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*SESAME Equation of State*  
*Number 7530, Basalt*

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*Prepared by Jo Ann Brown, Group T-1*

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*J. F. Barnes  
S. P. Lyon*



# SESAME EQUATION OF STATE NUMBER 7530, BASALT

by

J. F. Barnes and S. P. Lyon

## ABSTRACT

A full-range equation of state (EOS) for dry, nonporous basalt with a grain density of  $2.868 \text{ g/cm}^3$  has been constructed and placed on the SESAME library as material number 7530.

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As with most rocks, basalt is found with varying composition. It is an igneous rock, composed largely of complex minerals of the plagioclase feldspar and pyroxene groups; typically it contains very little identifiable quartz. In oxide abundance it is fairly similar to the diabbases and gabbros, other igneous rocks of about the same density but different texture. The particular molecular composition represented by equation-of-state (EOS) 7530 is given in Table I, where data are taken from Clark<sup>1</sup>; corresponding atomic abundance is shown in Table II. For this mixture the average atom, as used in the GRIZZLY<sup>2</sup> code, is calculated to have an atomic number  $\bar{Z} = 10.665$  and an atomic weight  $\bar{A} = 21.574$ . The EOS is constructed to have a reference density  $\rho_0 = 2.868 \text{ g/cm}^3$ , the assumed dry grain density of basalt. The EOS can be mixed with a suitable SESAME EOS for water if desired, and through the hydrocode setup the user can allow for the desired degree of porosity.

High pressure shock Hugoniot data on basalt are somewhat sparse, and since in fact the composition of the samples used in the existing

experiments was not as given in Table I anyway, we chose to use the more complete set of shock data on diabase given by McQueen, Marsh, and Fritz<sup>3</sup>. Ahrens and Gregson<sup>4</sup> showed that at the lower pressures where data exist the Hugoniot for gabbro, diabase, and basalt are in good agreement when account is taken of their differing initial density. We would expect the Hugoniot to agree also at higher pressures where the mineral makeup is "forgotten." Because the diabase samples had a density of 2.99 g/cm<sup>3</sup>, we constructed the EOS at that density and then scaled it to the basalt density given above. We assumed that the breaks in the experimental shock data reported in Reference 3 are due to a single phase change and approximated the  $U_s-U_p$  Hugoniot by three straight lines.

A new version of the "CHART JD" ion thermal (nuclear) model<sup>5</sup> that incorporates an improved treatment of the melting transition was used, along with the CHART-D<sup>6</sup> prescription for the variation of the Grüneisen parameter,  $\gamma$ , with compression. Reference  $\gamma$ , Debye temperature, cohesive energy, and melt temperature were simply computed as the number-weighted average of the major constituents, as shown in Table III. Although this is a crude procedure, better treatment for these quantities isn't warranted when one considers 1) the other approximations used in constructing equations of state for mixtures (such as the average atom approximation) and 2) the uncertainties of some of the entries in Table III. Note that, for example, since sound speeds and other data for calculation of  $\gamma_0$  and  $\Theta_D$  seem to be unavailable for ferrous oxide we used the calculated values for Fe<sub>2</sub>O<sub>3</sub>. It should also be noted that, as used here, cohesive energy is the energy required per mole of average atoms to separate a substance into its separate atoms at

0 K. The last line of Table III gives the calculated number-weighted averages of the quantities that we used as input to GRIZZLY. In construction of the cold curve, the Lennard-Jones factor was taken to be 0.185, which resulted in a critical temperature of about 6675 K.

Results are shown in Figures 1 through 4. Figure 1 shows selected pressure isotherms over the entire temperature range of the SESAME library table. Below the calculated critical isotherm van der Waal loops are obtained, and the 301 table in SESAME contains these loops. Figure 2 shows the corresponding isotherms with Maxwell equal-area construction. Data for effecting this replacement are stored in the 401 table of the library. Figure 3 shows the energy isotherms and Figure 4 the principal Hugoniot.

TABLE I

Chemical Composition of Basalt as Used in EOS 7530 (Ref. 1)

	<u>By Weight</u>	<u>By Number</u>
SiO <sub>2</sub>	50.83%	53.04%
CaO	10.42	11.65
MgO	6.34	9.86
Al <sub>2</sub> O <sub>3</sub>	14.07	8.65
FeO	9.00	7.86
H <sub>2</sub> O	0.91	3.17
Na <sub>2</sub> O	2.23	2.26
TiO <sub>2</sub>	2.03	1.59
Fe <sub>2</sub> O <sub>3</sub>	2.88	1.13
K <sub>2</sub> O	0.82	0.55
MnO	0.18	0.16
P <sub>2</sub> O <sub>5</sub>	0.23	0.10

TABLE II

Atomic Abundance as Used in EOS 7530

<u>Element</u>	<u>Abundance (By Number)</u>
O	60.11 %
Si	18.26
Al	5.96
Ca	4.01
Fe	3.48
Mg	3.39
H	2.18
Na	1.56
Ti	0.55
K	0.38
P	0.07
Mn	0.06

TABLE III

Estimates of the Grüneisen Parameter, Debye Temperature, Cohesive Energy, and Melt Temperature for the Major Constituents of Basalt and Their Resulting Weighted Averages

	$\gamma_o$	$\Theta_D$	$E_{coh}$	$T_m$
SiO <sub>2</sub>	0.653	950 K	146 kcal/mol	1883 K
CaO	2.40	640	127	2853
MgO	1.72	630	118	3125
Al <sub>2</sub> O <sub>3</sub>	1.595	1034	145	2288
FeO	(1.64)	(610)	110	1642
Fe <sub>2</sub> O <sub>3</sub>	<u>1.64</u>	<u>610</u>	<u>114</u>	<u>1838</u>
Basalt	1.17	851	137	2158



## REFERENCES

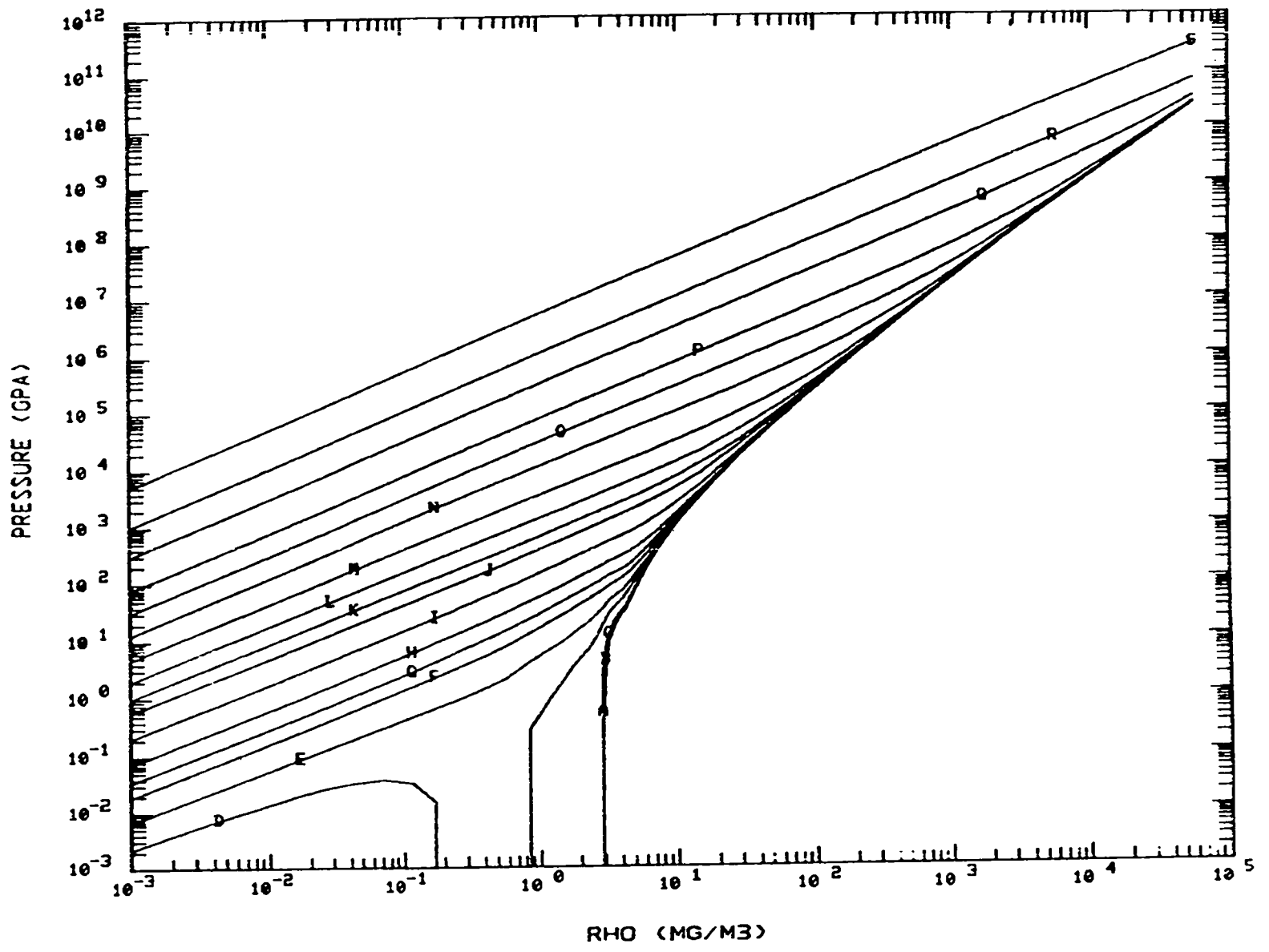
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2. J. Abdallah, Jr., "User's Manual for GRIZZLY," Los Alamos National Laboratory report LA-10244-M (September 1984).
3. R. G. McQueen, S. P. Marsh, and J. N. Fritz, *J. Geophys. Res.* 72, 4999 (1967).
4. T. J. Ahrens and V. G. Gregson, Jr., *J. Geophys. Res.* 69, 4839 (1964).
5. J. D. Johnson, Los Alamos National Laboratory, private communication, September 1986.
6. S. L. Thompson and H. S. Lawson, "Improvements in the Chart-D Radiation-Hydrodynamic Code III: Revised Analytic Equations of State," Sandia National Laboratories report SC-RR-710714 (March 1972).

changes ?

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TABLE 301

7530-1ST  
 TEMP (K)  
 A- 0.00+00  
 B- 2.98+02  
 C- 1.16+03  
 D- 5.80+03  
 E- 1.16+04  
 F- 2.32+04  
 G- 3.48+04  
 H- 5.80+04  
 I- 1.16+05  
 J- 2.32+05  
 K- 3.48+05  
 L- 5.80+05



M- 1.16+06  
 N- 2.90+06  
 O- 6.96+06  
 P- 1.74+07  
 Q- 6.96+07  
 R- 2.32+08  
 S- 1.16+09

T4 CRAY SES2D 1R

Fig. 1.

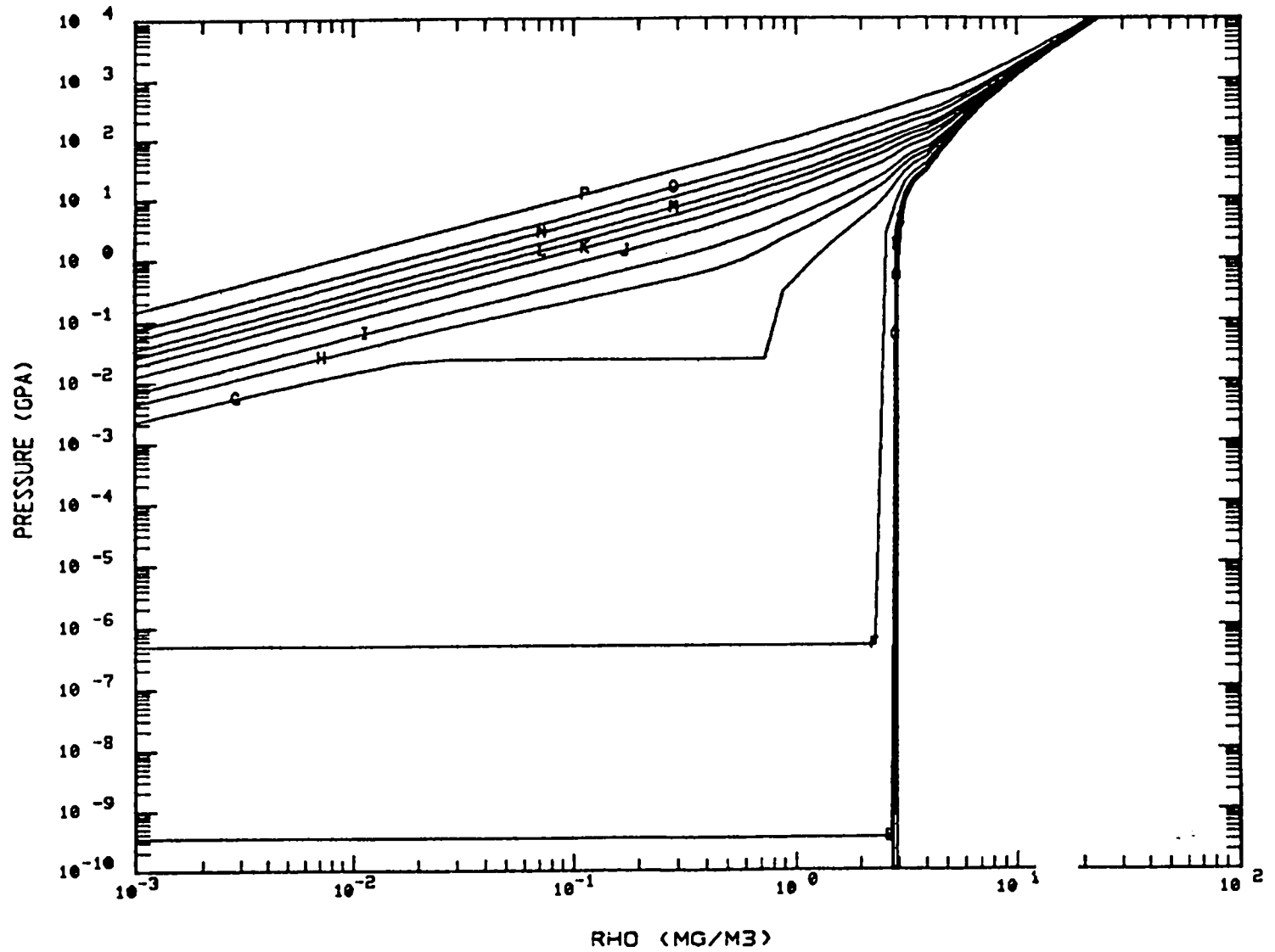
Selected pressure isotherms, containing van der Waal loops, for EOS 7530.

7530-IST  
 TEMP (K)  
 A-0.00+00  
 B-1.45+02  
 C-2.98+02  
 D-5.80+02  
 E-1.16+03  
 F-2.90+03  
 G-5.80+03  
 H-8.70+03  
 I-1.16+04  
 L-1.74+04  
 K-2.32+04  
 L-2.90+04

changes ?

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TABLE 301



M-3.48+04  
 N-4.64+04  
 O-5.80+04  
 P-9.28+04

Fig. 2.

Selected pressure isotherms for EOS 7530 with van der Waal loops replaced by calculated equilibrium vapor pressures.

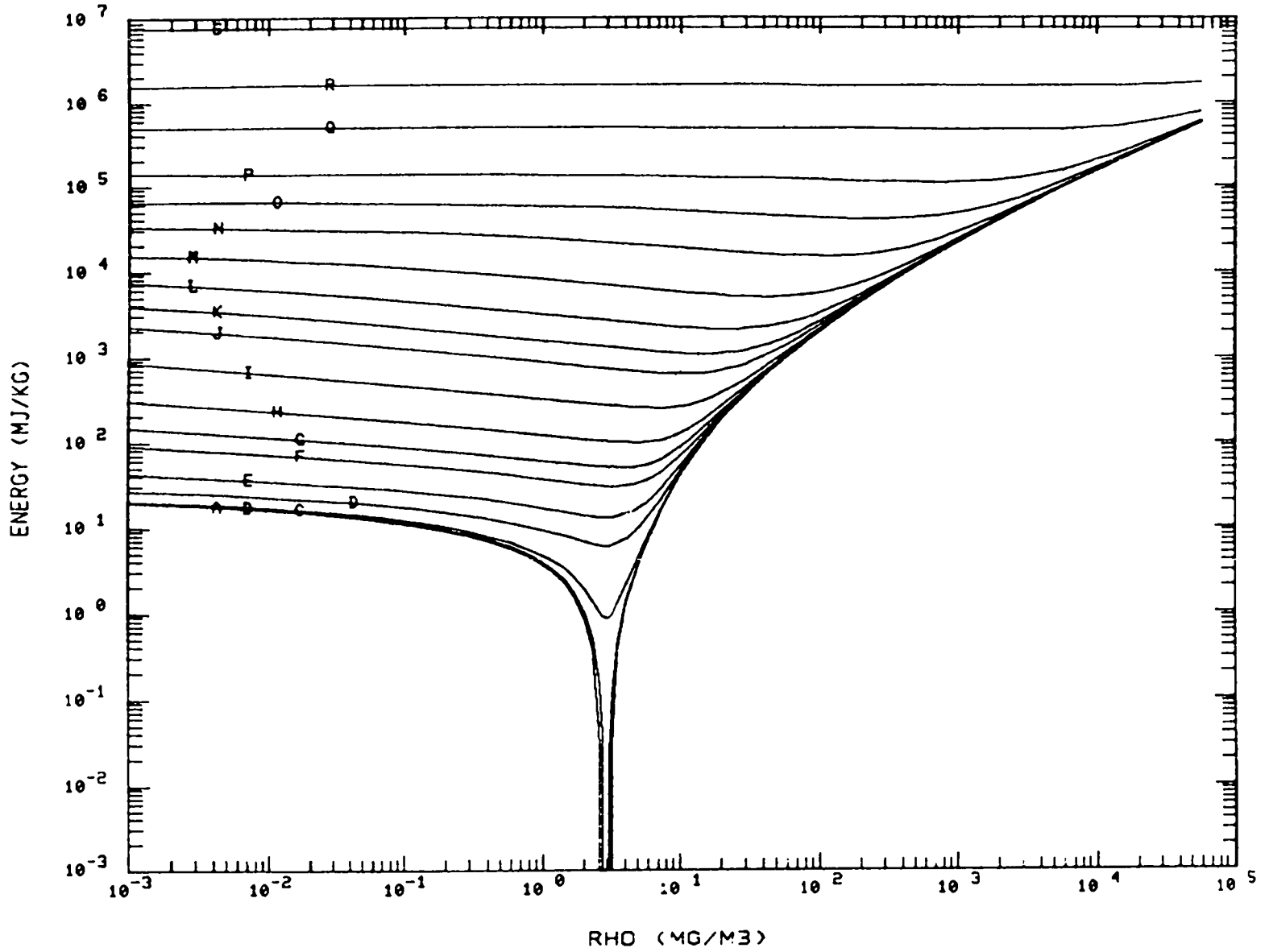
T4 CRAY SES2D 1R

7530-1ST  
 TEMP (K)  
 A-0.00+00  
 B-2.98+02  
 C-1.16+03  
 D-5.80+03  
 E-1.16+04  
 F-2.32+04  
 G-3.48+04  
 H-5.80+04  
 I-1.16+05  
 J-2.32+05  
 K-3.48+05  
 L-5.80+05

changes ?

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TABLE 301

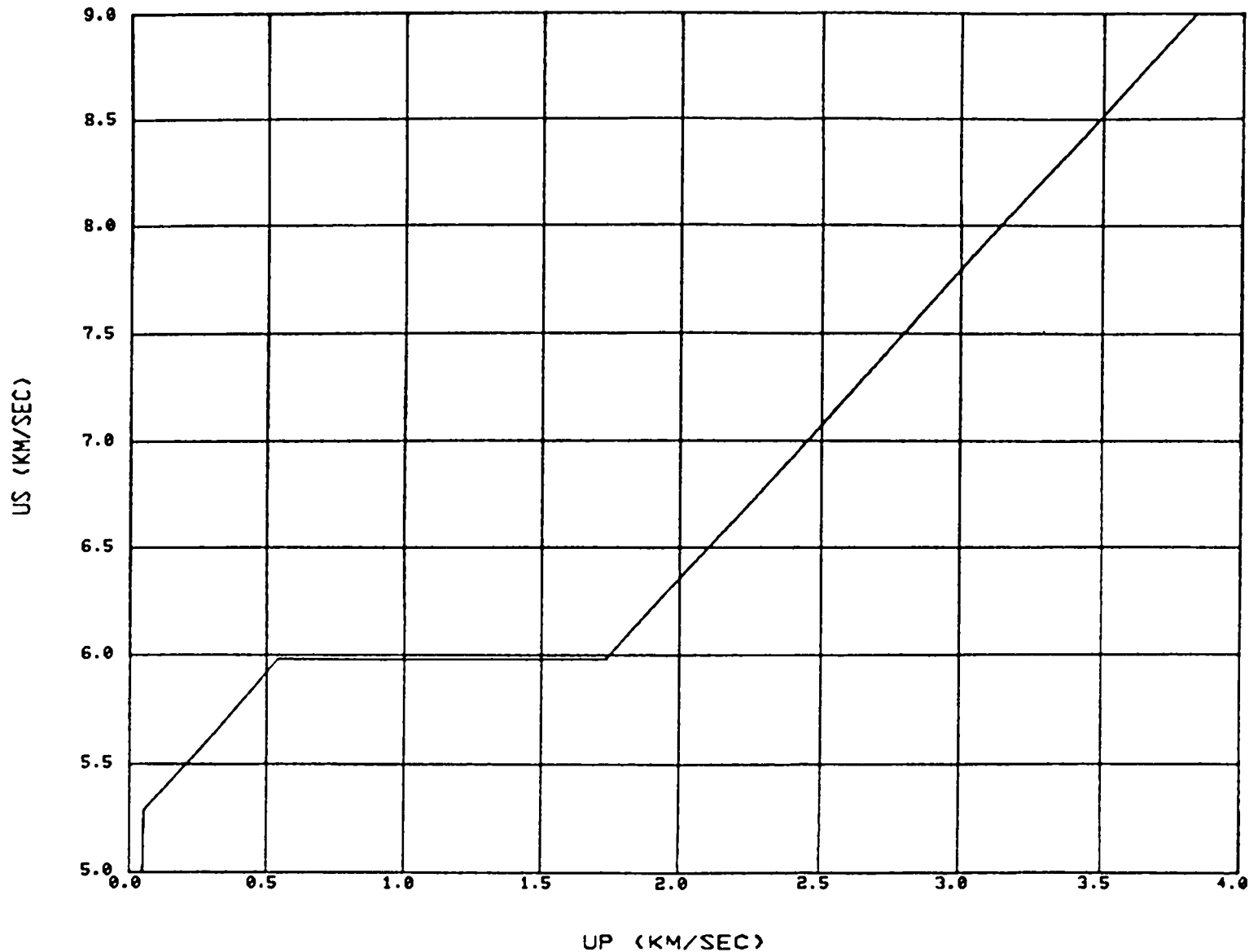


M-1.16+06  
 N-2.90+06  
 O-6.96+06  
 P-1.74+07  
 Q-6.96+07  
 R-2.32+08  
 S-1.16+09

Fig. 3.

Selected energy isotherms for EOS 7530.

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Fig. 4.

Shock velocity versus particle velocity on principal Hugoniot for EOS 7530.

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