251
3/13/79

DR. 2328

MASTER

UCRL-52610

EQUATIONS OF STATE OF SiO₂ AND H₂O MIXTURES

F. H. Ree

December 1, 1978

Work performed under the auspices of the U.S. Department of
Energy by the UCLLL under contract number W-7405-ENG-48

LAWRENCE
LIVERMORE
LABORATORY
University of California - Livermore

LAWRENCE LIVERMORE LABORATORY
University of California Livermore, California 94550

UCRL-52610

EQUATIONS OF STATE OF SiO₂ AND H₂O MIXTURES

F. H. Ree

MS. date: December 1, 1978

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

CONTENTS

Abstract	1
Introduction	1
Theoretical Formulation	2
Primary EOS Data of SiO_2 and H_2O	2
Mixture Model for SiO_2 and H_2O	3
Dynamic Effects in Shock Hugoniot Data of Silicate Rocks	8
Data Reduction	9
Results and Summary	17
Isotherms	17
Hugoniots	17
Isentropes	17
Dynamic Response of SiO_2 Mixtures	27
Acknowledgments	32
References	32

EQUATIONS OF STATE OF SiO₂ AND H₂O MIXTURES

ABSTRACT

We have developed equations of state (EOS) of silicon dioxide-water mixtures to allow realistic computer simulations of surface and underground nuclear explosions of different yields to be conducted. Because the amount of water contained in silicate rocks affects the size of craters and cavities formed by nuclear explosions, this factor must therefore be included in calculations of the EOS data of silicon dioxide-water mixtures. We have tabulated EOS for mixtures containing three different concentrations of water at densities between 10^{-5} and 140 Mg/m^3 and temperatures between 0.025 and 25,000 eV. The calculations were performed using an improved mixture model based on our earlier EOS data of silicon dioxide and water. The improved model makes allowances for a nonequilibrium dynamic effect that occurs more slowly than does the polymorphic phase change of silicate rocks. We have attempted to use these data to simulate the behavior of water-containing rocks during nuclear explosions.

INTRODUCTION

Equation-of-state (EOS) data for different rock-water compositions are required for computer simulations of surface or underground tests of nuclear devices. Butkovich¹ considered the effect of ground water on the size of craters and cavities formed by nuclear explosions, concluding that the vaporization of even small amounts of water (about 0.5 wt%) could generate substantial peak pressures in the surrounding rocks that would, in turn, create larger explosion cavities. We have produced EOS data for silicon dioxide-water mixtures over the greatest possible ranges of density (ρ) and temperature (T) for use in realistic simulations of surface or subsurface nuclear explosions of different yields in silicate rock formations.

Most existing EOS models for rocks or rock-water mixtures are limited in their suitability for this application. The simplest model is the perfect-gas Saha equation over an entire ρ -T plane.² Such a model clearly should not be used in the liquid or solid phase region because it produces an unrealistic Hugoniot in which the pressure (P) decreases with the compression.³ Another model is the Tillotson equation.^{4,5} This model consists of two analytical expressions for compressed and expanded density regions in the form $P(E,V)$, where E equals the specific internal energy and V equals the specific volume ($1/\rho$). Some parameters in the Tillotson equation are normalized to the principal Hugoniot over an experimentally accessible ρ -region, and the remaining parameters are adjusted to provide a smooth transition between the ideal-gas behavior at low density and the Thomas-Fermi models at high density. The gap between these two limiting ρ -T regions is obviously very large, and no theoretical justification exists to use the Tillotson equation to bridge this gap. The more elaborate model of Butkovich⁶ compresses material along the experimentally determined principal Hugoniot. The compressed material is released or expanded using a Grüneisen model for the liquid region and a model for the gaseous region that includes both the ionization and chemical dissociation components and that conforms to the perfect-gas Saha assumption. In a real situation, in which the rocks are shocked, released, and reshocked or isentropically recompressed, all of these models require modifications.

We previously developed theoretical EOS data for silicon dioxide⁷ and water⁸ that cover all (ρ -T) regions of any anticipated practical application. Using these data, we have now produced realistic EOS data for rock-water mixtures that are not restricted to the particular (ρ ,T) loci associated with existing models. We

based our EOS model on an improved mixture model described here. Our present EOS data cover a density range of 10^{-5} to 140 Mg/m^3 and a temperature range of 0.025 to 25,000 eV; this represents a nearly complete range of ρ and T . Water may be present either as water of hydration or as liquid trapped within or flowing in the rock formation, but only the weight percent is important in calculating EOS for purposes of this study.

During this investigation, evidence from the experimental Hugoniot of wet and dry rocks indicated that the transformation of the quartz phase (low P) to the stishovite phase (high P) occurs at a considerably higher pressure under nonequilibrium conditions (e.g. a shock wave) than the measured static transition pressure. This effect must be incorporated into an EOS model if the dynamic phenomenon to be simulated takes place in less time than the time required for the polymorphic phase changes.

THEORETICAL FORMULATION

PRIMARY EOS DATA OF SiO_2 AND H_2O

We have described our EOS generation procedure previously^{7,8} and a brief summary will suffice here. Our calculations use several computational programs based on theoretical models and experimental data, both of which describe various physical processes that occur in different ρ and T regions. Figures 1 and 2 show the ρ - T ranges for SiO_2 and H_2O , respectively, in which the models are used.^{7,8} Briefly, these are:

- **TIGER Region.** Within the TIGER region, the EOS properties are determined by the dissociation products of SiO_2 and H_2O as well as by the gaseous and condensed forms of SiO_2 and H_2O . The concentrations of these species (and therefore, the EOS data) are obtained by the TIGER code.⁹ The TIGER code uses Gibbs and stoichiometric conditions for the multi-component, multi-phase mixtures to solve the species concentrations. The gaseous species are assumed to obey the BKW equation.⁹

- **GRAY Region.** Within this region, we assume SiO_2 to be in either a molecular liquid, α -quartz, or stishovite phase. In the GRAY code,^{10,11} a SiO_2 molecule is considered as three hypothetical monatoms with an atomic weight of 60.06/3. The solid-state properties are calculated by the Grüneisen model, and the liquid-state properties are obtained by modifying the solid-state data by an entropy correction associated with the loss of order. The liquid-solid-mixed phase properties are determined by using the Lindemann rule. The GRAY code is normalized to the experimental Hugoniot data.

- **OCCIPITAL Region.** In this range, the SiO_2 and the H_2O molecules are assumed to be completely dissociated into electrons, ions, and neutral atomic species. Thermodynamic data are computed by the OCCIPITAL code^{2,12} which assumes that the mixtures behave like an ideal gas.

- **Experimental Region.** Within this region, there are three sets of accurate experimental data for water: the steam table for the low- ρ region of Schmidt¹³, the static compression data to 1 GPa and 1373 K of Burnam *et al.*,^{14,15} and the high pressure work of Bridgman.^{16,17}

- **TFCMIX and MASTER Regions.** The EOS data in the TFCMIX region¹⁸ are evaluated by the Thomas-Fermi theory with several modifications: corrections by Kirzhnits¹⁹ to include the wave nature of electrons and the electron exchange contribution, thermal correction of nuclei by Warren,²⁰ and a mixture model of SiO_2 and H_2O in which the values of V and E are assumed to be weighted sums of the values of V and E of individual atomic species at constant temperature and electron pressure. Within the MASTER region,²¹ the TFCMIX-generated data are modified using an improved 0 K-isotherm based on the experimental Hugoniot data. Such a modification is desirable because the electronic correlations and atomic shell structures absent in the Thomas-Fermi theory become significant at the low- P region.

To generate global EOS data, the theoretical data from the five regions above are used only within the boundaries shown in Figs. 1 and 2. By limiting the EOS data to the (ρ, T) regions indicated in Figs. 1 and 2, the theoretical pressure isotherms and isochores from the neighboring regions appear to be continuous. The "hole" region in which the theories become less valid is filled by interpolation of the theoretical data.

FIG. 1. Density and temperature regions of five theoretical codes (TIGER, OCCIPITAL, TFCMIX, MASTER, and GRAY) used to obtain EOS data of SiO_2 .¹ Data are taken at the locations within the individual regions indicated by *, O, X, —, and +.

MIXTURE MODEL FOR SiO_2 AND H_2O

To generate the EOS data of water-rock mixtures, one develops a mixture model based on the individual EOS data of SiO_2 and H_2O . The simplest model is the "additive-volume" model, developed by Lacey and Walton,²² which calculates E and V of a $\text{SiO}_2 + \text{H}_2\text{O}$ mixture using the following formulae:

$$V(P, T) = f_{\text{SiO}_2} V_{\text{SiO}_2}(P, T) + f_{\text{H}_2\text{O}} V_{\text{H}_2\text{O}}(P, T), \quad (1)$$

FIG. 2. Density and temperature regions of four theoretical codes (TIGER, OCCIPITAL, TFCMIX, and MASTER) and experimental data used to obtain EOS data of H_2O .² The data are taken at points shown by O, X, Y, +, and *.

$$E(P, T) = f_{\text{SiO}_2} E_{\text{SiO}_2}(V_{\text{SiO}_2}, T) + f_{\text{H}_2\text{O}} E_{\text{H}_2\text{O}}(V_{\text{H}_2\text{O}}, T), \quad (2)$$

where f_i is the weight fraction of the species i . The mixing is conducted at constant P and T .

We found that one important modification of the additive-volume model must be introduced near the liquid-vapor phase change of SiO_2 ; under these conditions, the entropy of mixing in the gaseous phase is no longer constant but depends on the amount of the condensed SiO_2 present. Such a modification takes into

account the experimental observation that the boiling temperature at constant pressure (or, alternately, the vapor pressure at constant temperature) is measured over a finite temperature (or pressure) range rather than at a single value. In other words, the sharp liquid-vapor phase change with a volume discontinuity observed for a one-component system no longer occurs in the two-component SiO_2 - H_2O mixture system, but is replaced by a range of pressures along which an isotherm contains a liquid-vapor phase change of SiO_2 .

This point can be explained in detail using an example of a 90 wt% SiO_2 and 10 wt% H_2O mixture, the composition of some naturally occurring hydrated minerals. The TIGER code was used to generate the EOS data for three separate systems: the SiO_2 + H_2O mixture, H_2O , and SiO_2 . It is assumed that the EOS data of the first system are essentially exact; these are compared with the additive-volume results obtained from the EOS data for the latter two systems. The TIGER calculation includes the gaseous species (Si , Si_2 , Si_3 , O , O_2 , H , H_2 , SiO , SiO_2 , OH , SiOH , $\text{Si}(\text{OH})_2$, SiH , and SiH_4), the liquids (Si , SiO_2 , and H_2O), and the solids (Si and SiO_2). The mixture system under consideration thus represents a reasonably realistic multiphase system that includes the effects of the expected chemical reactions. The reactions taking place among the dissociation products of SiO_2 and of H_2O , as well as those species (SiOH , $\text{Si}(\text{OH})_2$, SiH , and SiH_4) resulting from the exchanges between SiO_2 and H_2O molecules, have been considered here. Figures 3a and 3b show, respectively, the pressure and the energy isotherms for the mixture systems at $T = 2321, 2901, 3482, 4642, 5803, 6963$, and 9284 K. The solid curves are the SiO_2 + H_2O isotherms produced by TIGER; the points indicate the additive-volume calculations. Within the temperature region indicated in Fig. 3, SiO_2 undergoes the liquid-vapor phase change, but water exists only as vapor. The additive-volume theory is remarkably accurate in the density regions in which the system consists essentially of either pure water vapor and gaseous SiO_2 or of pure water vapor and pure liquid SiO_2 . Within the liquid-vapor transition of SiO_2 , however, the agreement between methods is not as good. Because the SiO_2 + H_2O system is binary, the Gibbs rule requires that the two independent variables (T and V , in this case) specify P and E even within the two-phase region. Therefore, in this example, the flat tie-line observed in pressure isotherms by the additive-volume theory for the pure SiO_2 system at the liquid-vapor transition region is not realistic and is replaced by an isotherm with a small positive slope in the mixture data generated by TIGER.

To formulate the correct isotherms, the following procedure was used. The Gibbs free energy (G^1) of the additive volume model is given by

$$G^1 = N_{\text{SiO}_2}^g \mu_{\text{SiO}_2}^g + N_{\text{SiO}_2}^l \mu_{\text{SiO}_2}^l + N_{\text{H}_2\text{O}} \mu_{\text{H}_2\text{O}} \quad (3)$$

where N_i and μ_i are the number of moles of i and the chemical potential of species i , respectively; the superscripts g and l denote the gas and liquid phases, respectively. Water is assumed to be in the vapor phase. Because G^1 does not contain an ideal mixing term for the gaseous SiO_2 and water vapor, this correction is included, and we obtain a corrected Gibbs free energy (G)

$$G = G^1 + \left[(N_{\text{SiO}_2}^g + N_{\text{H}_2\text{O}}) kT \right] \left[\xi \log_e \xi + (1 - \xi) \log_e (1 - \xi) \right] \quad (4)$$

where

$$\xi = N_{\text{SiO}_2}^g / (N_{\text{SiO}_2}^g + N_{\text{H}_2\text{O}}) .$$

When G is minimized with respect to $N_{\text{SiO}_2}^g$ at fixed values of $N_{\text{H}_2\text{O}}$ and N_{SiO_2} (where $N_{\text{SiO}_2} \equiv N_{\text{SiO}_2}^g + N_{\text{SiO}_2}^l$), one obtains a simple solution for the mole fraction ν where $\nu \equiv N_{\text{SiO}_2}^g / (N_{\text{SiO}_2}^g + N_{\text{H}_2\text{O}})$ of the SiO_2 vapor, i.e.

$$\nu = \exp \left[\frac{1}{RT} \int_{p_{\text{eq}}}^P (V_{\text{SiO}_2}^g - V_{\text{SiO}_2}^l) dP \right] \quad (5)$$

FIG. 3. (a) Pressure isotherms and (b) energy isotherms of a mixture system containing 10 wt% H_2O and 90 wt% SiO_2 at different temperatures. The solid lines are generated by TIGER; the points (o) are obtained from the additive-volume model using the EOS data of H_2O and SiO_2 obtained from TIGER. The data calculation by the improved additive-volume model described in this work agree nearly exactly with the TIGER-generated data.

where P_{eq} represents the vapor pressure of pure SiO_2 at the same temperature as the mixture isotherm under consideration.

The above analysis demonstrates an important consequence, namely, gaseous SiO_2 in the mixture system begins to condense at a pressure P' which is generally higher than the liquid-vapor transition pressure (P'_{eq}) for the pure SiO_2 system. The calculation of P' is performed iteratively by solving the equation:

$$\eta = \exp \left[\frac{1}{RT} \int_{P_{eq}}^{P'} (V_{\text{SiO}_2}^g - V_{\text{SiO}_2}^l) dP \right], \quad (6)$$

where $\eta = (N_{\text{SiO}_2})/(N_{\text{SiO}_2} + N_{\text{H}_2\text{O}})$. The value of η is a constant and, in this example, equals 0.7296.

By taking appropriate thermodynamic derivatives of G [Eq.(4)], we obtain

$$V(P, T) = f_{\text{SiO}_2}^g V_{\text{SiO}_2}^g(P, T) + (f_{\text{SiO}_2} - f_{\text{SiO}_2}^g) V_{\text{SiO}_2}^l(P, T) + f_{\text{H}_2\text{O}} V_{\text{H}_2\text{O}}(P, T), \quad (7)$$

$$E(P, T) = f_{\text{SiO}_2}^g E_{\text{SiO}_2}^g(V_{\text{SiO}_2}^g, T) + (f_{\text{SiO}_2} - f_{\text{SiO}_2}^g) E_{\text{SiO}_2}^l(V_{\text{SiO}_2}^l, T) + f_{\text{H}_2\text{O}} E_{\text{H}_2\text{O}}(V_{\text{H}_2\text{O}}, T), \quad (8)$$

where $f_{\text{SiO}_2}^g$ is the weight fraction of SiO_2 vapor and is related to ν by the expression

$$\nu = f_{\text{SiO}_2}^g / [f_{\text{SiO}_2} + f_{\text{H}_2\text{O}}(M_{\text{H}_2\text{O}}/M_{\text{SiO}_2})], \quad (9)$$

where M_{SiO_2} and $M_{\text{H}_2\text{O}}$ are the molecular weights of SiO_2 and H_2O , respectively.

To summarize, our procedure for generating the EOS data is as follows: We evaluate P' from Eq. (6). For values of $P \leq P'$, V and E are evaluated from Eqs. (7) and (8) by setting $f_{\text{SiO}_2} = f_{\text{SiO}_2}^g$; for values of $P > P'$, $f_{\text{SiO}_2}^g$ is evaluated from Eqs. (5) and (9). The use of $f_{\text{SiO}_2}^g$ in Eqs. (7) and (8) in turn gives V and E . In principle, the calculation of V and E depicted above must be performed for P above P' until a new high- P phase line (a solid phase) intersects the liquid-condensed phase line. At values of P above this intersection point, another complicated analysis is required. In practice, however, whenever P exceeds ten times P_{eq} the isotherm within the phase change region lies very close to the condensed side and no significant error results if the isotherm is assumed to be identical to the condensed-phase isotherm whenever $P > P''$, where $P'' = 100 P_{eq}$.

At temperatures sufficiently low that water vapor condenses, SiO_2 exists in the solid phase. In this case, we must consider a heterogeneous mixture consisting of three separate phases (i.e., condensed SiO_2 , condensed H_2O , and H_2O vapor) in equilibrium. Application of Gibbs rule shows that the $\text{SiO}_2 + \text{H}_2\text{O}$ mixture isotherms exhibit a first-order phase change with a sharp volume discontinuity in the pressure isotherms.

The theoretical formulation described in this section was programmed²³ and tested for the mixture of 90 wt% SiO_2 and 10 wt% H_2O and generated isotherms that were nearly identical to those produced by TIGER (Figs. 3a and b).

DYNAMIC EFFECTS IN SHOCK HUGONIOT DATA OF SILICATE ROCKS

From a thermodynamic point of view, the EOS data of SiO_2 or $\text{SiO}_2 + \text{H}_2\text{O}$ mixtures described in the previous sections can be used with reasonable confidence unless nonequilibrium conditions affect the experimental shock wave data. Unfortunately, a detailed comparison between theoretical and experimental Hugoniot data of rock-water systems revealed that such a nonequilibrium phenomenon occurred. The experimental Hugoniot data^{24,25} for quartz showed that a very large overdriving pressure in excess of that measured under static compression was required to dynamically transform quartz to the high pressure stishovite phase. The pressure (P_1) necessary to *initiate* this transformation depends on the density (ρ_0) of the quartz sample; if ρ_0 is 2.65, 1.77, 1.55, and 1.35 Mg/m^3 , then P_1 was found to be 14²⁴–19,²⁵ 15,²⁴ 9.1,²⁴ and 8.4 GPa, respectively. In contrast, crystalline quartz ($\rho_0 = 2.65 \text{ Mg/m}^3$) is transformed at 8.7 GPa under static compression. Although the values of P_1 were only roughly estimated from the data, they lead to the rather peculiar conclusion that the higher the initial density of the shocked sample, the higher the pressure that is required to transform the sample to the stishovite phase. This observation contradicts our intuitive view that a high- ρ_0 sample, the density of which approaches that of crystalline quartz, should transform closer (i.e., lower) to the static transition pressure. It must be stated that the overdriving pressure phenomenon is not limited to quartz; we found that a similar effect is also present in graphite Hugoniot.^{26,27} We believe this effect occurs for any material undergoing a large structural reordering during the phase change, since such a transition would take considerably more time than is available during the transit of a typical shock wave (about 1 μs).

A possible explanation at the molecular level of this peculiarity would be that these transformations involve a fairly extensive reordering of the structure and a large volume change. Under the shock compression, quartz is transformed to stishovite, which is about 38% more dense; quartz and stishovite occupy 0.377 and 0.233 m^3/Mg in the standard state at 300 K, respectively. In the case of low- ρ_0 quartz, the initial phase may be coesite, but this can be neglected in the present discussion. Therefore, unlike solid-solid transformations in metals, the transformation in the SiO_2 case requires appreciable atomic diffusion, and the rate of the transformation depends critically on the mechanism of nucleation. Nucleation will most probably occur heterogeneously near grain boundaries or dislocations where the defect energy is available to assist the nucleation. Obviously, the low- ρ_0 materials with less crystalline symmetry have more defects and thus more nucleation sites. Furthermore, because the growth of the new phase is a thermally activated process, the lower- ρ_0 materials, which are heated to higher temperatures by the shock wave, can be transformed more rapidly into the new phase.

The Hugoniot behavior can be explained on the following physical basis: low-density materials contain many nucleation sites, and, at the temperature generated by the shock wave, the nucleation time is short on the experimental time scale; pressures significantly higher than the static transformation pressure are not required to produce the stishovite phase. High density materials, however, contain fewer nucleation sites, and, at the shock temperature generated by a shock wave of a pressure corresponding to the static transformation pressure, these sites grow so slowly that no transformation occurs. The quartz phase is transformed to stishovite only if a shock wave of sufficient strength to provide adequate overdriving pressure (and high temperature) passes through the rock.

The nonequilibrium effect also causes serious difficulties in producing theoretical EOS data. A usual procedure for generating the EOS data of SiO_2 for example, is based on the experimental Hugoniot data for crystalline quartz, for which $\rho_0 = 2.65 \text{ Mg/m}^3$. Because the case $\rho_0 = 2.65 \text{ Mg/m}^3$ has a large overdriving pressure, hence a large associated value of U_s (shock velocity), the computed values of U_s for low- ρ_0 quartz (based on the crystalline quartz EOS) data are as much as 15% larger than the experimentally determined values of U_s within the transition region. A similar deviation is also present in the case of fully wet (80 wt% $\text{SiO}_2 + 20 \text{ wt% H}_2\text{O}$) sands as well as partially wet sands.

These observations are a manifestation of a nonthermodynamic phenomenon. However, the Hugoniot data (which show the overdriving pressure) are insensitive to the shock transit time of about 1 μsec . Therefore, this phenomenon must be regarded as essentially *time-independent* if one wishes to study a dynamic phenomenon that takes place within about 1 μsec . "Pseudo" thermodynamic data within this range of P and

T can be generated (see below) by individually modifying the EOS data to correctly reproduce experimental Hugoniot of materials with different densities (and different H₂O contents). A more rigorous method implements a suitable constitutive relation into a hydrocode itself. The former approach requires generation of a large number of EOS data to accommodate all different initial conditions. However, this approach fulfills our immediate need to provide the EOS data to the user, so we will follow this path as a near-term solution. It must be re-emphasized here that the EOS data generated in this manner are applicable only for a dynamic process in which shock wave propagation is an important part of the hydrosimulation.

There are many ways to normalize the EOS data to agree with the experimental Hugoniot data. The procedure described below is relatively simple and easy to put into practice:

1) Assume that the nonequilibrium effect alters only the Hugoniot pressure (P_H) but not the Hugoniot energy (E_H).

2) Evaluate the Hugoniot temperature (T_H) by superimposing the E_H vs. ρ data on the theoretical isotherm data.

3) Calculate $\Delta P(\rho, T_H) = P'_H - P_H$, where P'_H is predicted from the uncorrected EOS data basis at (ρ, T_H) .

4) Replace $P^{\text{old}}(\rho, T)$ in the theoretically generated EOS data with $P^{\text{new}}(\rho, T) = P^{\text{old}}(\rho, T) - \Delta P$ for all T and all ρ within the (ρ, T) -region in which the dynamic correction is needed.

Our physical picture under assumption (1) is that: the system in question is in mechanical disequilibrium. The pressure buildup in the quartz phase occurs because a finite time is required for the second phase (stishovite) to nucleate and grow. However, because there is no contrary evidence, we assume that the same shock energy is necessary to achieve a given compression with or without the nonequilibrium effect. The validity of the latter assumption is probably closely tied with the correctness of the assumption that the mixture system is in thermal equilibrium. At any rate, the density interval in which the dynamic correction is needed is relatively small. In the case of the SiO₂ + H₂O mixtures considered in this report, it applies to the interval between 3.5 and 4 Mg/m³.

DATA REDUCTION

We have considered SiO₂ + H₂O mixtures with three different water contents: 96 wt% SiO₂ + 4 wt% H₂O, 90 wt% SiO₂ + 10 wt% H₂O, and 80 wt% SiO₂ + 20 wt% H₂O. The third mixture system represents that of rock nearly saturated with water. The specific volumes (V_0) of these systems at room temperature and 1 atm (0.101325 MPa) are calculated by adding the corresponding specific volumes of SiO₂ and H₂O weighted by their weight fractions. The normal densities ($\rho_0 = 1/V_0$) of these systems at 300 K and 0.1 MPa are: 2.485, 2.274, and 1.991 Mg/m³, respectively.

In this work, the energies of SiO₂ and H₂O at 0 K and 1 atm serve as the reference points for all energy values. We approximate the energy shifts $\Delta E [= E_{298.15 \text{ K at 1 atm}} - E_{0 \text{ K at 1 atm}}]$ of SiO₂ and H₂O by substituting the corresponding enthalpy differences $\Delta H [= H_{298.15 \text{ K at 1 atm}} - H_{0 \text{ K at 1 atm}}]$. The quantity ΔH can be obtained from the JANAF table.²⁸ For example, in the case of 80 wt% SiO₂ + 20 wt% H₂O, ΔE is determined as follows:

$$\begin{aligned}\Delta E &= 0.8\Delta H_{\text{SiO}_2} + 0.2\Delta H_{\text{H}_2\text{O}} \\ &= (0.8)(1.151 \times 10^{-4}) + (0.2)(5.497 \times 10^{-4}) \\ &= 2.020 \times 10^{-4} \text{ MJ/g}.\end{aligned}$$

Therefore, 2.02×10^{-4} MJ/g must be added to all values of E if the original values are referenced from ρ_0 at 1 atm. By using the above convention, no negative energy values occur during most hydrocode calculations. This is useful in some cases, since some hydrocodes do not allow negative energies.

TABLE 1. Complete list of density and temperature values used to generate EOS data.

Density (ρ), Mg/m ³		Temperature (T), eV		
1×10^{-5}	1.5×10^{-2}	2.2	0.025	100
1.5×10^{-5}	2×10^{-2}	2.274 ^b	0.03	150
2×10^{-5}	2.5×10^{-2}	2.3	0.035	250
2.5×10^{-5}	3×10^{-2}	2.4	0.04	400
3×10^{-5}	4×10^{-2}	2.485 ^c	0.05	600
4×10^{-5}	5×10^{-2}	2.5	0.07	1 000
5×10^{-5}	6×10^{-2}	2.65	0.1	1 500
6×10^{-5}	8×10^{-2}	3	0.13	2 500
8×10^{-5}	0.1	3.5	0.15	4 000
1×10^{-4}	0.125	4	0.18	6 000
1.5×10^{-4}	0.15	4.5	0.2	10 000
2×10^{-4}	0.2	5	0.25	15 000
2.5×10^{-4}	0.25	5.5	0.3	25 000
3×10^{-4}	0.3	6	0.4	
4×10^{-4}	0.4	6.5	0.5	
5×10^{-4}	0.5	7	0.6	
6×10^{-4}	0.6	8	0.7	
8×10^{-4}	0.6309	10	0.8	
1×10^{-3}	0.8	12.5	1	
1.25×10^{-3}	0.9	15	1.5	
1.5×10^{-3}	1	20	2.5	
2×10^{-3}	1.02	25	4	
2.5×10^{-3}	1.04	30	6	
3×10^{-3}	1.14	40	8	
4×10^{-3}	1.18	50	10	
5×10^{-3}	1.25	60	15	
6×10^{-3}	1.5	80	25	
8×10^{-3}	1.991 ^a	100	40	
1×10^{-2}	2	125	60	
1.25×10^{-2}	2.157	140	80	

^aThis density value (ρ_0) was used only for 80 wt% SiO₂ + 20 wt% H₂O mixture.

^bThis density value (ρ_0) was used only for 90 wt% SiO₂ + 10 wt% H₂O mixture.

^cThis density value (ρ_0) was used only for 96 wt% SiO₂ + 4 wt% H₂O mixture.

Because the improved mixture model for the SiO₂ + H₂O mixtures uses P and T as independent variables, the resulting EOS data are obtained over irregular density grids. Final EOS data over uniform density grids are obtained by interpolation and are generated in tabular forms containing 88 ρ -points and 43 T-points to give 3784 data points (Table 1).

Tables 2 through 7 list the values of P and E at selected values of T and ρ for the three SiO₂ + H₂O mixtures. These data are selected from the EOS tables on file²⁹ which are constructed to be used with the LLL hydrocodes.

TABLE 2. Values of P (in TPa) for selected values of ρ and T of 96 wt% SiO₂ + 4 wt% H₂O (abstracted from the complete EOS table²³).

Density, Mg/m ³	Temperature, eV									
	0.025	0.05	0.08	0.097	0.1	0.15	0.25	0.5	0.8	0.8
0.00001	5.232E-11	7.944E-11	1.137E-10	1.591E-10	2.272E-10	3.416E-10	6.914E-09	1.019E-08	1.662E-08	2.463E-08
0.0001	5.538E-10	7.406E-10	1.066E-09	1.508E-09	2.143E-09	3.221E-09	3.161E-08	6.406E-08	1.408E-07	2.169E-07
0.001	2.300E-09	7.504E-09	1.072E-08	1.501E-08	2.146E-08	3.228E-08	7.005E-08	7.138E-07	1.369E-06	1.861E-06
0.025	2.640E-09	1.668E-07	2.697E-07	3.708E-07	5.098E-07	6.175E-07	1.420E-06	2.843E-06	2.843E-06	4.272E-06
0.06	2.340E-09	2.956E-07	6.525E-07	9.258E-07	1.354E-06	2.089E-06	3.457E-06	4.832E-06	4.725E-05	9.933E-05
0.1	2.340E-09	2.956E-07	1.090E-06	1.570E-06	2.37E-06	3.442E-06	5.866E-06	7.019E-06	5.315E-05	1.768E-04
0.15	2.340E-09	2.956E-07	1.664E-06	2.405E-06	3.657E-06	5.347E-06	9.266E-06	1.177E-05	5.836E-05	2.047E-04
0.25	2.340E-09	2.956E-07	2.800E-06	4.182E-06	6.605E-06	9.579E-06	1.612E-05	2.043E-05	6.564E-05	3.612E-04
0.5	2.340E-09	2.956E-07	6.970E-06	1.63E-05	1.691E-05	2.647E-05	4.929E-05	5.962E-05	1.69E-04	4.419E-04
0.8	2.340E-09	2.956E-07	9.163E-06	1.690E-05	2.792E-05	5.024E-05	7.415E-05	9.195E-05	1.633E-04	4.722E-04
1	2.340E-09	2.956E-07	9.488E-06	2.379E-05	3.946E-05	6.268E-05	1.295E-04	1.597E-04	2.381E-04	5.337E-04
1.14	2.340E-09	2.956E-07	9.47E-06	2.147E-05	4.963E-05	1.108E-04	1.880E-04	2.727E-04	2.925E-04	6.335E-04
1.25	2.340E-09	2.956E-07	9.406E-06	3.266E-05	5.951E-05	1.361E-04	2.444E-04	3.833E-04	3.597E-04	7.147E-04
1.5	2.340E-09	2.956E-07	9.405E-06	4.529E-05	5.195E-05	2.044E-04	4.107E-04	5.122E-04	5.945E-04	9.943E-04
2	2.340E-09	5.217E-07	1.17E-05	1.305E-04	2.906E-04	6.054E-04	1.297E-03	1.626E-03	2.311E-03	3.182E-03
2.2	2.340E-09	5.217E-07	1.431E-05	2.299E-04	3.100E-04	1.191E-03	2.531E-03	3.40E-03	4.374E-03	5.581E-03
2.48	1.190E-07	2.040E-04	5.519E-04	1.022E-03	1.599E-03	3.582E-03	6.059E-03	7.161E-03	9.332E-03	1.125E-02
3	6.645E-03	7.317E-03	9.243E-03	9.116E-03	1.812E-02	1.168E-02	1.607E-02	1.758E-02	2.055E-02	2.311E-02
4	1.579E-02	2.013E-02	2.493E-02	2.14E-02	2.390E-02	2.614E-02	3.362E-02	3.588E-02	4.001E-02	4.393E-02
6	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	2.174E-01	2.198E-01	2.244E-01	2.288E-01
10	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01	1.17E-01
140	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02

Density, Mg/m ³	Temperature, eV									
	0.7	1	1.5	2.5	4	10	25	100	1 000	10 000
0.00001	3.975E-08	6.900E-08	1.495E-07	3.033E-07	6.635E-07	2.729E-06	9.252E-06	5.044E-05	3.368E-04	5.368E-03
0.0001	1.975E-07	6.148E-07	1.244E-06	2.779E-06	5.735E-06	2.360E-05	8.012E-05	5.009E-04	5.368E-03	5.368E-02
0.001	3.490E-06	5.610E-06	1.017E-05	2.419E-05	4.840E-05	2.012E-04	8.198E-04	4.052E-03	5.362E-02	5.368E-01
0.025	7.842E-06	1.17E-05	2.353E-05	4.407E-05	9.201E-05	3.919E-04	1.710E-03	1.052E-02	1.335E-01	1.342E+01
0.06	1.17E-05	2.717E-05	4.957E-05	1.093E-04	2.031E-04	6.634E-04	3.776E-03	2.526E-02	3.199E+00	3.222E+01
0.1	5.975E-04	4.462E-04	6.30E-04	1.679E-03	3.265E-03	1.361E-02	5.866E-02	4.103E-01	5.323E+00	5.366E+01
0.15	4.544E-04	7.196E-04	1.225E-03	2.356E-03	4.651E-03	1.950E-02	8.332E-02	5.990E-01	7.971E+00	6.048E+01
0.25	1.47E-03	1.97E-03	3.07E-03	5.70E-03	7.400E-03	3.417E-02	1.701E-01	9.053E-01	1.325E+01	1.342E+02
0.6	2.264E-03	3.441E-03	4.661E-03	7.603E-03	1.663E-02	8.541E-02	3.189E-01	2.207E+00	3.147E+01	3.215E+02
0.8	3.200E-03	4.740E-03	6.169E-03	1.150E-02	2.140E-02	1.889E-01	4.102E-01	2.093E+00	4.187E+01	4.286E+02
1	2.676E-03	6.200E-03	8.288E-03	1.390E-02	2.538E-02	3.252E-01	5.154E-01	3.568E+00	5.226E+01	5.356E+02
1.14	4.772E-03	7.332E-03	9.636E-03	1.533E-02	2.733E-02	1.475E-01	5.825E-01	4.035E+00	5.951E+01	6.105E+02
1.25	3.919E-03	6.067E-03	9.597E-03	1.663E-02	2.932E-02	1.590E-01	6.344E-01	4.401E+00	6.529E+01	6.694E+02
1.5	3.232E-03	5.739E-03	1.166E-02	1.665E-02	3.332E-02	1.665E-01	5.522E-01	3.807E+00	7.811E+01	6.832E+02
2	5.495E-03	1.268E-02	1.717E-02	2.688E-02	4.334E-02	2.384E-01	9.859E-01	6.656E+00	1.039E+02	1.071E+03
2.2	1.554E-03	1.313E-02	3.453E-02	4.853E-02	4.853E-02	2.555E-01	1.095E-01	7.500E+00	1.141E+02	1.178E+03
2.48	1.516E-02	2.862E-02	2.585E-02	3.673E-02	5.739E-02	2.995E-01	1.214E+00	6.420E+00	1.287E+02	1.331E+03
3	2.812E-02	3.410E-02	3.992E-02	5.109E-02	7.771E-02	3.572E-01	1.462E+00	1.087E+01	1.07E+02	1.686E+03
4	5.100E-02	6.650E-02	6.777E-02	8.401E-02	1.292E-01	4.951E-01	1.958E+00	1.325E+01	2.057E+02	2.141E+03
6	2.434E-01	2.578E-01	2.912E-01	2.277E-01	4.121E-01	9.719E-01	3.050E+00	1.963E+01	3.669E+02	3.289E+03
10	1.37E+01	1.333E+01	1.345E+01	1.337E+01	1.499E+01	1.800E+01	2.563E+01	8.413E+01	1.245E+02	1.335E+03
140	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.057E-02	5.229E-02	5.423E-02	7.791E-02	6.779E+03	7.447E+04

TABLE 3. Values of E (in MJ/g) for selected values of ρ and T of 96 wt% $\text{SiO}_2 + 4$ wt% H_2O (abstracted from the complete EOS table²⁹).

Density, g/cm ³	Temperature, °C									
	0.05	0.055	0.06	0.07	0.1	0.15	0.25	0.3	0.4	0.5
0.0000	2.253E-04	2.515E-04	3.296E-04	4.974E-04	6.674E-04	2.067E-03	1.631E-02	1.762E-02	2.680E-02	3.314E-02
0.0001	2.253E-04	2.535E-04	3.432E-04	5.160E-04	6.822E-04	2.066E-03	1.666E-02	1.747E-02	2.702E-02	3.333E-02
0.001	1.722E-04	2.623E-04	3.690E-04	5.585E-04	7.409E-04	2.067E-03	4.120E-03	1.59E-02	2.610E-02	2.357E-02
0.005	1.340E-04	2.007E-04	4.141E-04	6.227E-04	8.383E-04	2.069E-03	3.707E-03	4.43E-03	1.722E-02	2.831E-02
0.05	1.332E-04	2.594E-04	4.204E-04	6.453E-04	8.691E-04	2.069E-03	3.735E-03	4.52E-03	1.340E-02	1.946E-02
0.1	1.329E-04	2.354E-04	4.372E-04	6.593E-04	8.866E-04	2.070E-03	3.767E-03	4.717E-03	1.105E-02	1.916E-02
0.15	1.327E-04	2.240E-04	4.644E-04	6.700E-04	9.051E-04	2.070E-03	3.763E-03	4.694E-03	9.432E-03	1.856E-02
0.25	1.326E-04	2.160E-04	4.533E-04	6.062E-04	9.275E-04	2.071E-03	3.759E-03	4.673E-03	7.734E-03	1.509E-02
0.3	1.325E-04	2.091E-04	4.670E-04	7.145E-04	9.697E-04	2.067E-03	3.744E-03	4.642E-03	6.779E-03	1.065E-02
0.4	1.325E-04	2.069E-04	4.507E-04	7.245E-04	9.837E-04	2.064E-03	3.735E-03	4.629E-03	6.647E-03	9.500E-03
1	1.325E-04	2.061E-04	4.563E-04	7.326E-04	9.905E-04	2.061E-03	3.720E-03	4.622E-03	6.511E-03	8.930E-03
1.14	1.325E-04	2.057E-04	4.490E-04	7.373E-04	1.005E-03	2.050E-03	3.724E-03	4.616E-03	6.531E-03	8.763E-03
1.25	1.325E-04	2.055E-04	4.429E-04	7.404E-04	1.011E-03	2.057E-03	3.723E-03	4.616E-03	6.503E-03	8.647E-03
1.5	1.325E-04	2.058E-04	4.399E-04	7.450E-04	1.025E-03	2.054E-03	3.716E-03	4.611E-03	6.459E-03	8.445E-03
2	1.325E-04	2.059E-04	4.274E-04	7.649E-04	1.063E-03	2.044E-03	3.715E-03	4.622E-03	6.349E-03	8.113E-03
2.3	1.325E-04	2.173E-04	4.645E-04	7.308E-04	1.091E-03	2.045E-03	3.720E-03	4.652E-03	6.276E-03	7.849E-03
2.68	1.325E-04	2.070E-04	5.181E-04	9.296E-04	1.133E-03	2.042E-03	3.709E-03	4.734E-03	6.200E-03	7.639E-03
3	2.371E-04	4.795E-04	7.214E-04	1.085E-03	1.324E-03	2.124E-03	4.140E-03	5.112E-03	6.090E-03	7.097E-03
4	1.750E-03	1.927E-03	2.147E-03	2.517E-03	2.749E-03	2.981E-03	3.212E-03	3.443E-03	3.674E-03	3.905E-03
6	8.466E-03	8.647E-03	9.407E-03	9.216E-03	9.670E-03	1.044E-02	1.209E-02	1.280E-02	1.451E-02	1.595E-02
10	5.929E-01	5.910E-01	5.942E-01	5.950E-01	5.957E-01	5.964E-01	5.971E-01	5.978E-01	5.985E-01	5.992E-01
140	3.100E+00	3.100E+00	3.100E+00	3.100E+00	3.100E+00	3.100E+00	3.100E+00	3.100E+00	3.100E+00	3.100E+00

Density, g/cm ³	Temperature, °C									
	0.7	1	1.5	2.5	4	10	25	100	1000	10000
0.0000	4.132E-02	5.764E-02	1.122E-01	1.765E-01	4.074E-01	1.524E+01	4.273E+00	1.061E+01	9.945E+01	8.243E+02
0.0001	3.033E-02	4.914E-02	8.609E-02	1.547E-01	3.158E-01	1.141E+01	3.065E+00	1.043E+01	9.939E+01	8.243E+02
0.001	3.499E-02	4.567E-02	6.550E-02	1.294E-01	2.305E-01	9.493E-01	3.474E+00	1.731E+01	9.939E+01	8.243E+02
0.005	2.690E-02	3.670E-02	5.160E-02	9.034E-02	1.536E-01	5.059E-01	2.549E+00	1.370E+01	9.980E+01	8.242E+02
0.05	2.524E-02	3.484E-02	4.900E-02	8.105E-02	1.302E-01	1.167E-01	2.212E+00	1.255E+01	9.989E+01	8.237E+02
0.1	2.466E-02	3.329E-02	4.609E-02	7.771E-02	1.297E-01	4.794E-01	1.980E+00	1.200E+01	9.976E+01	8.237E+02
0.15	2.394E-02	3.222E-02	4.743E-02	7.477E-02	1.297E-01	4.557E-01	1.809E+00	1.136E+01	9.964E+01	8.237E+02
0.25	2.334E-02	3.096E-02	4.665E-02	7.129E-02	1.163E-01	4.291E-01	1.643E+00	1.057E+01	9.967E+01	8.239E+02
0.3	1.954E-02	3.057E-02	4.353E-02	6.625E-02	1.054E-01	3.057E-01	1.459E+00	9.202E+00	9.944E+01	8.267E+02
0.4	1.680E-02	3.102E-02	4.421E-02	6.405E-02	1.014E-01	3.681E-01	1.364E+00	8.912E+00	9.942E+01	8.263E+02
1	1.537E-02	3.129E-02	4.277E-02	6.054E-02	9.604E-02	3.534E-01	1.316E+00	8.646E+00	9.907E+01	8.261E+02
1.14	1.461E-02	3.105E-02	4.230E-02	5.807E-02	9.379E-02	3.440E-01	1.206E+00	8.494E+00	9.902E+01	8.259E+02
1.25	1.410E-02	3.077E-02	4.059E-02	5.610E-02	9.145E-02	3.301E-01	1.205E+00	8.349E+00	9.464E+01	8.250E+02
1.5	1.314E-02	2.790E-02	3.552E-02	5.245E-02	8.706E-02	3.266E-01	1.200E+00	8.100E+00	9.426E+01	8.257E+02
2	1.172E-02	2.001E-02	2.744E-02	4.740E-02	8.100E-02	3.072E-01	1.149E+00	7.051E+00	9.364E+01	8.253E+02
2.3	1.000E-02	1.710E-02	2.594E-02	4.625E-02	7.941E-02	3.005E-01	1.139E+00	7.743E+00	9.342E+01	8.252E+02
2.68	8.630E-03	1.460E-02	2.511E-02	4.506E-02	7.777E-02	2.919E-01	1.112E+00	7.636E+00	9.313E+01	8.250E+02
3	1.067E-02	1.400E-02	2.519E-02	4.392E-02	7.595E-02	2.824E-01	1.085E+00	7.308E+00	9.265E+01	8.247E+02
4	1.252E-02	1.665E-02	2.666E-02	4.421E-02	7.493E-02	2.686E-01	1.036E+00	7.089E+00	9.194E+01	8.243E+02
6	2.063E-02	2.532E-02	3.255E-02	5.150E-02	8.110E-02	2.539E-01	9.634E-01	6.660E+00	9.067E+01	8.236E+02
10	3.057E-01	3.112E-01	3.164E-01	3.395E-01	3.691E-01	5.033E-01	9.956E-01	5.529E+00	6.522E+01	8.204E+02
140	3.201E+00	3.206E+00	3.212E+00	3.222E+00	3.249E+00	3.397E+00	3.700E+00	6.559E+00	7.709E+01	8.139E+02

TABLE 4. Values of P (in TPa) for selected values of ρ and T of 90 wt% SiO₂ + 10 wt% H₂O (abstracted from the complete EOS table²⁹).

Density, Mg/m ³	Temperature, eV									
	0.025	0.035	0.05	0.07	0.1	0.15	0.25	0.5	0.8	0.9
0.00001	1.357E-10	1.087E-10	7.405E-11	5.177E-11	3.490E-11	2.075E-11	1.622E-09	1.151E-08	1.176E-08	2.401E-08
0.0001	1.353E-09	1.075E-09	7.344E-10	5.141E-10	3.474E-10	2.064E-10	1.619E-08	1.146E-08	1.170E-08	2.395E-08
0.001	2.340E-08	1.872E-08	1.304E-08	9.141E-09	6.149E-09	3.642E-09	1.645E-07	1.104E-07	1.104E-07	2.242E-07
0.01	2.340E-07	1.872E-07	1.304E-07	9.141E-08	6.149E-08	3.642E-08	1.645E-06	1.104E-06	1.104E-06	2.242E-06
0.06	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
0.1	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
0.15	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
0.25	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
0.5	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
0.8	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
1	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
1.14	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
1.25	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
1.5	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
2	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
2.2	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
2.48	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
3	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
4	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
6	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
25	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05
160	2.340E-06	1.872E-06	1.304E-06	9.141E-07	6.149E-07	3.642E-07	1.645E-05	1.104E-05	1.104E-05	2.242E-05

Density, Mg/m ³	Temperature, eV									
	0.7	1	1.5	2.5	4	10	25	100	1000	10000
0.00001	4.149E-08	3.173E-08	2.297E-08	1.621E-08	1.149E-08	6.149E-09	3.173E-09	1.621E-09	8.149E-10	4.149E-10
0.0001	4.149E-07	3.173E-07	2.297E-07	1.621E-07	1.149E-07	6.149E-08	3.173E-08	1.621E-08	8.149E-09	4.149E-09
0.001	4.149E-06	3.173E-06	2.297E-06	1.621E-06	1.149E-06	6.149E-07	3.173E-07	1.621E-07	8.149E-08	4.149E-08
0.01	4.149E-05	3.173E-05	2.297E-05	1.621E-05	1.149E-05	6.149E-06	3.173E-06	1.621E-06	8.149E-07	4.149E-07
0.025	6.999E-05	5.149E-05	3.649E-05	2.599E-05	1.849E-05	1.049E-05	5.149E-06	2.599E-06	1.249E-06	6.999E-07
0.06	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
0.1	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
0.15	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
0.25	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
0.5	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
0.8	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
1	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
1.14	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
1.25	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
1.5	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
2	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
2.2	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
2.48	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
3	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
4	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
6	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
25	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06
160	0.000149	0.000109	7.999E-05	5.599E-05	3.999E-05	2.249E-05	1.149E-05	5.999E-06	2.999E-06	1.499E-06

TABLE 5. Values of E (in MJ/g) for selected values of ρ and T of 90 wt% SiO₂ + 10 wt% H₂O (abstracted from the complete EOS table²⁹).

Density, Mg/m ³	Temperature, eV									
	0.025	0.033	0.05	0.07	0.1	0.15	0.25	0.3	0.4	0.5
0.0001	3.905E-04	4.247E-04	5.236E-04	6.947E-04	8.938E-04	2.788E-03	1.643E-02	2.124E-02	2.578E-02	3.492E-02
0.001	3.695E-04	4.292E-04	5.373E-04	7.198E-04	9.286E-04	2.785E-03	6.502E-03	1.174E-02	2.415E-02	2.931E-02
0.01	1.377E-04	4.305E-04	5.621E-04	7.621E-04	9.867E-04	2.785E-03	4.434E-03	1.435E-02	2.134E-02	2.666E-02
0.03	1.682E-04	3.878E-04	6.006E-04	8.341E-04	1.084E-03	2.276E-03	4.118E-03	5.737E-03	1.728E-02	1.122E-02
0.05	1.535E-04	3.889E-04	6.197E-04	8.556E-04	1.115E-03	2.267E-03	4.044E-03	5.172E-03	1.132E-02	7.400E-02
0.1	1.599E-04	2.668E-04	6.264E-04	8.683E-04	1.155E-03	2.266E-03	4.044E-03	5.172E-03	1.047E-02	1.367E-02
0.15	1.589E-04	2.768E-04	6.305E-04	8.782E-04	1.151E-03	2.264E-03	4.044E-03	5.074E-03	6.527E-03	1.659E-02
0.25	1.587E-04	2.672E-04	6.328E-04	8.799E-04	1.170E-03	2.364E-03	4.044E-03	4.061E-03	4.061E-03	1.485E-02
0.3	1.586E-04	2.596E-04	5.856E-04	9.041E-04	1.149E-03	2.359E-03	4.001E-03	4.444E-03	7.312E-03	1.062E-02
0.4	1.586E-04	2.582E-04	5.577E-04	9.048E-04	1.120E-03	2.374E-03	3.967E-03	4.744E-03	5.211E-03	9.982E-03
0.5	1.586E-04	2.574E-04	5.114E-04	9.407E-04	1.121E-03	2.374E-03	3.967E-03	4.966E-03	4.966E-03	9.982E-03
1	1.586E-04	2.578E-04	5.327E-04	9.368E-04	1.114E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.500E-03
1.14	1.586E-04	2.567E-04	5.274E-04	9.355E-04	1.115E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.496E-03
1.3	1.586E-04	2.563E-04	5.181E-04	9.355E-04	1.115E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.496E-03
1.5	1.586E-04	2.563E-04	5.181E-04	9.355E-04	1.115E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.496E-03
2	1.586E-04	2.486E-04	5.476E-04	9.041E-04	1.124E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.496E-03
2.3	1.586E-04	2.289E-04	5.809E-04	9.144E-04	1.127E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.496E-03
2.6	1.582E-04	3.677E-04	6.265E-04	9.144E-04	1.127E-03	2.374E-03	3.967E-03	4.744E-03	4.744E-03	9.496E-03
3	4.062E-04	6.753E-04	9.687E-04	1.257E-03	1.257E-03	1.257E-03	1.257E-03	1.257E-03	1.257E-03	9.496E-03
4	2.231E-03	2.732E-03	2.708E-03	8.353E-03	2.391E-03	1.257E-03	1.257E-03	1.257E-03	1.257E-03	1.257E-03
6	9.885E-03	1.018E-02	1.039E-02	1.091E-02	1.124E-02	1.124E-02	1.124E-02	1.124E-02	1.124E-02	1.124E-02
23	3.162E-01	3.164E-01	3.166E-01	3.169E-01	3.171E-01	3.171E-01	3.171E-01	3.171E-01	3.171E-01	3.171E-01
100	3.321E+00	3.322E+00	3.322E+00	3.324E+00	3.324E+00	3.324E+00	3.324E+00	3.324E+00	3.324E+00	3.324E+00

Density, Mg/m ³	Temperature, eV									
	0.7	1	1.5	2.5	4	10	25	100	1 000	10 000
0.0001	4.299E-02	6.822E-02	1.218E-01	1.892E-01	4.177E-01	1.757E+00	4.712E+00	1.17E+01	1.005E+02	5.387E+02
0.001	4.028E-02	5.126E-02	9.245E-02	1.667E-01	5.274E-01	1.177E+00	2.749E+00	1.17E+01	1.005E+02	6.347E+02
0.01	3.692E-02	4.978E-02	6.807E-02	1.403E-01	8.747E-01	1.247E+00	2.749E+00	1.17E+01	1.005E+02	6.347E+02
0.03	2.871E-02	3.874E-02	5.408E-02	9.637E-02	1.654E-01	6.088E-01	2.749E+00	1.17E+01	1.005E+02	6.347E+02
0.06	2.685E-02	3.657E-02	5.200E-02	8.763E-02	1.488E-01	4.350E-01	2.749E+00	1.17E+01	1.005E+02	6.347E+02
0.1	2.681E-02	3.514E-02	5.086E-02	8.473E-02	1.368E-01	4.350E-01	2.749E+00	1.17E+01	1.005E+02	6.347E+02
0.15	2.542E-02	3.402E-02	5.010E-02	7.955E-02	1.324E-01	4.350E-01	1.17E+01	1.17E+01	1.17E+01	6.347E+02
0.25	2.471E-02	3.267E-02	4.913E-02	7.555E-02	1.240E-01	4.350E-01	1.17E+01	1.17E+01	1.17E+01	6.347E+02
0.3	2.558E-02	3.122E-02	4.744E-02	6.765E-02	1.115E-01	4.005E-01	1.17E+01	1.17E+01	1.17E+01	6.412E+02
0.4	1.889E-02	3.263E-02	4.595E-02	6.621E-02	1.061E-01	3.818E-01	1.404E+00	5.03E+00	4.755E+01	6.403E+02
1	1.639E-02	3.268E-02	4.513E-02	6.181E-02	1.005E-01	3.646E-01	1.757E+00	6.783E+00	4.234E+01	6.403E+02
1.14	1.547E-02	3.288E-02	4.219E-02	5.886E-02	9.636E-02	3.557E-01	1.757E+00	6.637E+00	4.600E+01	6.404E+02
1.3	1.485E-02	3.113E-02	3.936E-02	5.710E-02	9.367E-02	3.514E-01	1.762E+00	6.783E+00	4.755E+01	6.403E+02
1.5	1.398E-02	2.680E-02	3.354E-02	5.362E-02	9.033E-02	3.366E-01	1.756E+00	6.783E+00	5.565E+01	6.402E+02
2	1.241E-02	2.821E-02	2.831E-02	4.964E-02	8.520E-02	3.189E-01	1.767E+00	6.002E+00	9.485E+01	6.399E+02
2.3	1.192E-02	1.689E-02	2.778E-02	4.851E-02	8.354E-02	3.107E-01	1.765E+00	6.783E+00	9.435E+01	6.397E+02
2.6	1.197E-02	1.728E-02	2.764E-02	4.789E-02	8.263E-02	3.071E-01	1.752E+00	7.751E+00	9.433E+01	6.396E+02
3	1.250E-02	1.651E-02	2.880E-02	4.717E-02	8.124E-02	2.961E-01	1.725E+00	7.755E+00	9.388E+01	6.392E+02
4	1.453E-02	1.821E-02	2.940E-02	4.627E-02	8.048E-02	2.820E-01	1.674E+00	7.242E+00	9.312E+01	6.386E+02
6	2.547E-02	2.863E-02	3.654E-02	5.660E-02	7.919E-02	2.682E-01	1.601E+00	6.821E+00	9.193E+01	6.382E+02
23	3.322E-01	3.334E-01	3.478E-01	3.662E-01	3.967E-01	5.481E-01	1.844E+00	5.781E+00	6.656E+01	6.349E+02
100	3.338E+00	3.341E+00	3.348E+00	3.351E+00	3.358E+00	3.369E+00	3.378E+00	3.389E+00	3.399E+00	3.409E+00

TABLE 6. Values of P (in TPa) for selected values of ρ and T of 80 wt% SiO₂ + 20 wt% H₂O (abstracted from the complete EOS table²⁹).

Density, Mg/m ³	Temperature, eV									
	0.025	0.035	0.05	0.07	0.1	0.15	0.25	0.3	0.4	0.5
0.00001	2.516E-10	3.972E-10	5.683E-10	7.957E-10	1.136E-09	1.708E-09	0.765E-09	1.441E-08	2.163E-08	3.358E-08
0.0001	2.340E-09	3.750E-09	5.358E-09	7.502E-09	1.072E-08	1.610E-08	5.408E-08	1.136E-07	2.169E-07	3.630E-07
0.001	2.340E-09	3.740E-08	5.354E-08	7.501E-08	1.074E-07	1.611E-07	2.984E-07	9.512E-07	1.708E-06	2.738E-06
0.015	2.340E-09	2.956E-07	4.180E-07	6.073E-07	2.795E-06	4.161E-06	7.076E-06	9.988E-06	3.766E-05	5.390E-05
0.05	2.340E-09	2.956E-07	3.022E-06	4.474E-06	7.043E-06	1.043E-05	1.758E-05	2.718E-05	7.339E-05	1.264E-04
0.1	2.340E-09	2.956E-07	4.831E-06	7.425E-06	1.184E-05	1.641E-05	3.071E-05	3.795E-05	6.753E-05	2.294E-04
0.25	2.340E-09	2.956E-07	9.408E-06	1.814E-05	2.941E-05	4.273E-05	8.239E-05	1.026E-04	1.792E-04	4.795E-04
0.4	2.340E-09	2.956E-07	5.488E-06	4.183E-05	7.719E-05	1.416E-04	2.618E-04	3.299E-04	5.299E-04	6.924E-04
0.6	2.340E-09	2.956E-07	5.488E-06	4.183E-05	7.719E-05	1.416E-04	2.618E-04	3.299E-04	5.299E-04	6.924E-04
0.8	2.340E-09	2.956E-07	4.405E-06	4.776E-05	1.127E-04	2.122E-04	4.405E-04	6.658E-04	8.649E-04	1.300E-03
1	2.340E-09	2.956E-07	4.405E-06	4.776E-05	1.127E-04	1.779E-04	7.108E-04	9.988E-04	1.365E-03	1.933E-03
1.14	2.340E-09	2.956E-07	5.488E-06	8.179E-05	2.066E-04	4.483E-04	6.749E-04	1.237E-03	1.854E-03	2.544E-03
1.35	2.340E-09	2.956E-07	5.488E-06	8.179E-05	2.066E-04	4.483E-04	1.136E-03	1.980E-03	2.352E-03	3.161E-03
1.5	2.340E-09	2.956E-07	5.488E-06	8.179E-05	4.194E-04	5.749E-04	2.162E-03	2.568E-03	4.009E-03	5.131E-03
2	1.000E-07	1.827E-04	5.344E-04	1.072E-03	1.377E-03	6.715E-03	2.723E-03	1.073E-02	1.073E-02	1.228E-02
2.3	1.508E-04	1.032E-03	1.757E-03	2.727E-03	3.774E-03	5.749E-03	7.742E-03	1.144E-02	1.452E-02	1.674E-02
2.48	4.869E-04	3.249E-03	4.889E-03	7.599E-03	8.894E-03	1.011E-02	1.422E-02	1.788E-02	2.116E-02	2.382E-02
3	1.427E-03	1.404E-03	1.404E-03	1.404E-03	1.404E-03	1.404E-03	1.404E-03	1.404E-03	1.404E-03	1.404E-03
4	3.964E-04	4.458E-03	4.458E-03	4.458E-03	4.458E-03	4.458E-03	4.458E-03	4.458E-03	4.458E-03	4.458E-03
5	2.679E-04	1.474E-03	1.474E-03	1.474E-03	1.474E-03	1.474E-03	1.474E-03	1.474E-03	1.474E-03	1.474E-03
25	1.540E-04	1.540E-03	1.540E-03	1.540E-03	1.540E-03	1.540E-03	1.540E-03	1.540E-03	1.540E-03	1.540E-03
140	5.494E-04	5.494E-03	5.494E-03	5.494E-03	5.494E-03	5.494E-03	5.494E-03	5.494E-03	5.494E-03	5.494E-03

Density, Mg/m ³	Temperature, eV									
	0.7	1	1.5	2.5	4	10	25	100	1 000	10 000
0.00001	5.179E-08	0.470E-08	1.923E-07	4.747E-07	7.747E-07	3.611E-06	1.013E-05	5.761E-05	5.634E-04	5.634E-03
0.0001	4.974E-07	7.835E-07	1.174E-06	2.744E-06	7.071E-06	2.720E-05	6.721E-05	5.322E-04	5.632E-03	5.634E-02
0.001	4.683E-06	7.204E-06	1.240E-05	2.077E-05	6.047E-05	2.342E-04	9.126E-04	5.150E-03	5.628E-02	5.634E-01
0.015	9.704E-05	1.579E-04	2.749E-04	4.774E-04	1.197E-03	4.144E-03	1.937E-02	1.160E-01	1.402E+00	1.408E+01
0.05	2.297E-04	3.725E-04	6.411E-04	1.170E-03	2.697E-03	1.070E-02	4.194E-02	2.684E-01	3.358E+00	3.380E+01
0.1	1.924E-04	2.244E-04	4.174E-04	1.194E-03	4.174E-03	2.679E-02	4.363E-01	5.687E+00	5.632E+00	5.632E+01
0.25	1.128E-03	1.703E-03	2.774E-03	6.044E-03	6.044E-03	4.270E-02	1.954E-01	1.038E+00	1.391E+01	1.408E+02
0.4	3.127E-03	4.534E-03	6.754E-03	1.179E-02	2.194E-02	1.002E-01	3.664E-01	2.391E+00	3.309E+01	3.375E+02
0.6	3.442E-03	4.405E-03	6.967E-03	1.531E-02	2.539E-02	1.206E-01	4.168E-01	3.144E+00	4.405E+01	4.485E+02
1	4.052E-03	6.407E-03	1.171E-02	1.875E-02	3.398E-02	1.590E-01	5.341E-01	3.687E+00	5.496E+01	5.624E+02
1.14	4.821E-03	9.740E-03	1.707E-02	1.143E-02	3.707E-02	1.783E-01	6.722E-01	4.403E+00	6.262E+01	6.410E+02
1.35	5.680E-03	1.093E-02	1.451E-02	1.777E-02	4.053E-02	1.932E-01	7.332E-01	4.605E+00	6.861E+01	7.029E+02
1.5	6.169E-03	1.429E-02	1.697E-02	2.053E-02	4.939E-02	2.274E-01	8.718E-01	5.714E+00	6.222E+01	6.434E+02
2	1.662E-02	2.335E-02	2.959E-02	4.275E-02	7.804E-02	1.874E-01	1.142E+00	7.475E+00	1.089E+02	1.118E+03
2.3	2.174E-02	2.865E-02	3.542E-02	5.445E-02	9.908E-02	3.717E-01	1.567E+00	1.201E+01	1.201E+02	1.237E+03
2.48	2.986E-02	3.721E-02	4.579E-02	6.019E-02	9.591E-02	1.761E-01	1.404E+00	9.287E+00	1.363E+02	1.405E+03
3	4.408E-02	5.540E-02	6.749E-02	8.078E-02	1.243E-01	4.562E-01	1.795E+00	1.75E+01	1.632E+02	1.686E+03
4	8.897E-02	1.029E-01	1.168E-01	1.470E-01	2.074E-01	6.455E-01	2.297E+00	1.456E+01	2.168E+02	2.248E+03
6	3.138E-01	3.272E-01	3.693E-01	4.201E-01	5.307E-01	1.176E+00	3.623E+00	2.161E+01	3.236E+02	3.370E+03
25	1.561E+01	1.569E+01	1.579E+01	1.606E+01	1.653E+01	1.853E+01	2.545E+01	5.283E+01	1.316E+02	1.402E+04
140	5.495E+02	5.500E+02	5.509E+02	5.700E+02	5.716E+02	5.836E+02	6.438E+02	8.435E+02	7.149E+03	7.878E+04

TABLE 7. Values of E (in MJ/g) for selected values of ρ and T of 80 wt% SiO₂ + 20 wt% H₂O (abstracted from the complete EOS table²⁹).

Density, Mg/m ³	Temperature, eV									
	0.06	0.15	0.3	0.7	1	1.5	2.5	5	10	15
0.0001	6.66E-04	7.15E-04	8.70E-04	1.02E-03	1.27E-03	1.47E-03	1.67E-03	1.87E-03	2.07E-03	2.27E-03
0.001	6.012E-04	7.153E-04	8.40E-04	1.07E-03	1.31E-03	1.51E-03	1.71E-03	1.91E-03	2.11E-03	2.31E-03
0.01	2.40E-04	7.20E-04	8.71E-04	1.09E-03	1.31E-03	1.51E-03	1.71E-03	1.91E-03	2.11E-03	2.31E-03
0.025	2.037E-04	4.702E-04	9.11E-04	1.14E-03	1.34E-03	1.54E-03	1.74E-03	1.94E-03	2.14E-03	2.34E-03
0.05	2.027E-04	3.90E-04	9.107E-04	1.174E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
0.1	2.024E-04	3.721E-04	9.102E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
0.25	2.022E-04	3.525E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
0.5	2.021E-04	3.045E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
1	2.021E-04	3.435E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
1.14	2.021E-04	3.421E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
1.25	2.021E-04	3.420E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
1.5	2.021E-04	3.420E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
2	2.020E-04	3.420E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
2.3	1.970E-04	4.109E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
2.48	2.760E-04	3.162E-04	8.707E-04	1.173E-03	1.37E-03	1.57E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03
3	8.790E-04	1.195E-03	1.509E-03	1.77E-03	1.97E-03	2.17E-03	2.37E-03	2.57E-03	2.77E-03	2.97E-03
4	2.964E-03	3.219E-03	3.520E-03	3.821E-03	4.122E-03	4.423E-03	4.724E-03	5.025E-03	5.326E-03	5.627E-03
6	1.263E-02	1.274E-02	1.285E-02	1.296E-02	1.307E-02	1.318E-02	1.329E-02	1.340E-02	1.351E-02	1.362E-02
25	3.605E-01	3.607E-01	3.611E-01	3.615E-01	3.619E-01	3.623E-01	3.627E-01	3.631E-01	3.635E-01	3.639E-01
140	3.549E+00	3.549E+00	3.549E+00	3.549E+00	3.549E+00	3.549E+00	3.549E+00	3.549E+00	3.549E+00	3.549E+00

Density, Mg/m ³	Temperature, eV									
	0.7	1	1.5	2.5	4	10	25	100	1000	10000
0.0001	4.504E-02	6.444E-02	1.727E-01	7.107E-01	2.11E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.001	4.339E-02	5.402E-02	1.017E-01	1.77E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.01	4.022E-02	4.906E-02	7.494E-02	1.77E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.025	3.170E-02	4.229E-02	5.031E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.05	2.947E-02	3.901E-02	5.643E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.1	2.055E-02	3.024E-02	5.047E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.25	2.716E-02	4.535E-02	6.210E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
0.5	2.231E-02	3.502E-02	5.013E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
1	1.937E-02	3.498E-02	4.799E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
1.14	1.765E-02	3.451E-02	4.444E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
1.25	1.696E-02	3.175E-02	4.014E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
1.5	1.651E-02	2.975E-02	3.773E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
2	1.550E-02	2.650E-02	3.393E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
3	1.440E-02	2.207E-02	3.219E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
2.3	1.451E-02	2.103E-02	3.206E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
2.48	1.436E-02	2.074E-02	3.217E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
3	1.506E-02	2.035E-02	3.252E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
4	1.769E-02	2.220E-02	3.391E-02	1.040E-01	5.7E-01	1.14E-01	6.40E-02	3.60E-02	2.00E-02	1.10E-02
6	2.807E-02	3.568E-02	4.343E-02	6.532E-02	9.940E-02	2.904E-01	1.064E-01	7.001E-01	3.405E+01	6.625E+01
25	3.776E-01	3.047E-01	3.916E-01	4.130E-01	4.505E-01	6.005E-01	1.130E-01	1.650E+01	6.604E+01	6.552E+02
140	3.965E+00	3.571E+00	3.580E+00	3.659E+00	3.693E+00	3.666E+00	4.195E+00	7.296E+00	8.113E+01	8.529E+02

RESULTS AND SUMMARY

ISOTHERMS

The final pressure and energy isotherms are shown in Figs. 4a and 4b, respectively, for the 96 wt% $\text{SiO}_2 + 4 \text{ wt}\% \text{H}_2\text{O}$ system. The corresponding plots for the 90 wt% $\text{SiO}_2 + 10 \text{ wt}\% \text{H}_2\text{O}$ and the 80 wt% $\text{SiO}_2 + 20 \text{ wt}\% \text{H}_2\text{O}$ systems are shown in Figs. 5 and 6, respectively. To illustrate the three-dimensional nature of P and E, we have plotted $\log_e P$ and $\log_e E$ as functions of $\log_e \rho$ and $\log_e T$ ($T \leq 100 \text{ eV}$) for three $\text{SiO}_2 + \text{H}_2\text{O}$ systems (Figs. 7-9).

The isotherms in Figs. 5 to 16 describe a region below $T = 0.0585 \text{ eV}$ where the liquid-vapor transition of water takes place and a higher T-region between 0.1 and 1 eV where SiO_2 undergoes a similar phase change. In spite of the relatively small amount of water contained in the 96 wt% $\text{SiO}_2 + 4 \text{ wt}\% \text{H}_2\text{O}$ mixture, it is evident that the final EOS data is rather sensitive to the presence of water. Therefore, an underground explosion in rock containing a small amount of water is expected to create a larger explosion cavity because of the increase in the cavity pressure due to vaporized water.

HUGONIOTS

Hugoniots of $\text{SiO}_2 + \text{H}_2\text{O}$ mixtures were measured by Anderson³⁰ for three different compositions of SiO_2 and H_2O : 96 wt% $\text{SiO}_2 + 4 \text{ wt}\% \text{H}_2\text{O}$, 90 wt% $\text{SiO}_2 + 10 \text{ wt}\% \text{H}_2\text{O}$, and 81 wt% $\text{SiO}_2 + 19 \text{ wt}\% \text{H}_2\text{O}$. These compositions are either identical or very nearly equivalent to those for which the EOS data in this work was calculated. However, the samples used by Anderson in the first two cases were porous and their densities were thus slightly lower ($\rho_0 = 1.72$ and 1.96 Mg/m^3 , respectively) than samples without pores ($\rho_0 = 2.485$ and 2.274 Mg/m^3 , respectively). The third case did not deal with porous samples. Figures 10a and 10b plot Anderson's data and the theoretical Hugoniots, both with and without the nonequilibrium correction mentioned earlier for the 96 wt% $\text{SiO}_2 + 4 \text{ wt}\% \text{H}_2\text{O}$ mixture. Similar plots for the other two mixtures are shown in Figs. 11 and 12. The theoretical calculations for the 96 wt% $\text{SiO}_2 + 4 \text{ wt}\% \text{H}_2\text{O}$ and the 90 wt% $\text{SiO}_2 + 10 \text{ wt}\% \text{H}_2\text{O}$ mixtures were conducted assuming that the porous samples have the same energies initially as those of the fully compacted samples and that the pores are very weak; negligibly small applied pressure can thus collapse the pores. Figures 10, 11, and 12 show that the theoretical (including the nonequilibrium correction) and the experimental data agree satisfactorily. Further refinements in the theoretical data are possible, but because the experimental error is probably as large as the observed deviations between the theoretical and the experimental data, such refinements were not included. It should be noted that the SiO_2 data used to generate the EOS data of the $\text{SiO}_2 + \text{H}_2\text{O}$ mixtures incorporate a correction factor for the nonequilibrium effect. Although this factor is appropriate for a system of dry, nonporous, crystalline quartz, it is too large for porous SiO_2 and $\text{SiO}_2 + \text{H}_2\text{O}$ mixtures. As a result, the Hugoniots (dashed lines, Figs. 10-12) lie above the observed data points. It was therefore necessary to compensate for the excessive correction so that the Hugoniot data for water-containing rocks would agree with the observed data.

ISENTROPES

In Fig. 13, we show the expansion isentropes of the 80 wt% $\text{SiO}_2 + 20 \text{ wt}\% \text{H}_2\text{O}$ mixture starting from ρ_0 at four different initial temperatures (T_0). We plotted these isentropes to show the effect of T_0 on the trajectories of the isentropes. The isentrope for $T_0 = 10 \text{ eV}$ lies entirely within the (ρ, T) range in which both SiO_2 and H_2O exist only as gases, whereas the isentrope for $T_0 = 1 \text{ eV}$ lies primarily within the liquid-gas transition range of SiO_2 in which H_2O is still completely in the vapor phase. The expansion isentrope for $T_0 = 0.1 \text{ eV}$ lies in a region composed mostly with liquid $\text{SiO}_2 + \text{gaseous H}_2\text{O}$. The expansion isentrope for $T_0 = 0.04 \text{ eV}$ initially decreases sharply with density. Within this portion, SiO_2 and

FIG. 4. (a) Pressure and (b) energy isotherms of 96 wt% SiO_2 + 4 wt% H_2O mixture. There are 43 isotherms denoted by T_i ($i = 1, 2, \dots, 43$):

0.025 eV	0.6 eV	100 eV
0.03	0.7	150
0.035	0.8	250
0.04	1	400
0.05	1.5	600
0.07	2.5	1 000
0.1	4	1 500
0.13	6	2 500
0.15	8	4 000
0.18	10	6 000
0.2	15	10 000
0.25	25	15 000
0.3	40	25 000
0.4	60	
0.5	80

FIG. 5. (a) Pressure and (b) energy isotherms of 90 wt% SiO_2 + 10 wt% H_2O mixture. There are 43 isotherms (see Fig. 4).

FIG. 6. (a) Pressure and (b) energy isotherms of 80 wt% SiO_2 + 20 wt% H_2O mixture. There are 43 isotherms (See Fig. 4).

FIG. 7. (a) $\log_e P$ (in TPa) and (b) $\log_e E$ (in MJ/g) of 96 wt% SiO_2 + 4 wt% H_2O mixture as functions of $\log_e \rho$ (in Mg/m^3) and $\log_e T$ (in eV) (to $T = 100$ eV).

FIG. 8. (a) $\log_e P$ (in TPa) and (b) $\log_e E$ (in MJ/g) of 90 wt% SiO_2 + 10 wt% H_2O mixture as functions of $\log_e \rho$ (in Mg/m^3) and $\log_e T$ (in eV) (to $T = 100 \text{ eV}$).

FIG. 9. (a) $\log_e P$ (in TPa) and (b) $\log_e E$ (in MJ/g) of 80 wt% SiO_2 + 20 wt% H_2O mixture as functions of $\log_e \rho$ (in Mg/m^3) and $\log_e T$ (in eV) (to $T = 100$ eV).

FIG. 10. (a) Shock-velocity vs particle velocity and (b) Hugoniot pressure vs density of porous 96 wt% SiO₂ + 4 wt% H₂O mixture. Solid lines represent the renormalized Hugoniot for the mixture which take into account the nonequilibrium effect of the mixture. Dashed lines represent the Hugoniot based on crystalline quartz (with the nonequilibrium correction) and H₂O data. Dots represent the experimental data of Anderson.³⁰ The initial density of the porous samples is 1.72 Mg/m³; the normal density of the mixture without the pores is 2.485 Mg/m³.

FIG. 11. (a) Shock-velocity vs particle velocity and (b) Hugoniot pressure vs density of porous 90 wt% SiO_2 + 10 wt% H_2O mixture. Solid lines represent the renormalized Hugoniot for the mixture which take into account the nonequilibrium effect of the mixture. Dashed lines represent the Hugoniot based on crystalline quartz (with the nonequilibrium correction) and H_2O data. Dots represent the experimental data of Anderson.³⁰ The initial density of the porous samples is 1.96 Mg/m^3 ; the normal density of the mixture without the pores is 2.274 Mg/m^3 .

FIG. 12. (a) Shock-velocity vs particle velocity and (b) Hugoniot pressure vs density of 80 wt% SiO_2 + 20 wt% H_2O mixture. Solid lines represent the renormalized Hugoniot for the mixture which take into account the nonequilibrium effect of the mixture. Dashed lines represent the Hugoniot based on crystalline quartz (with the nonequilibrium correction) and H_2O data. Dots represent the experimental data of 81 wt% SiO_2 + 19 wt% H_2O system (fully saturated sands) obtained by Anderson.³⁰ In the Hugoniot calculations, the initial density is taken to be same as the normal density of the mixture (1.991 Mg/m^3).

FIG. 13. Expansion isentropes of 80 wt% SiO_2 + 20 wt% H_2O mixture with initial (ρ_0, T_0) points at $\rho_0 = 1.991 \text{ Mg/m}^3$ and $T_0 = 0.04, 0.1, 1, \text{ and } 10 \text{ eV}$. The isentropes (solid lines) are superimposed over isotherms of the mixture (dotted lines) to illustrate that the trajectories of the isentropes pass through the phase change regions of SiO_2 or H_2O in the mixture.

H_2O exist in the solid and liquid phases, respectively. At greater density, the isentrope flattens out in a manner similar to one of the isotherms of the 80 wt% SiO_2 + 20 wt% H_2O mixture. Within this region, water undergoes the liquid-vapor phase change while SiO_2 remains in the solid phase. The vapor pressure of SiO_2 can be neglected, and most of the pressure of the isentrope is attributable to the vapor pressure of water. Figure 13 shows that soil located at different positions from the center of an underground test can attain a wide variety of different thermodynamic states, depending on distance from the center. It also shows that all physically possible thermodynamic phases of the rock-water mixtures must be included in the EOS data to realistically simulate a surface or subsurface explosion.

DYNAMIC RESPONSE OF SiO_2 MIXTURES

When an explosion occurs inside water-containing rocks, each region surrounding the explosion center experiences different pressures, temperatures, and compression histories. These histories depend on the yield of high explosive, the water content of the rocks, and the speed of propagation of the disturbance from zones closer to the explosion center. Such complex dynamic behavior may be simulated using a hydrodynamic code. In fact, the chief motivation of the present work is the need to provide satisfactory EOS data of hydrous rocks required in such a study.

FIG. 14. Snapshots of density profiles at 1, 3, 5, and 7 ms after 92.6-kt-yield explosion in (a) fully compacted dry rock ($\rho_0 = 2.65 \text{ Mg/m}^3$) and (b) fully saturated rock ($\rho_0 = 1.991 \text{ Mg/m}^3$).

FIG. 15. Pressure vs density trajectories of two zones in a 90 wt% SiO_2 + 10 wt% H_2O rock. The zones are located initially at 5.3 m (*) and 10 m (+) from the center of a 92.6-kt-yield explosion. Twenty-five isotherms generated in this work (dashed lines) are superimposed on the trajectories (see Fig. 4 for isotherm values).

We describe below a limited exemplary study of this type by simulating the first 10 ms of a simplest underground explosion. Initially, we deposit an energy of 92.6 kt in an iron sphere with a radius of 46 cm surrounded by rock strata with varying amounts of water. Because we are concerned with the early-time phenomenology of the explosion where the pressure generally remains above 6 GPa, the material strength of rocks will be ignored in the following discussion. In Figs. 14a and 14b, "snapshots" of the density are shown at 1, 3, 5, and 7 ms after the explosion for two cases, i.e., the fully compacted dry rock ($\rho_0 = 2.65 \text{ Mg/m}^3$) and the fully water-saturated rock ($\rho_0 = 1.991 \text{ Mg/m}^3$). The profiles appear qualitatively different near the shock front at $t = 5$ and 7 ms. In the case of the dry rock, the profiles in Fig. 14a consist of two distinct regions: the region near the shock front where $\rho \geq \rho_0$ and the high-T and low- ρ "fireball" region near the

FIG. 16. Pressure vs density trajectories of zone initially 10 m from center of 92.6-kt-yield explosion in rocks of different water content.

explosion center. Because the fully compacted rock is less compressible than hydrated rocks, the shock heating at $t = 5$ ms or later is insufficient to vaporize the rock, and the disturbance propagates through the solid region. We thus expect the shock front to break away from the gaseous fireball region near the explosion center. In the case of water-bearing rocks, a relatively weak shock strength of about 3 GPa is sufficient to vaporize water along the release path of the shock. Thus, except for the compressed region near the shock front, the pressure along the release path in the rock media depends on the materials that have been vaporized, namely, SiO_2 and H_2O in the central fireball region and water vapor for most of the remaining portion. The profiles in Fig. 14b therefore show only a gas-like behavior. At later times ($t \geq 0.01$ s), when the attenuated strength of the shock cannot vaporize water, we should expect to see profiles characteristic of a condensed phase because the shock propagates only through the condensed medium.

In Fig. 15, we fix two zones, initially at $x_0 = 5.3$ and 10 m from the explosion center, in fully saturated rock and look at the trajectories of P vs ρ after the shock wave arrives at these zones. The dashed lines indicate the isotherms of the 80 wt% SiO_2 and 20 wt% H_2O mixture at the indicated temperatures. The trajectory for $x_0 = 5.3$ m traces entirely along the gaseous phases of SiO_2 and H_2O , whereas SiO_2 remains in the liquid or solid phase along the release path for $x_0 = 10$ m. Figure 16 shows the P vs ρ/ρ_0 release paths at the zone at $x_0 = 10$ m in rocks with the four different water contents considered in this work. As expected, the dry rock is compressed the least and is thus heated the least. It exhibits the lowest pressure at low-compression (low ρ/ρ_0) of the four samples because of the lack of water vapor. The fully saturated rock achieves the greatest compression and hence greatest heating; it exhibits the greatest pressure at low compression because it contains large amounts of water vapor. Figure 17 demonstrates that this effect is closely related to the magnitude of the radial displacement of the medium; the motion of the zone initially at $x_0 = 20$ m is shown as

FIG. 17. Radial displacements of zone initially 20 m from the center of a 92.6-kt-yield explosion for rocks of different water content.

a function of time for the four different hydrous rocks. Because the low-density, water-containing medium undergoes a larger shock compression (Fig. 16), it causes large displacement. At 7.5 ms after the explosion (or 5.5 ms after the shock wave arrives at $x_0 = 20$ m), the difference in the displacements between the dry rock and the fully saturated rock is about 1.2 m. This difference increases with time at 7.5 ms, although it eventually approaches a constant value. The water content of rocks thus affects the size of the explosion cavity by two different but important mechanisms: first, a combined effect due to the low boiling point of water and an inherently low strength of water-containing rocks and, second, the low density of water-containing rocks that allows these strata to be displaced outward more easily.

ACKNOWLEDGMENTS

I thank G. Nutt of the D Division for supporting this work. L. Wong, S. Weaver, the late C. Werner, K. Long and B. Brown of the H Division have stored the rock-water mixture EOS data developed here into the EOS libraries of L.L.L. hydrocodes. The improved additive-volume code described in this work is based on the conventional additive-volume code developed by S. Lacey and D. Walton of the K Division, and the necessary improvement was coded by G. Haggin of the H Division.

REFERENCES

1. T. R. Butkovich, "The Influence of Water in Rocks on Effects of Underground Nuclear Explosions," *J. Geophys. Res.* **76**, 1993 (1971).
2. J. L. M. Cortez and C. S. Lacey, *MIX-A Code to Combine Equation-of-State Tables*, Lawrence Livermore Laboratory, Livermore, Calif., Internal Document UCON 75-11 (1975).*
3. M. Kamegai, *H-Division Quarterly Report*, Lawrence Livermore Laboratory, Livermore, Calif. UCRL-50028-75-4 (1975), p. 36.
4. J. H. Tillotson, *Metallic Equations of State for Hypervelocity Impact*, Air Force Special Weapons Center, Dept. of Defense, Washington, D.C. GA-3216 (1962).
5. T. J. Flanagan, *The Hugoniot Equation of State of Materials for the Ferris Wheel Program*, Sandia Laboratories, Albuquerque, N. Mex., USAEC Report SC-M-66-451 (1966).
6. T. R. Butkovich, "Calculation of the Shock Wave from an Underground Explosion in Granite," *J. Geophys. Res.* **70**, 885 (1965).
7. F. H. Ree, *Equation of State of the Silicon Dioxide System*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-52153 (1976).
8. F. H. Ree, *Equation of State of Water*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-52190 (1976).
9. M. Cowperthwaite and W. H. Zwisler, *TIGER Program Documentation*, Stanford Research Institute, Palo Alto, Calif., Publication No. Z106, Vol. I (1973), Vols. II-IV (1974).
10. R. Grover, "Liquid Metal Equation-of-State on Scaling," *J. Chem. Phys.* **55**, 3435 (1971).
11. E. B. Royce, GRAY, *Three-Phase Equation-of-State for Metals*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-51121 (1971).
12. C. A. Rouse, "Ionization Equilibrium Equation-of-State. V. Twenty-two Element Mixtures at Stellar Temperatures and Densities," *Astrophys. J.* **137**, 1286 (1963) and references cited therein.
13. E. Schmidt, *Properties of Water and Steam in SI-Units* (Springer-Verlag, New York Inc., 1969).
14. C. W. Burnham, J. R. Holloway, and N. F. Davis, *Thermodynamic Properties of H₂O to 1000°C and 1 kbar*, The Geological Society of America Special Paper No. 132 (1969).
15. C. W. Burnham, J. R. Holloway, and N. F. Davis, *Thermodynamic Properties of Water to 1,000°C and 10,000 Bars*, Pennsylvania State University, University Park, Penn., Research and Development Progress Report No. 414 (1969).

16. M. H. Rice and J. M. Walsh, "Equation of State of Water to 250 Kilobars," *J. Chem. Phys.* **26**, 824 (1957).
17. G. A. Gurtman, J. W. Kirsch, and C. R. Hastings, "Analytical Equation of State for Water Compressed to 300 kbar," *J. Appl. Phys.* **42**, 851 (1971).
18. K. Johnson, *TFCMIX*, Lawrence Livermore Laboratory, Livermore, Calif., Internal Document HTN-252 (1976).*
19. S. L. McCarthy, *The Kirzhnits Corrections to the Thomas-Fermi Equation-of-State*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-14363 (1965).
20. D. T. Warren, *Nuclear Correction for Genesis*, Lawrence Livermore Laboratory, Livermore, Calif., UCID-15316 (1968).
21. K. Johnson, *MASTER*, Lawrence Livermore Laboratory, Livermore, Calif., Internal Document HTN-260 (1976).*
22. S. L. Lacey and O. R. Walton, *MIX—A Code to Combine Equation of State Tables*, Lawrence Livermore Laboratory, Livermore, Calif., Internal Document UCON. T1-18, K-Division (1977).*
23. G. Haggin and F. H. Ree, *MIX*, Lawrence Livermore Laboratory, Livermore, Calif., Internal Document HTN-293 (1978).*
24. R. F. Trunin, G. V. Simakov, M. A. Podarets, B. N. Moiseyev, and L. V. Popov, "Dynamic Compressibility of Quartz and Quartzite at High Pressure," *Acad. Sci. USSR Phys. Solid Earth* No. 1, 13 (1971).
25. R. G. McQueen, J. N. Fritz, and S. P. Marsh, "On the Equation of State of Stishovite," *J. Geophys. Res.* **68**, 3219 (1963).
26. R. G. McQueen and S. P. Marsh, in *Behavior of Dense Media under High Dynamic Pressure* (Gordon and Breach Science Publishers, New York, 1968) pp. 207-216.
27. W. H. Gust and D. A. Young, "Shock Compression of Pyrolytic, Ceylon Natural, and a Hot-Pressed Synthetic Graphite to 120 GPa," to be published in the proceedings of the Sixth AIRAPT International High Pressure Conference, Boulder, Colo., July 25-29, 1977.
28. D. R. Stull and H. Prophet, eds., *JANAF Thermochemical Data*, NSRDS-NBS 37 (1971), 2nd Ed. (U. S. Government Printing Office, Washington, D.C.), Catalog No. C 13.48:37.
29. The entire EOS tables are available from the author upon request.
30. Unpublished data by G. D. Anderson quoted in M. van Thiel, *Compendium of Shock Wave Data*, Lawrence Livermore Laboratory, Livermore, Calif., UCRL-50108 Vols. 1-3 Rev. 1 (1977).

KMG:ld

*Readers who desire further information on LLL internal documents should address their inquiries to: Technical Information Department, Lawrence Livermore Laboratory, Livermore, California 94550.