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SESAME Equation of State Number 7530, Basalt

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by

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ABSTRACT

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

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 diabases 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[1]; corresponding atomic abundance is shown in Table II. For this mixture the average atom, as used in the GRIZZLY[2] 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 ρ_0 = 2.868 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[3]. Ahrens and Gregson[4] showed that at the lower pressures where data exist the Hugoniots for gabbro, diabase, and basalt are in good agreement when account is taken of their differing initial density. We would expect the Hugoniots to agree also at higher pressures where the mineral makeup is "forgotten." Because the diabase samples had a density of 2.99 g/cm^3, 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[5] that incorporates an improved treatment of the melting transition was used, along with the CHART-D[6] 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 γ_o and Θ_D seem to be unavailable for ferrous oxide we used the calculated values for Fe_2O_3. 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)

	By Weight	By Number
SiO_2	50.83%	53.04%
CaO	10.42	11.65
MgO	6.34	9.86
$A\ell_2O_3$	14.07	8.65
FeO	9.00	7.86
H_2O	0.91	3.17
Na_2O	2.23	2.26
TiO_2	2.03	1.59
Fe_2O_3	2.88	1.13
K_2O	0.82	0.55
MnO	0.18	0.16
P_2O_5	0.23	0.10

TABLE II

Atomic Abundance as Used in EOS 7530

Element	Abundance (By Number)
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

	γ_o	Θ_D	E_{coh}	T_m
SiO_2	0.653	950 K	146 kcal/mol	1883 K
CaO	2.40	640	127	2853
MgO	1.72	630	118	3125
$A\ell_2O_3$	1.595	1034	145	2288
FeO	(1.64)	(610)	110	1642
Fe_2O_3	1.64	610	114	1838
Basalt	1.17	851	137	2158

REFERENCES

1. K. F. Clark, "Mineral Composition of Rocks," in Handbook of Physical Properties of Rocks, Volume I, R. S. Carmichael, Ed. (CRC Press, Inc., Boca Raton, Florida, 1984), p.70.

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).

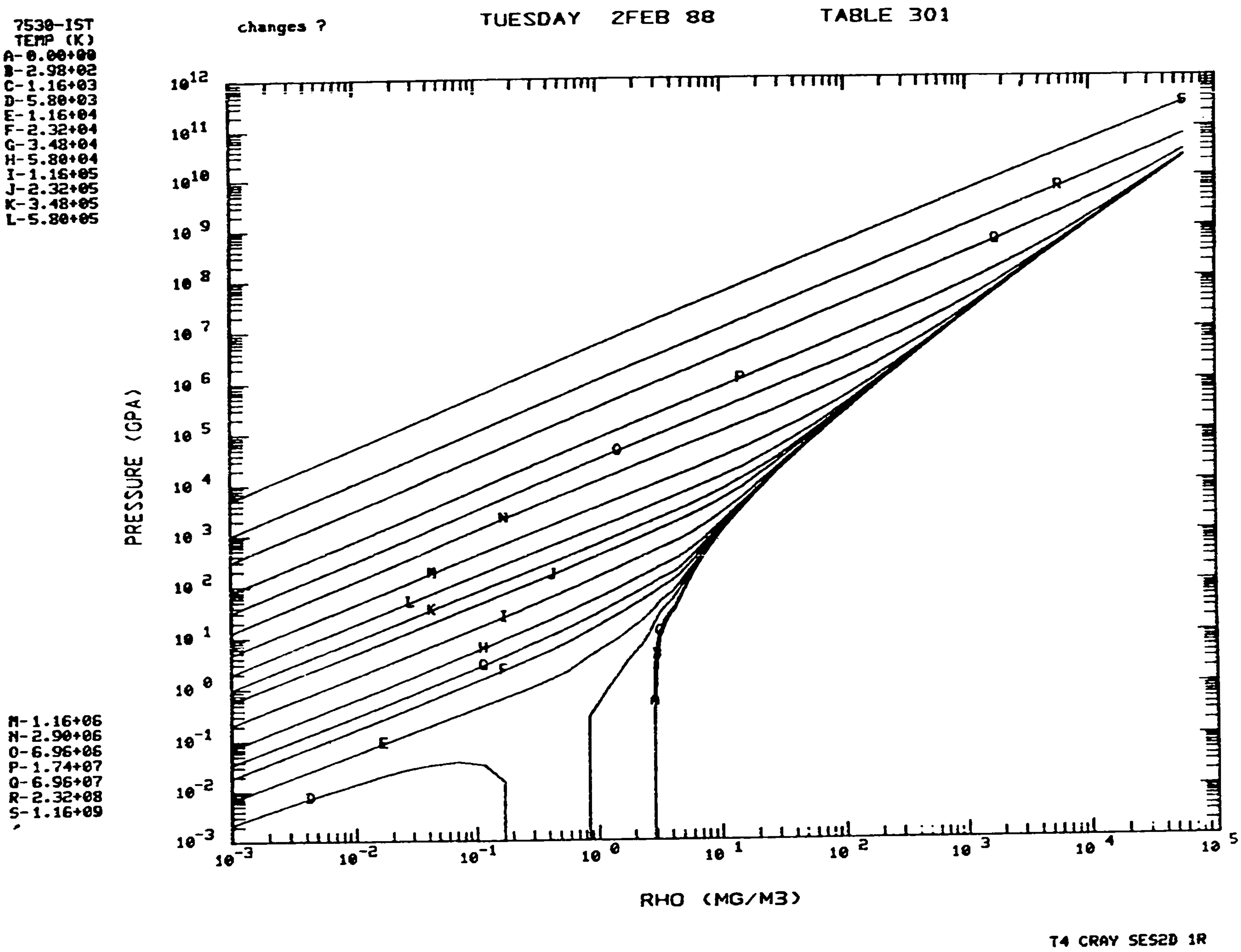

Fig. 1.

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

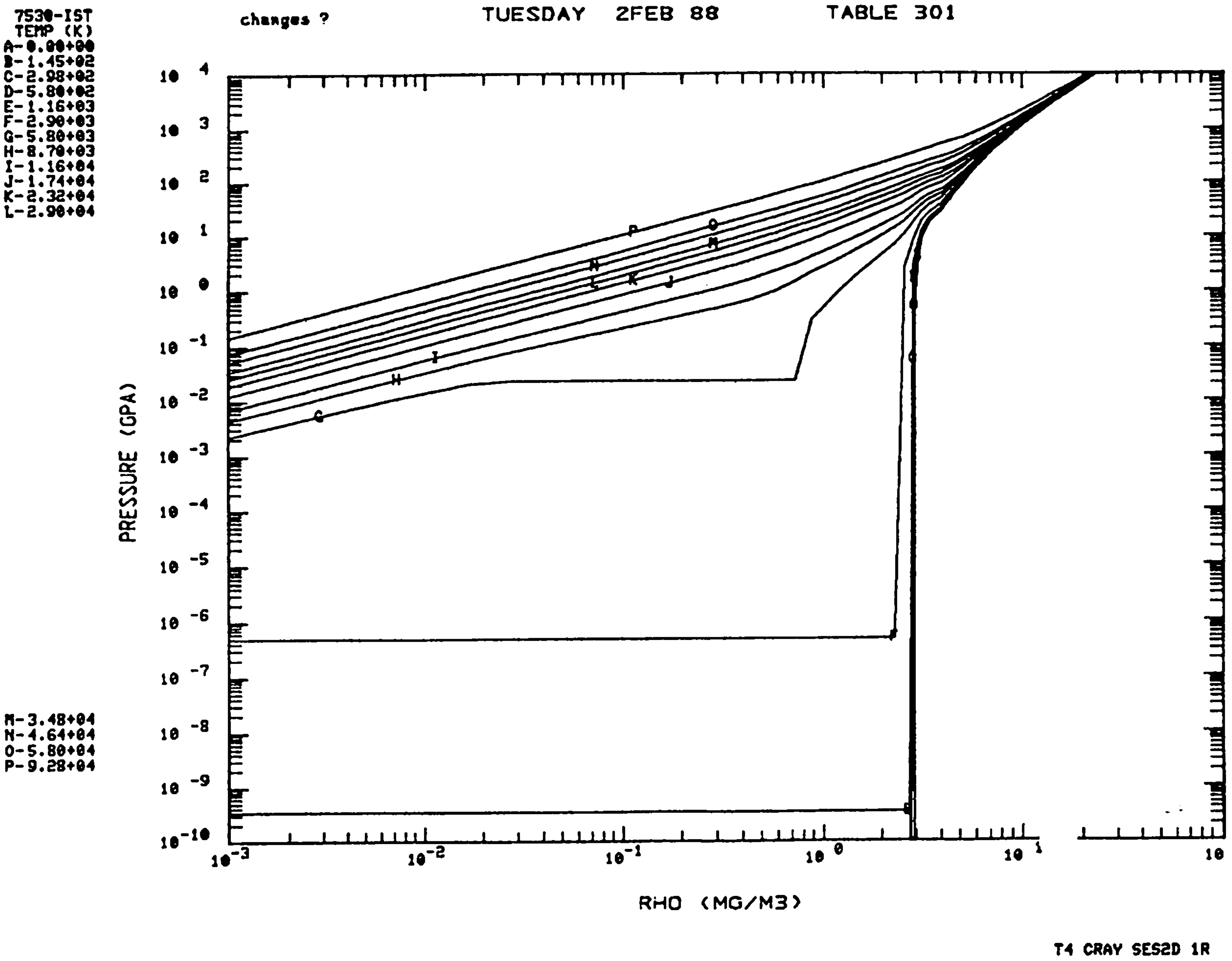

Fig. 2.

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

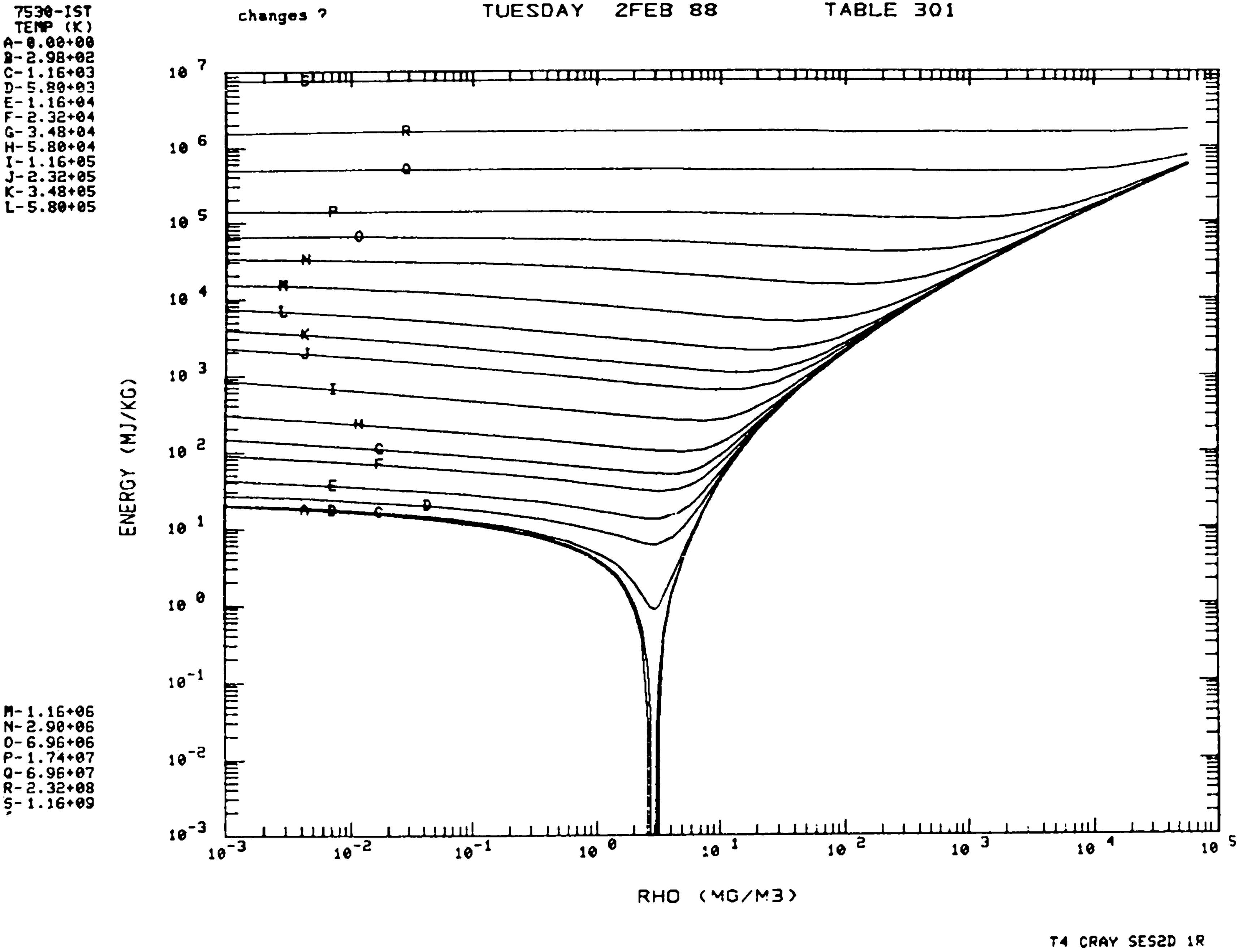

Fig. 3.

Selected energy isotherms for EOS 7530.

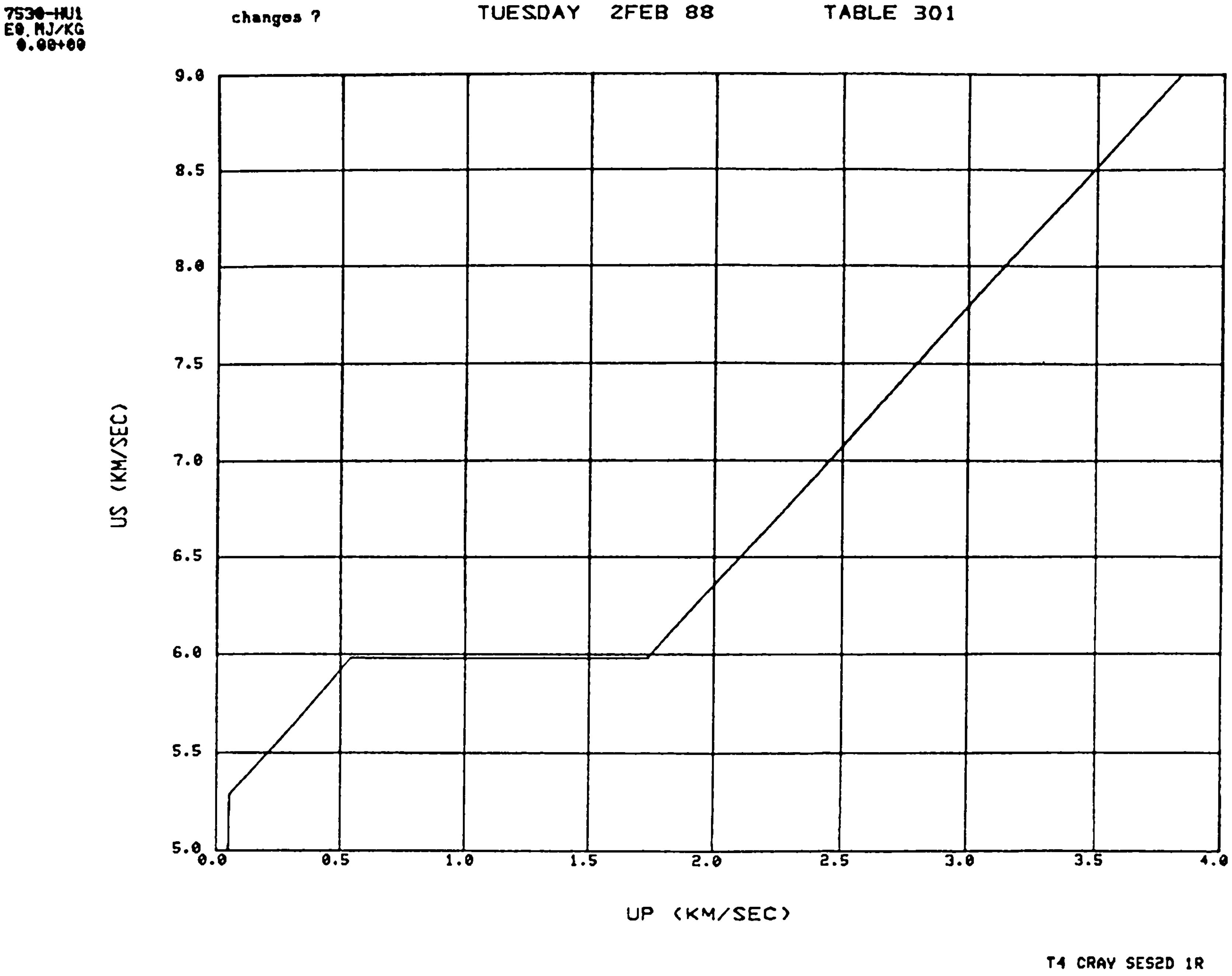

Fig. 4.

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

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