamma_G 3RT D_e(x) T \quad (7)$$

from which we obtain

$$\left. \frac{\partial P}{\partial \eta} \right)_{\eta=1} = B_o + \rho_o \gamma_o 3RT \left[D_e(x) + \frac{\partial D_e(x)}{\partial \eta} \right] \quad (8)$$

We have denoted the bulk modulus at zero degrees by B_o and γ_o is the value of the Grüneisen parameter at $\eta = 1$. In the present calculations we have set $\frac{\partial \gamma_G}{\partial \eta} = 0$ since we know that in some manner γ_G decreases from γ_o as η either decreases or increases from unity. This actually produces a slight cusp in our isotherms at normal density, and is a matter for further investigation.

The second term in the brackets is evaluated from the definitions of the Debye function and the Grüneisen parameter as

$$\left. \frac{\partial D_e(x)}{\partial \eta} \right)_{\eta=1} = 3\gamma_o x \left[\frac{1}{e^x - 1} - \frac{D_e(x)}{x} \right]$$

For matching to the imperfect gas, from Eq. (6) we have

$$\left. \frac{\partial P}{\partial \eta} \right)_{\eta=1} = B_o + RT \left[\rho_o + 2b(T) + 3c(T) \right] \quad (9)$$

For each isotherm, through equating the pressures at $\eta = 1$ as given by Eqs. (6) and (7), and the derivatives as given by Eqs. (8) and (9) the coefficients $b(T)$ and $c(T)$ are easily evaluated.

Pressure isotherms generated by Eq. (6) display a critical point below which they possess the familiar Van der Waals form. In order to show the general validity of the approach we show in Table I the critical temperatures calculated for a few metals and reported earlier [3]. In the table we compare our results with those predicted by Young and Alder [4] on a hard-sphere/Van der Waals model, and with Grosse and coworkers' estimates based on extrapolation of various experimental data, as quoted in the preceding reference.

For detailed calculations on sodium we have used the input parameters listed in Table II. With this input, using our standard techniques for calculating the cold curve we calculate a critical temperature of 2727 K, a pressure of 0.0378 GPa and a density of 0.116 g/cm^3 . These are in fair agreement with the best estimates from experimental data [5]. Somewhat better agreement in critical pressure and density can be obtained by altering the cold curve slightly. In Fig. 2 we compare $P_c(\eta)$, computed from Eq. (1) with parameters prescribed according to considerations discussed above, with the curve that results from ascribing 3% of the binding energy to a longer-range force so that the cold curve has an additional term falling off as η^3 . (The total binding energy is preserved.) In this manner we have obtained the values shown in Table III, where we have also listed the best experimental estimates as cited above.

Below the critical temperature a Maxwell equal-area construction, carried out numerically for each isotherm, yields the corresponding vapor pressure. In Fig. 3 we compare two calculated vapor pressures with the experimental or estimated values in a general depiction of typical calculated isotherms. Over a very wide range of vapor pressure the calculated

values never depart far from experiment; at 1000 K the calculated value is 7.2×10^{-6} GPa as compared to the experimental value of 1.8×10^{-5} GPa. Since the vapor saturation density at 1000 K is calculated to be about 2×10^{-5} g/cm³, the Maxwell construction has been performed over such a range that the shape of the isotherm as given by Eq. (6) has been rather severely tested.

Actually, the experimental vapor pressures, adjusted to terminate at our calculated critical point have been entered into our tabular equation of state as finally constructed and presented here. To complete the hydrodynamic description we require the specific internal energy; this is calculated along each isotherm through integration of the basic thermodynamic relation

$$P = \rho_0 \eta^2 \left(\frac{\partial E}{\partial \eta} \right)_T + T \left(\frac{\partial P}{\partial T} \right)_\eta .$$

At the higher temperatures an error in our formulation, and an area for improvement, become apparent. The thermal energy, which above the critical isotherm is easily seen to be given by

$$E_\theta = - \frac{1}{\rho_0} \int_1^\eta RT^2 \left[\frac{\partial b}{\partial T} \eta^2 + \frac{\partial c}{\partial T} \eta^3 \right] \frac{d\eta}{\eta^2} + E_\theta(\eta = 1)$$

$$= \frac{RT^2}{\rho_0} \left[\frac{\partial b}{\partial T} (1 - \eta) + \frac{1}{2} \frac{\partial c}{\partial T} (1 - \eta^2) \right] + E_\theta(\eta = 1) ,$$

cannot possibly reduce as $\eta \rightarrow 0$ to the ideal gas value unless $\frac{\partial b}{\partial T}$ or $\frac{\partial c}{\partial T}$ are negative. From our calculations this can only occur if γ_G is allowed to decrease with increasing temperature. Although this in fact is known

to happen, we do not know the relationship; it seems preferable at this time to work with a thermodynamically consistent equation of state even if there is a known error of this sort.

The resulting equation of state is given in Table IV.

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TABLE I
CRITICAL TEMPERATURE (K)

<u>Element</u>	<u>Calc.</u>	<u>Young & Alder</u>	<u>Exper/Grosse</u>
Al	8480	7151	8550
Ni	9133	9576	6000
Pt	13704	12526	14650
Mo	18966	14588	17000

TABLE II

INPUT PARAMETERS FOR SODIUM EQUATION OF STATE

Atomic Number	$Z = 11$
Atomic Weight	$Z = 22.9898$
Density at Zero Kelvin	$\rho_0 = 1.011 \text{ g/cm}^3$
Bulk Modulus	$B_0 = 7.70 \text{ GPa}$
Binding Energy	$E_{\text{coh}} = 26.04 \text{ kcal/mol}$
Grüneisen Ratio	$\gamma_G = 1.17$
Debye Temperature	$\theta_D = 158 \text{ K}$

TABLE III

CALCULATED CRITICAL CONSTANTS AND EXPERIMENTAL ESTIMATES

	<u>Calculated</u>	<u>Estimated</u>
Temperature (K)	2738.	2733.
Pressure (GPa)	0.0421	0.0413
Density (g/cm ³)	0.136	0.1796

TABLE IV

SODIUM EQUATION OF STATE

COMPRESSION	T = 300 K			T = 500 K		
	PRESSURE (GPA)	ENERGY (KJ/G)		PRESSURE (GPA)	ENERGY (KJ/G)	
.00001	5.451E-18	2.405E-10		7.608E-11	5.117E-01	
.00002	5.451E-18	2.294E-10		7.608E-11	5.116E-01	
.00005	5.451E-18	1.905E-10		7.608E-11	5.116E-01	
.00010	5.451E-18	1.795E-10		7.608E-11	5.115E-01	
.00020	5.451E-18	1.744E-10		7.608E-11	5.115E-01	
.00050	5.451E-18	1.714E-10		7.608E-11	5.115E-01	
.00100	5.451E-18	1.704E-10		7.608E-11	5.115E-01	
.00200	5.451E-18	1.699E-10		7.608E-11	5.115E-01	
.00500	5.451E-18	1.696E-10		7.608E-11	5.115E-01	
.01000	5.451E-18	1.695E-10		7.608E-11	5.115E-01	
.02000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.05000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.10000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.15000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.20000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.25000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.30000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.35000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.40000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.45000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.50000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.55000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.60000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.65000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.70000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.75000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.80000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.85000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.90000	5.451E-18	1.694E-10		7.608E-11	5.115E-01	
.95000	7.493E-11	1.582E-10		1.907E-01	4.947E-01	
1.00000	3.143E-01	2.657E-01		5.689E-01	4.809E-01	
1.05000	7.202E-01	2.719E-01		9.745E-01	4.869E-01	
1.10000	1.174E+00	2.959E-01		1.428E+00	5.107E-01	
1.15000	1.674E+00	3.365E-01		1.928E+00	5.511E-01	
1.20000	2.217E+00	3.924E-01		2.470E+00	6.067E-01	

TABLE IV (continued)

COMPRESSION	T= 750 K		T=1000 K	
	PRESSURE (GPA)	ENERGY (KJ/G)	PRESSURE (GPA)	ENERGY (KJ/G)
.0001	2.843E-07	1.259E+00	3.657E-06	5.265E+00
.0002	2.843E-07	1.042E+00	7.313E-06	5.265E+00
.0005	2.843E-07	9.118E-01	1.737E-05	5.060E+00
.0010	2.843E-07	8.683E-01	1.737E-05	3.112E+00
.0020	2.843E-07	8.466E-01	1.737E-05	2.138E+00
.0050	2.843E-07	8.336E-01	1.737E-05	1.553E+00
.0100	2.843E-07	8.292E-01	1.737E-05	1.358E+00
.0200	2.843E-07	8.271E-01	1.737E-05	1.261E+00
.0300	2.843E-07	8.258E-01	1.737E-05	1.203E+00
.0500	2.843E-07	8.253E-01	1.737E-05	1.183E+00
.0600	2.843E-07	8.251E-01	1.737E-05	1.173E+00
.0800	2.843E-07	8.250E-01	1.737E-05	1.167E+00
.1000	2.843E-07	8.249E-01	1.737E-05	1.165E+00
.1500	2.843E-07	8.249E-01	1.737E-05	1.165E+00
.2000	2.843E-07	8.249E-01	1.737E-05	1.165E+00
.2500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.3000	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.3500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.4000	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.4500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.5000	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.5500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.6000	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.6500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.7000	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.7500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.8000	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.8500	2.843E-07	8.249E-01	1.737E-05	1.164E+00
.9000	1.597E-01	7.980E-01	1.515E-01	1.122E+00
.9500	4.941E-01	7.649E-01	4.461E-01	1.065E+00
1.0000	8.887E-01	7.513E-01	7.980E-01	1.036E+00
1.0500	1.294E+00	7.571E-01	1.209E+00	1.022E+00
1.1000	1.748E+00	7.808E-01	1.614E+00	1.028E+00
1.1500	2.247E+00	8.211E-01	2.068E+00	1.052E+00
1.2000	2.789E+00	8.767E-01	2.567E+00	1.092E+00
			3.109E+00	1.147E+00

TABLE IV (continued)

COMPRESSION	T=1250 K		T=1500 K	
	PRESSURE (GPA)	ENERGY (KJ/G)	PRESSURE (GPA)	ENERGY (KJ/G)
.00001	4.571E-06	5.410E+00	5.485E-06	5.748E+00
.00002	9.142E-06	5.410E+00	1.097E-05	5.748E+00
.00005	2.286E-05	5.410E+00	2.743E-05	5.748E+00
.00010	4.573E-05	5.410E+00	5.487E-05	5.748E+00
.00020	9.150E-05	5.410E+00	1.098E-04	5.748E+00
.00050	2.002E-04	4.921E+00	2.749E-04	5.748E+00
.00100	2.002E-04	3.227E+00	5.511E-04	5.748E+00
.00200	2.002E-04	2.380E+00	9.848E-04	5.331E+00
.00500	2.002E-04	1.872E+00	9.846E-04	3.296E+00
.01000	2.002E-04	1.702E+00	9.846E-04	2.617E+00
.02000	2.002E-04	1.617E+00	9.846E-04	2.278E+00
.05000	2.002E-04	1.567E+00	9.846E-04	2.075E+00
.10000	2.002E-04	1.550E+00	9.846E-04	2.007E+00
.15000	2.002E-04	1.544E+00	9.846E-04	1.984E+00
.20000	2.002E-04	1.541E+00	9.846E-04	1.973E+00
.25000	2.002E-04	1.540E+00	9.846E-04	1.966E+00
.30000	2.002E-04	1.538E+00	9.846E-04	1.962E+00
.35000	2.002E-04	1.538E+00	9.846E-04	1.959E+00
.40000	2.002E-04	1.537E+00	9.846E-04	1.956E+00
.45000	2.002E-04	1.536E+00	9.846E-04	1.954E+00
.50000	2.002E-04	1.536E+00	9.846E-04	1.953E+00
.55000	2.002E-04	1.536E+00	9.846E-04	1.953E+00
.60000	2.002E-04	1.535E+00	9.847E-04	1.952E+00
.70000	2.002E-04	1.535E+00	9.847E-04	1.950E+00
.75000	2.003E-04	1.535E+00	2.714E-03	1.947E+00
.80000	1.608E-01	1.466E+00	1.827E-01	1.831E+00
.85000	4.197E-01	1.392E+00	4.099E-01	1.737E+00
.90000	7.326E-01	1.339E+00	6.878E-01	1.663E+00
.95000	1.102E+00	1.306E+00	1.019E+00	1.610E+00
1.00000	1.530E+00	1.293E+00	1.406E+00	1.577E+00
1.05000	1.935E+00	1.299E+00	1.850E+00	1.564E+00
1.10000	2.389E+00	1.299E+00	2.256E+00	1.570E+00
1.15000	2.888E+00	1.322E+00	2.709E+00	1.593E+00
1.20000	3.430E+00	1.363E+00	3.209E+00	1.634E+00
		1.418E+00	3.750E+00	1.689E+00

TABLE IV (continued)

COMPRESSION	T=1750 K		T=2000 K	
	PRESSURE (GPA)	ENERGY (KJ/G)	PRESSURE (GPA)	ENERGY (KJ/G)
.0001	6.399E-06	6.348E+00	7.313E-06	6.652E+00
.0002	1.280E-05	6.348E+00	1.463E-05	6.652E+00
.0005	3.200E-05	6.348E+00	3.657E-05	6.652E+00
.0010	6.402E-05	6.348E+00	7.316E-05	6.652E+00
.0020	1.281E-04	6.348E+00	1.464E-04	6.652E+00
.0050	3.207E-04	6.348E+00	3.665E-04	6.652E+00
.0100	6.430E-04	6.348E+00	7.348E-04	6.652E+00
.0200	1.291E-03	6.347E+00	1.476E-03	6.652E+00
.0500	3.145E-03	6.240E+00	3.697E-03	6.649E+00
.01000	3.145E-03	4.315E+00	7.176E-03	6.631E+00
.02000	3.145E-03	3.353E+00	7.722E-03	4.923E+00
.05000	3.145E-03	2.776E+00	7.722E-03	3.711E+00
.10000	3.145E-03	2.583E+00	7.722E-03	3.307E+00
.15000	3.145E-03	2.519E+00	7.722E-03	3.173E+00
.20000	3.145E-03	2.487E+00	7.722E-03	3.105E+00
.25000	3.145E-03	2.468E+00	7.722E-03	3.065E+00
.30000	3.145E-03	2.455E+00	7.722E-03	3.038E+00
.35000	3.145E-03	2.446E+00	7.722E-03	3.019E+00
.40000	3.145E-03	2.439E+00	7.722E-03	3.004E+00
.45000	3.145E-03	2.434E+00	7.722E-03	2.993E+00
.50000	3.145E-03	2.430E+00	7.722E-03	2.984E+00
.55000	3.145E-03	2.426E+00	9.229E-03	2.973E+00
.60000	3.145E-03	2.423E+00	1.103E-01	2.789E+00
.65000	5.656E-02	2.357E+00	2.469E-01	2.628E+00
.70000	2.129E-01	2.219E+00	4.231E-01	2.490E+00
.75000	4.126E-01	2.103E+00	6.425E-01	2.374E+00
.80000	6.592E-01	2.008E+00	9.087E-01	2.279E+00
.85000	9.561E-01	1.935E+00	1.224E+00	2.206E+00
.90000	1.306E+00	1.882E+00	1.592E+00	2.153E+00
.95000	1.710E+00	1.849E+00	2.014E+00	2.120E+00
1.00000	2.171E+00	1.835E+00	2.492E+00	2.106E+00
1.05000	2.576E+00	1.841E+00	2.897E+00	2.112E+00
1.10000	3.030E+00	1.864E+00	3.350E+00	2.136E+00
1.15000	3.529E+00	1.905E+00	3.850E+00	2.176E+00
1.20000	4.071E+00	1.960E+00	4.392E+00	2.231E+00

TABLE IV (continued)

COMPRESSION	T=2250 K		T=2500 K	
	PRESSURE (GPA)	ENERGY (KJ/G)	PRESSURE (GPA)	ENERGY (KJ/G)
.0001	8.227E-06	6.862E+00	9.141E-06	7.079E+00
.0002	1.648E-05	6.862E+00	1.828E-05	7.079E+00
.0005	4.114E-05	6.862E+00	4.572E-05	7.079E+00
.0010	8.231E-05	6.862E+00	9.145E-05	7.079E+00
.0020	1.647E-04	6.862E+00	1.830E-04	7.079E+00
.0050	4.124E-04	6.862E+00	4.582E-04	7.079E+00
.0100	8.267E-04	6.862E+00	9.186E-04	7.079E+00
.0200	1.661E-03	6.861E+00	1.845E-03	7.078E+00
.0500	4.166E-03	6.858E+00	4.634E-03	7.075E+00
.1000	8.135E-03	6.840E+00	9.095E-03	7.057E+00
.2000	1.664E-02	6.771E+00	1.665E-02	6.987E+00
.5000	1.553E-02	4.914E+00	2.716E-02	6.416E+00
1.0000	1.553E-02	4.209E+00	2.716E-02	5.332E+00
1.5000	1.553E-02	3.974E+00	2.716E-02	4.972E+00
2.0000	1.553E-02	3.857E+00	2.716E-02	4.791E+00
2.5000	1.553E-02	3.786E+00	2.716E-02	4.683E+00
3.0000	1.553E-02	3.739E+00	2.716E-02	4.611E+00
3.5000	1.553E-02	3.706E+00	3.225E-02	4.505E+00
4.0000	1.553E-02	3.680E+00	6.753E-02	4.217E+00
4.5000	1.554E-02	3.661E+00	1.232E-01	3.957E+00
5.0000	7.129E-02	3.453E+00	2.031E-01	3.724E+00
5.5000	1.602E-01	3.244E+00	3.112E-01	3.515E+00
6.0000	2.809E-01	3.060E+00	4.514E-01	3.331E+00
6.5000	4.373E-01	2.899E+00	6.276E-01	3.171E+00
7.0000	6.333E-01	2.761E+00	8.435E-01	3.032E+00
7.5000	8.725E-01	2.645E+00	1.102E+00	2.916E+00
8.0000	1.158E+00	2.551E+00	1.407E+00	2.822E+00
8.5000	1.493E+00	2.477E+00	1.761E+00	2.748E+00
9.0000	1.879E+00	2.424E+00	2.166E+00	2.695E+00
9.5000	2.319E+00	2.391E+00	2.623E+00	2.652E+00
1.0000	2.813E+00	2.378E+00	3.133E+00	2.645E+00
1.0500	3.218E+00	2.383E+00	3.539E+00	2.655E+00
1.1000	3.671E+00	2.407E+00	3.992E+00	2.678E+00
1.1500	4.171E+00	2.447E+00	4.491E+00	2.718E+00
1.2000	4.712E+00	2.502E+00	5.033E+00	2.774E+00

TABLE IV (continued)

COMPRESSION	T=2750 K		T=3000 K	
	PRESSURE (GPA)	ENERGY (KJ/G)	PRESSURE (GPA)	ENERGY (KJ/G)
.0J001	1.006E-05	7.732E+00	1.097E-05	8.0C3E+00
.0J002	2.011E-05	7.732E+00	2.194E-05	8.0C3E+00
.0J005	5.029E-05	7.732E+00	5.486E-05	8.0C3E+00
.0J010	1.006E-04	7.732E+00	1.097E-04	8.0C3E+00
.0J020	2.013E-04	7.732E+00	2.196E-04	8.003E+00
.0J050	5.040E-04	7.732E+00	5.498E-04	8.0C3E+00
.0J100	1.010E-03	7.732E+00	1.102E-03	8.0C3E+00
.0J200	2.030E-03	7.732E+00	2.214E-03	8.0C3E+00
.0J500	5.103E-03	7.728E+00	5.571E-03	7.999E+00
.01000	1.005E-02	7.711E+00	1.101E-02	7.982E+00
.02000	1.866E-02	7.641E+00	2.067E-02	7.912E+00
.05000	3.442E-02	7.331E+00	4.011E-02	7.601E+00
.10000	4.230E-02	6.783E+00	5.580E-02	7.054E+00
.15000	4.320E-02	6.286E+00	6.647E-02	6.557E+00
.20000	4.600E-02	5.845E+00	8.081E-02	6.116E+00
.25000	5.570E-02	5.450E+00	1.037E-01	5.721E+00
.30000	7.609E-02	5.096E+00	1.386E-01	5.367E+00
.35000	1.106E-01	4.776E+00	1.890E-01	5.048E+00
.40000	1.629E-01	4.488E+00	2.582E-01	4.759E+00
.45000	2.364E-01	4.228E+00	3.495E-01	4.495E+00
.50000	3.349E-01	3.995E+00	4.666E-01	4.266E+00
.55000	4.621E-01	3.787E+00	6.131E-01	4.058E+00
.60000	6.219E-01	3.603E+00	7.925E-01	3.874E+00
.65000	8.180E-01	3.442E+00	1.008E+00	3.713E+00
.70000	1.054E+00	3.304E+00	1.264E+00	3.575E+00
.75000	1.332E+00	3.188E+00	1.562E+00	3.459E+00
.80000	1.657E+00	3.093E+00	1.906E+00	3.364E+00
.85000	2.030E+00	3.019E+00	2.298E+00	3.291E+00
.90000	2.453E+00	2.966E+00	2.739E+00	3.238E+00
.95000	2.927E+00	2.934E+00	3.232E+00	3.205E+00
1.00000	3.454E+00	2.920E+00	3.775E+00	3.191E+00
1.05000	3.860E+00	2.926E+00	4.180E+00	3.197E+00
1.10000	4.313E+00	2.949E+00	4.634E+00	3.221E+00
1.15000	4.812E+00	2.989E+00	5.133E+00	3.261E+00
1.20000	5.354E+00	3.045E+00	5.675E+00	3.316E+00

TABLE IV (continued)

COMPRESSION	T=3250 K		T=3500 K	
	PRESSURE (GPA)	ENERGY (KJ/G)	PRESSURE (GPA)	ENERGY (KJ/G)
.0001	1.188E-05	8.274E+00	1.280E-05	8.545E+00
.0002	2.377E-05	8.274E+00	2.560E-05	8.545E+00
.0005	5.943E-05	8.274E+00	6.400E-05	8.545E+00
.0010	1.189E-04	8.274E+00	1.280E-04	8.545E+00
.0020	2.379E-04	8.274E+00	2.562E-04	8.545E+00
.0050	5.956E-04	8.274E+00	6.414E-04	8.545E+00
.0100	1.194E-03	8.274E+00	1.286E-03	8.545E+00
.0200	2.399E-03	8.274E+00	2.584E-03	8.545E+00
.0500	6.040E-03	8.270E+00	6.508E-03	8.541E+00
.1000	1.197E-02	8.252E+00	1.293E-02	8.523E+00
.02000	2.268E-02	8.183E+00	2.469E-02	8.454E+00
.05000	4.580E-02	7.872E+00	5.149E-02	8.143E+00
.10000	6.930E-02	7.324E+00	8.280E-02	7.596E+00
.15000	8.973E-02	6.828E+00	1.130E-01	7.099E+00
.20000	1.156E-01	6.387E+00	1.504E-01	6.658E+00
.25000	1.516E-01	5.993E+00	1.996E-01	6.264E+00
.30000	2.012E-01	5.638E+00	2.637E-01	5.909E+00
.35000	2.674E-01	5.319E+00	3.458E-01	5.590E+00
.40000	3.535E-01	5.030E+00	4.488E-01	5.301E+00
.45000	4.627E-01	4.770E+00	5.759E-01	5.041E+00
.50000	5.984E-01	4.537E+00	7.302E-01	4.808E+00
.55000	7.640E-01	4.329E+00	9.150E-01	4.600E+00
.60000	9.630E-01	4.145E+00	1.133E+00	4.416E+00
.65000	1.199E+00	3.984E+00	1.389E+00	4.255E+00
.70000	1.474E+00	3.846E+00	1.684E+00	4.117E+00
.75000	1.792E+00	3.730E+00	2.022E+00	4.001E+00
.80000	2.156E+00	3.635E+00	2.405E+00	3.907E+00
.85000	2.566E+00	3.562E+00	2.835E+00	3.833E+00
.90000	3.026E+00	3.509E+00	3.313E+00	3.780E+00
.95000	3.536E+00	3.476E+00	3.840E+00	3.747E+00
1.00000	4.096E+00	3.463E+00	4.417E+00	3.734E+00
1.05000	4.501E+00	3.468E+00	4.822E+00	3.740E+00
1.10000	4.955E+00	3.492E+00	5.275E+00	3.763E+00
1.15000	5.454E+00	3.532E+00	5.775E+00	3.833E+00
1.20000	5.996E+00	3.587E+00	6.317E+00	3.859E+00

TABLE IV (continued)

COMPRESSION	T=3750 K			T=4000 K		
	PRESSURE (GPA)	ENERGY (KJ/G)		PRESSURE (GPA)	ENERGY (KJ/G)	
.0001	1.371E-05	8.816E+00		1.463E-05	9.019E+00	
.0002	2.743E-05	8.816E+00		2.925E-05	9.019E+00	
.0005	6.857E-05	8.816E+00		7.314E-05	9.019E+00	
.0010	1.372E-04	8.816E+00		1.463E-04	9.019E+00	
.0020	2.745E-04	8.816E+00		2.928E-04	9.019E+00	
.0050	6.873E-04	8.816E+00		7.331E-04	9.019E+00	
.0100	1.378E-03	8.816E+00		1.470E-03	9.019E+00	
.0200	2.768E-03	8.816E+00		2.953E-03	9.019E+00	
.0500	6.977E-03	8.812E+00		7.445E-03	9.015E+00	
.1000	1.389E-02	8.794E+00		1.485E-02	8.958E+00	
.0200	2.670E-02	8.725E+00		2.871E-02	8.620E+00	
.0500	5.718E-02	8.414E+00		6.287E-02	8.076E+00	
.1000	9.630E-02	7.867E+00		1.098E-01	7.583E+00	
.1500	1.363E-01	7.370E+00		1.595E-01	7.145E+00	
.2000	1.852E-01	6.929E+00		2.200E-01	6.753E+00	
.2500	2.475E-01	6.535E+00		2.955E-01	6.402E+00	
.3000	3.262E-01	6.180E+00		3.888E-01	6.086E+00	
.3500	4.242E-01	5.861E+00		5.026E-01	5.801E+00	
.4000	5.441E-01	5.572E+00		6.394E-01	5.545E+00	
.4500	6.891E-01	5.313E+00		8.022E-01	5.315E+00	
.5000	8.619E-01	5.079E+00		9.937E-01	5.110E+00	
.5500	1.066E+00	4.871E+00		1.217E+00	4.930E+00	
.6000	1.304E+00	4.687E+00		1.474E+00	4.772E+00	
.6500	1.579E+00	4.527E+00		1.770E+00	4.632E+00	
.7000	1.894E+00	4.388E+00		2.105E+00	4.525E+00	
.7500	2.252E+00	4.272E+00		2.482E+00	4.434E+00	
.8000	2.654E+00	4.178E+00		2.904E+00	4.365E+00	
.8500	3.103E+00	4.104E+00		3.371E+00	4.315E+00	
.9000	3.599E+00	4.051E+00		3.886E+00	4.286E+00	
.9500	4.144E+00	4.019E+00		4.449E+00	4.276E+00	
1.0000	4.738E+00	4.005E+00		5.058E+00	4.282E+00	
1.0500	5.143E+00	4.011E+00		5.464E+00	4.306E+00	
1.1000	5.596E+00	4.034E+00		5.917E+00	4.346E+00	
1.1500	6.096E+00	4.074E+00		6.416E+00	4.401E+00	
1.2000	6.637E+00	4.130E+00		6.958E+00		

Figure Captions

- Fig. 1. Calculated zero-temperature isotherm and shock Hugoniot for sodium.**
- Fig. 2. Calculated pressure with- and without long-range force.**
- Fig. 3. Calculated pressure isotherms for sodium.**

Fig. 1. Calculated zero-temperature isotherm and shock Hugoniot for sodium.

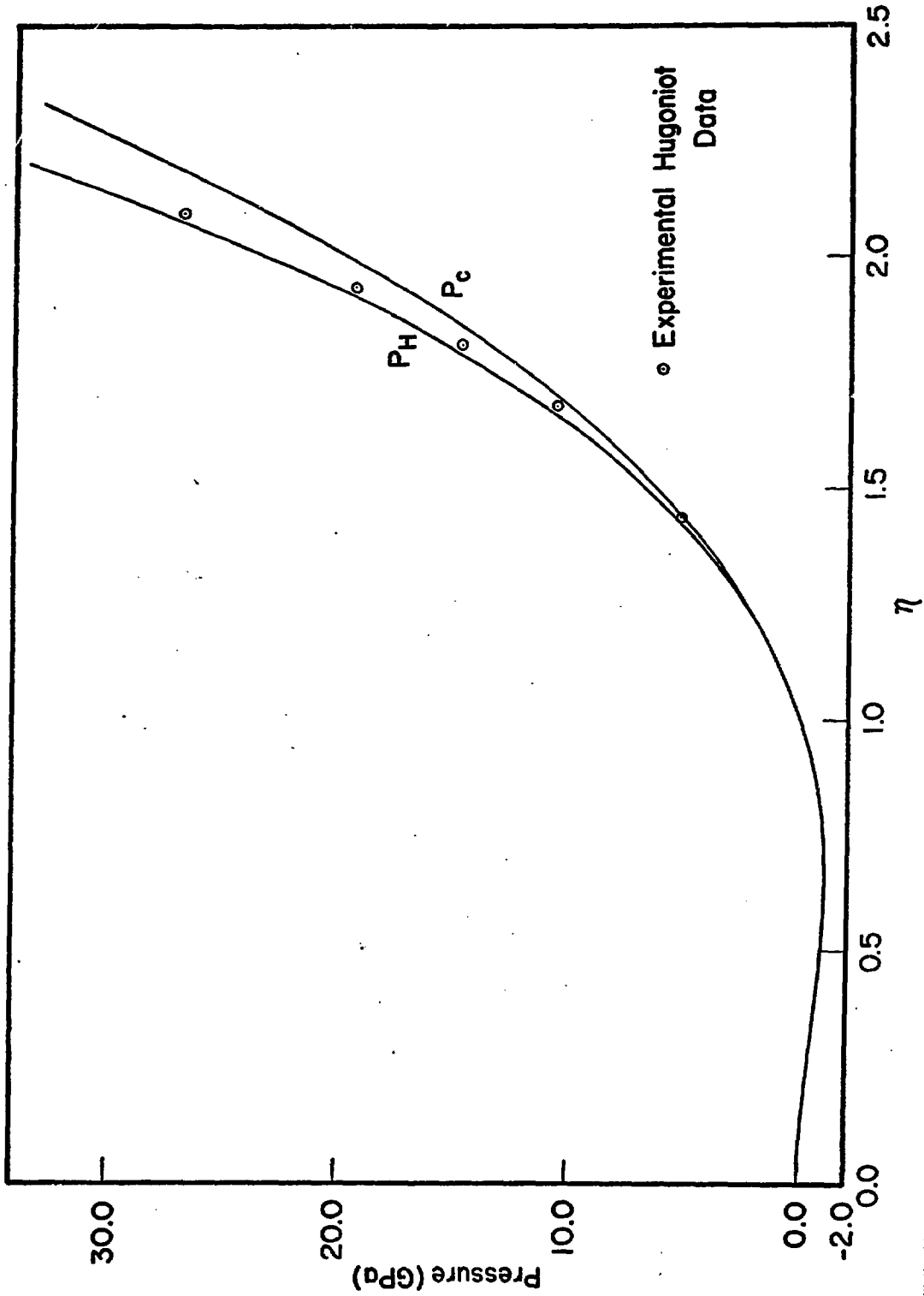


Fig. 2. Calculated pressure with- and without long-range force.

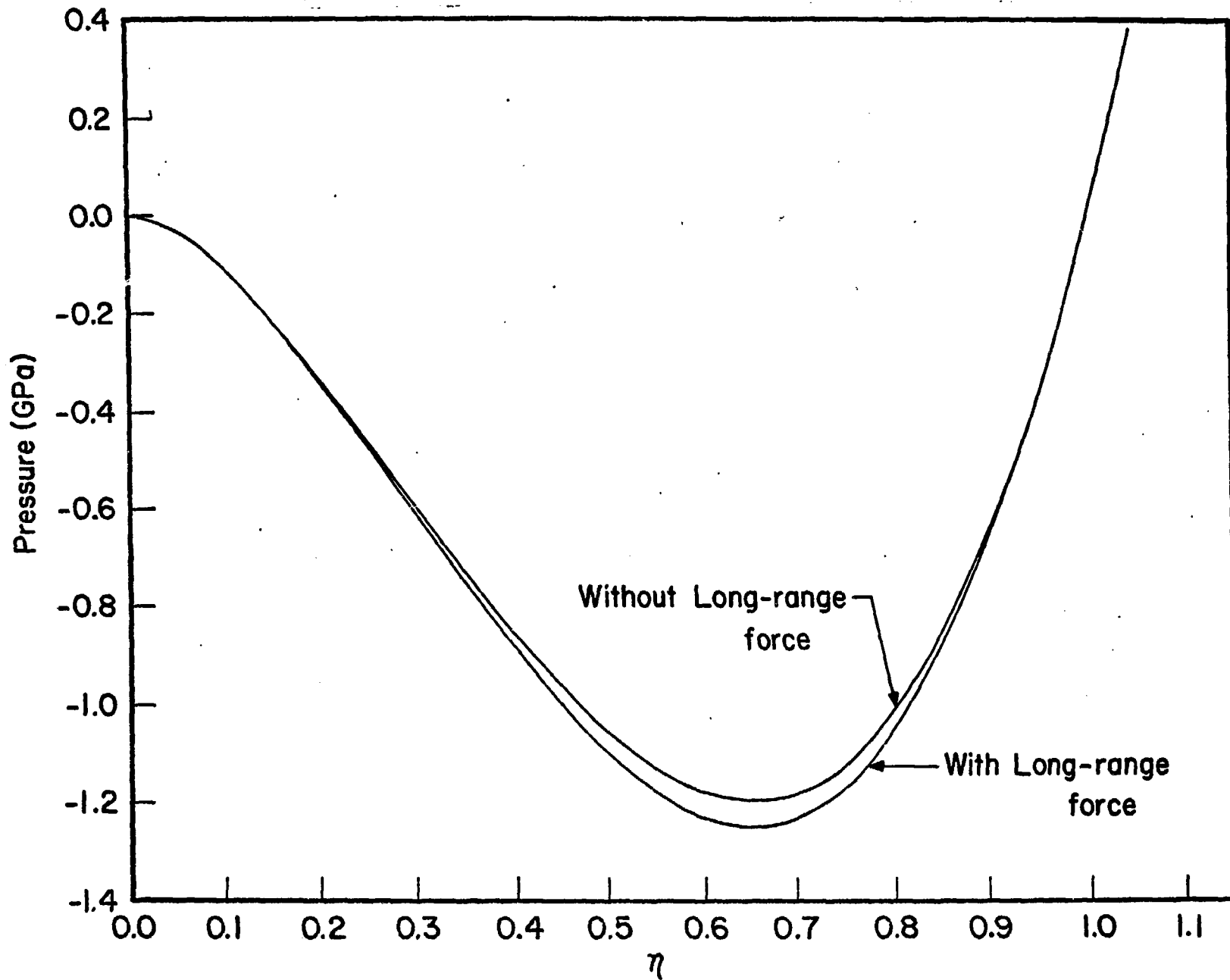


Fig. 3. Calculated pressure isotherms for sodium.

