

SHOCK VAPORIZATION OF ANHYDRITE AND GLOBAL COOLING FROM K/T

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We present new data on the vaporization criterion of anhydrite, the amount of sulfur dioxide injected into the atmosphere during the Chicxulub impact and its effect on the global climate. Determined from the analyses of the shock wave experiments, the values of the entropies of incipient (S_I) and complete (S_V) vaporization for anhydrite are $1.65 \pm 0.12 \text{ kJ}(\text{kg.K})^{-1}$ and $3.17 \pm 0.12 \text{ kJ}(\text{kg.K})^{-1}$, respectively and the corresponding pressures for the incipient (P_I) and the complete vaporization (P_V) are $32.5 \pm 2.5 \text{ GPa}$ and $122 \pm 13 \text{ GPa}$ respectively. Along with this criterion, the use of the results of the 2-D hydrodynamic simulations of Ivanov et. al. [1] for the Chicxulub impact, and the radiative transfer model of Pope et. al. [2] yields the drop in the global average surface temperature in the range of 12-19 K for 9-9.5 years at the K/T boundary.

It is now widely accepted that the world wide extinction of many marine and terrestrial biota at the K/T boundary is related to the impact on Earth by a large bolide at the Chicxulub site. The decrease in the solar insolation introduced by the sulfuric acid aerosols formed from the SO_2 and SO_3 injected into the atmosphere due to the shock induced vaporization of the anhydrite present at the impact site could result in global cooling and cause severe environmental stress for prolonged period of time. This prompted active research on the effect of shock devolatilization of anhydrite.

To determine the vaporization criterion of anhydrite, Yang and Ahrens [3] carried out shock wave experiments on porous anhydrite samples up to 75 GPa using a propellant gun. In these experiments, the shocked material after adiabatic expansion impacted against a Al witness plate backed by a LiF window. The particle velocity history of the Al/LiF interface was monitored using a VISAR interferometer. In the present study, we have reanalyzed the experimental data using an improved equation of state (eos) of the porous anhydrite and the vaporization products, and also by using the entropy criterion for vaporization of material under shock compression.

The analyses was carried out by performing numerical simulations using a 1-D lagrangian finite difference code WONDY [4], which integrates the equations of conservation of mass, momentum

and energy. The eos of the porous anhydrite was constructed using the p- α model of Herrmann [5], which uses the eos of the nondistended material as the reference state. The eos of the porous material is described as $p=f(v/\alpha, E)$, where $p=f(v_s, E)$, $\alpha=v_s/v$, and v_s and v are the specific volumes of the solid and the porous materials at same pressure (p) and energy density (E). The parameter α is given by the distension relation described differently in three different regions: Above some shock pressure, P_s , all the pores are assumed to be closed ($\alpha=1$); below some elastic pressure, P_e , the change in α is assumed to be due to elastic deformation of the pores; for loading between P_s and P_e , the pores are assumed to collapse irreversibly and crushing distension relation is employed. The continuity conditions are imposed on the three p- α relations at the boundaries of these region. For 30% porous anhydrite $P_s \sim 4 \text{ GPa}$ and $P_e \sim 0.1 \text{ GPa}$ were used.

The eos of the vaporized material had the form that is continuous with the Mie-Gruneisen equation at normal solid density. The eos reduces to an ideal gas equation for the low density expanded material.

The entropy increase at a given compression was calculated using relation $\Delta S = \Delta S_{tr} + C_v \ln(T_H/T_S)$, with C_v assumed to be $3R$; ΔS_{tr} is zero if there is no phase transition, otherwise it is the entropy of the high pressure phase relative to that of the low pressure phase at room temperature and pressure; T_H and T_S are the temperatures along Hugoniot and isentrope at the same compression.

Numerical simulations were carried out for various values of S_I and S_V . The best agreement between the simulated and the experimental profiles (figure 1) was obtained for $S_I = 1.65 \pm 0.12 \text{ kJ}(\text{kg.K})^{-1}$ and $S_V = 3.17 \pm 0.12 \text{ kJ}(\text{kg.K})^{-1}$. These values are less than $2.12 \text{ kJ}(\text{kg.K})^{-1}$ and $3.73 \text{ kJ}(\text{kg.K})^{-1}$ that are estimated from the extrapolated thermodynamic data at room pressure and high temperature. The pressure of incipient and complete vaporization for single crystal anhydrite corresponding to the new entropy values are $32 \pm 2.5 \text{ GPa}$ and $122 \pm 13 \text{ GPa}$, respectively.

For estimating the amount of the degassed sulfur we need to know the amount of anhydrite

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shocked above the vaporization pressure. Ivanov et. al. [1] carried out 2-D numerical simulations to model a crater of diameter 180 km and 300 km in a two layer medium (3 km of tuff overlying a granite basement) and determined the cumulative volume of the sediment compressed above given pressure. Recently, O'Keefe and Ahrens [6] constrained the size of the Chicxulub crater to be 100 ± 5 km. For this crater size, we applied hydrodynamic scaling to the results of Ivanov et. al. [1] and found that $66-93 \text{ km}^3$ and $26-44 \text{ km}^3$ of sediment were shocked above 32.5 GPa and 122 GPa, respectively. Assuming 30% anhydrite content in the upper layer, the amount of the sulfur dioxide injected into the atmosphere is found to be 11-39 Gt. The resulting global temperature decrease and the life of the sulfate aerosol cloud were determined by extrapolating the results of the Pope et. al. [2]. The global temperature decrease is found to be 12-19 K and the sulfate clouds would have lasted for 9-9.5 years. These values are somewhat lower than 31 K and 12 years reported by Pope et. al. [2] and the difference largely arises from our determination of the smaller transient crater volume.

We agree with Pope et. al. [2] that the sulfur oxide injection into atmosphere would have caused global cooling to $\sim 0^\circ \text{C}$ resulting in the severe environmental stress on the biota for about a decade at the K/T boundary.

Summary of Results	
S_I	$1.65\pm 0.12 \text{ kJ}(\text{kg}\cdot\text{K})^{-1}$
S_V	$3.17\pm 0.12 \text{ kJ}(\text{kg}\cdot\text{K})^{-1}$
P_I	$32.5\pm 2.5 \text{ GPa}$
P_V	$122\pm 13 \text{ GPa}$
SO_2 loading in atmosphere*	11-39 (>200) Gt
Global temperature drop*	12-19 (31) K
Life of sulfate aerosols*	9-9.5 (12) yr

* Results of Pope et. al. [2] are given in parenthesis

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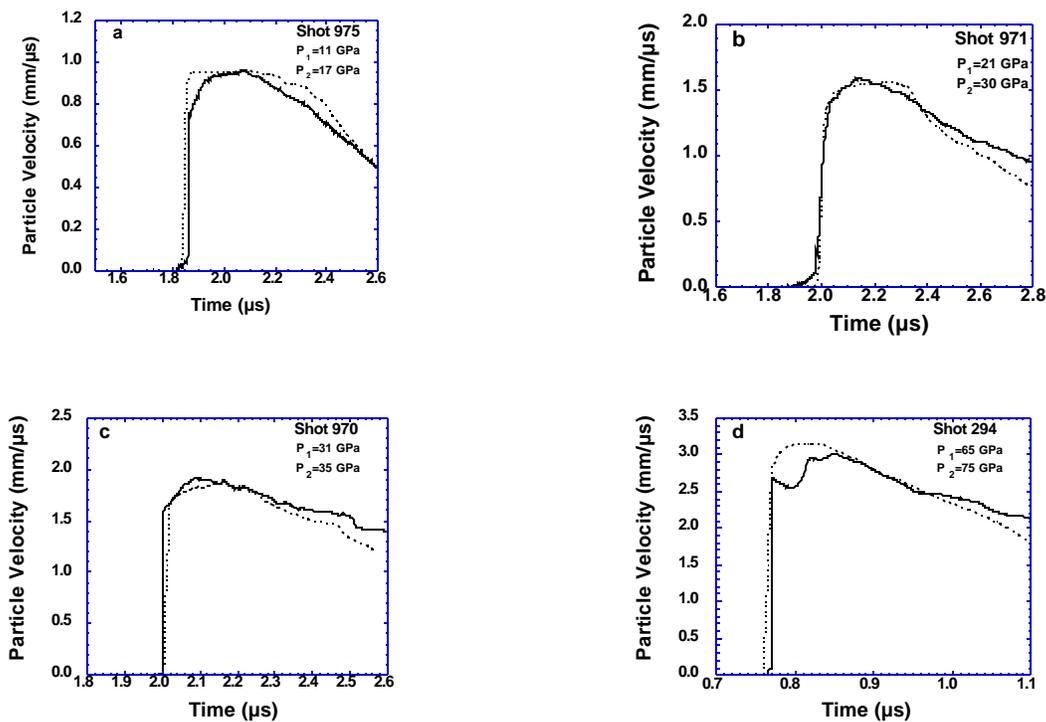


Fig. 1 Comparison of the numerical simulations (dotted lines) and experimental results (solid lines) for four shock adiabatic expansion experiments (P_1 and P_2 are initial- and recompression-shock pressures). The best agreement is obtained for $S_I = 1.65\pm 0.12 \text{ kJ}(\text{kg}\cdot\text{K})^{-1}$ and $S_V = 3.17\pm 0.12 \text{ kJ}(\text{kg}\cdot\text{K})^{-1}$. The profiles reported upon initial analysis [3] of these data demonstrated erroneous oscillations which we now understand to have arisen from too large a change in grid spacing in different media.