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POLYSTYRENE FOAM PRODUCTS EQUATION OF STATE AS A FUNCTION OF POROSITY AND FILL GAS

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Abstract. An accurate EOS for polystyrene foam is necessary for analysis of numerous experiments in shock compression, inertial confinement fusion, and astrophysics. Plastic to gas ratios vary between various samples of foam, according to the density and cell-size of the foam. A matrix of compositions has been investigated, allowing prediction of foam response as a function of the plastic-to-air ratio. The EOS code CHEETAH allows participation of the air in the decomposition reaction of the foam. Differences between air-filled, Ar-blown, and CO_2-blown foams are investigated, to estimate the importance of allowing air to react with products of polystyrene decomposition. O_2-blown foams are included in some comparisons, to amplify any consequences of reaction with oxygen in air. He-blown foams are included in some comparisons, to provide an extremum of density. Product pressures are slightly higher for oxygen-containing fill gases than for non-oxygen-containing fill gases. Examination of product species indicates that CO_2 decomposes at high temperatures.

Keywords: Polystyrene, Equation of State, Foam composition.
PACS: 64.30.Jk, 82.70.Rr, 51.35.+a.

INTRODUCTION

Polystyrene (PS) foam is used in many experimental assemblies as a moderator of shock propagation and to fix dimensions. The Equation of State (EOS) of polystyrene foam is well-established at moderate temperatures.

Recent experiments in the warm dense matter regime [1] required EOS reflecting both plasma properties and properties of molecular condensates from the plasma. Attempts at hydrodynamic simulation of these experiments showed that, for organics at the threshold of dissociation, neither conventional nor plasma EOS were applicable, but that condensation of molecular species must be treated directly. EOS were generated for the epoxy component of the experimental assembly using the Cheetah thermochemical code, [2] and proved adequate to provide accurate hydrodynamic modeling of the experiment. [3] In these regimes, PS foam was treated as solid PS, since compaction is complete at the experimental pressures. Existing plasma EOS were successfully used for the PS foam component in the experimental simulations. However, it is likely that the air present in the original foam will participate in the EOS, reacting with PS to form a variety of species which will affect the EOS at temperatures only slightly lower than those treated. [1]

In addition, many foam manufacturers are striving to produce foams containing only CO_2, since the process for production of these foams eliminates the chlorinated or fluorinated hydrocarbons that carry a high environmental price, and are necessary for the production of many air-filled PS foams. The difference in the product Hugoniot between air- and CO_2-filled PS foams is reported.

POLYSTYRENE FOAM

PS foams have a variety of industrial and scientific applications, and fall roughly into two types: expanded foams, as used in coffee cups, and extruded foams, such as the high density closed-cell foams commonly used in experimental configurations.

Air is incorporated into foams by imposing it during the molding or extrusion of the plastic into a foam product. Porosity may be generated by dissolution of a solvent, or blowing agent, such as pentane or a chlorinated hydrocarbon, in the solid polystyrene. The solvent expands during heating, creating cells which can then be occupied and stabilized by air. CO_2 may be incorporated by inclusion of CO_2-generating compounds or moieties into the polystyrene, and release of the CO_2 during heating. These schemes generate porosity without requiring the use of hydrocarbons or chlorinated hydrocarbons, providing economic and environmental advantages over the traditional blowing schemes.

Polystyrene foams are generally closed-cell foams, since most applications call for the strength and insulation properties typical of closed-cell structures. Sophisticated schemes such as high-internal phase emulsion (HIPE) [4] are used to make foams with higher densities, varying cell morphologies, and incorporation of dopants. Depressurization of a PS saturated with gas is a route to foams containing nitrogen, and provides a second avenue to foams containing CO_2. [5]

Polystyrene foams have densities between about 0.02 g/cc and 0.2 g/cc, corresponding to compositions between about 95.2 wt. % PS and 99.5 wt. % PS. A foam comprising 95 wt. % PS is about 1.6% PS by volume, and one with 99.5 wt. % PS is about 5% PS by volume. A technique such as HIPE can produce foams with densities as high as 0.5 g/cc. [5]

VARIATION WITH FILL GASES

Variation of fill gases has an observable effect on the EOS of the PS foam products. Changes in the Hugoniot are examined, as representative of variation in the EOS.

Examination of the PV Hugoniots for reaction products of PS filled with the several gases shows differences between the fill gases. (Figure 1.) Although some differences are attributable to variations in the gas Hugoniot, as for helium, some are due to variations in chemical behavior, with the PS/O_2 and PS/air exerting more pressure than expected from mixing the PS Hugoniot with that of the gas. This elevated pressure suggests reaction with the O_2, or with O_2 in air.

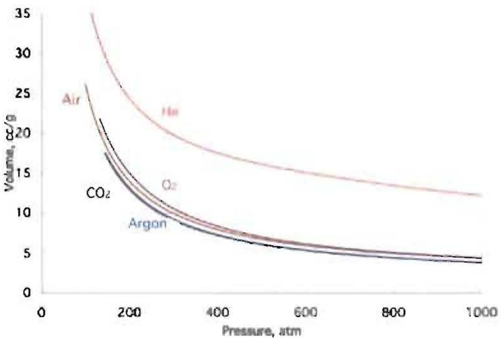

FIGURE 1. Hugoniot of products produced from PS/gas mixtures at initial densities that vary according to the density of the fill gas.

To reduce differences arising from the varying initial densities of the fill gases, the initial density is adjusted to 0.06 g/cc for all. Again, the PV Hugoniot reflects the elevated pressure arising in PS/O_2 and PS/air foams, relative to foams with inert fills. (Figure 2.)

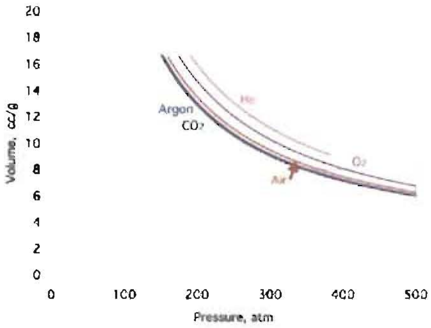

FIGURE 2. P-V Hugoniots of 97% PS/3% gas mixtures (by weight) with initial densities fixed to 0.06 g/cc for all.

Temperature differences are pronounced between products of reaction with the various fill gases, with products of oxygen- and air-filled foams showing much higher temperatures than those of other gases (Figure 3.)

These differences become more pronounced for larger fractions of fill gases.

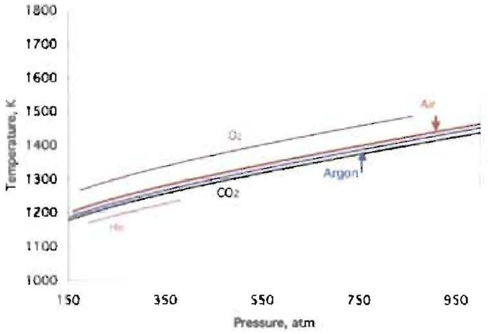

FIGURE 3. P-T Hugoniots of 97% PS/ 3% gas mixtures (by weight) with all initial densities fixed to 0.06 g/cc.

VARIATION WITH GAS CONTENT

Gas content has a marked effect on the products Hugoniots for PS foams. Heating in compression is greater for foams with a higher gas content. This effect dominates chemical differences.

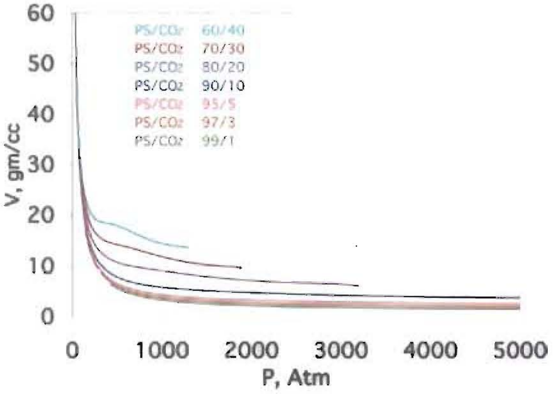

FIGURE 4. P-V Hugoniots for PS/Air at various fractions of gas. The slight change in curvature appears to be related to reaction of CO_2 to produce CO.

PRODUCT SPECIES

Product species can be examined directly, as reported by the Cheetah code at each step in calculation of the EOS. Products along the Hugoniot are compared.

The plethora of products and the variation in product ratios with temperature along the Hugoniot require some selectivity in comparison of products. The defining characteristics of reaction are not those associated with combustion, because the concentration of gas is small relative to that of PS, prohibiting complete oxidation of the PS to CO_2 and H_2O. Three metrics are used to estimate the extent of reaction between the PS and fill gas: the ratio of gaseous products to solid, production of hydrocarbons, and the presence of CO and H_2O, products specific to particular fill gases.

The majority of carbon in products takes the form of soot, as can be seen in Figure 5, comparing solid and gaseous products. Foams with smaller gas contents or inert fill produce more soot than foams with CO_2 or air. Air-blown PS produces the least soot, as carbon is consumed in gaseous products.

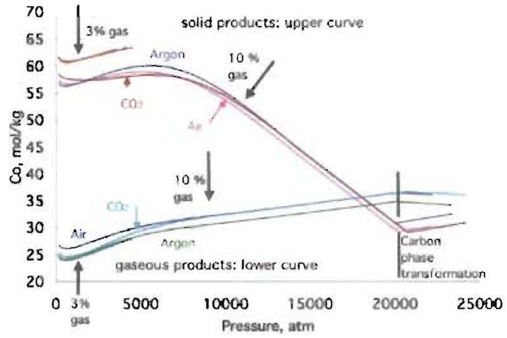

FIGURE 5. Change of pressure of solid and gaseous products with variation in initial gas fill, for two compositions: 97% PS and 90% PS. The solid products for 97% PS (3% gas) are indistinguishable from products with 10% argon gas.

Production of CH_4, shown in Figure 6 as representative of hydrocarbons, is a function of fill gas. The most CH_4 is produced by foam filled with argon, followed by CO_2, then air. Variation in other hydrocarbons C_2H_2, C_2H_4, and C_2H_6, varies by a few percent, with argon-filled PS producing the highest concentration, then CO_2. Air-filled PS produces the least hydrocarbon products, probably as a consequence of consumption of the carbon in formation of a variety of gaseous products where air or oxygen is present.

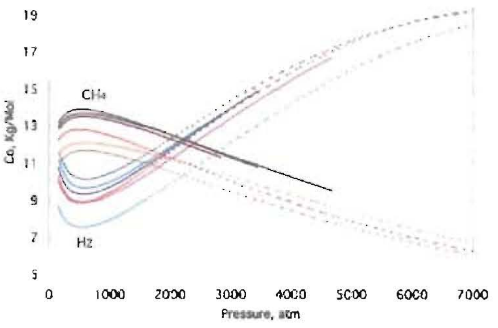

FIGURE 6. Major products as a function of pressure for two compositions, 97% PS, solid, and 90% PS, dotted lines. From the top, CH_4; Ar, CO_2, air (3 wt%) , Ar, CO_2, air (10 wt%), H2; air (10 %), air (3%), Ar (3%), Ar (10 %), CO_2(3%), CO_2(10 %).

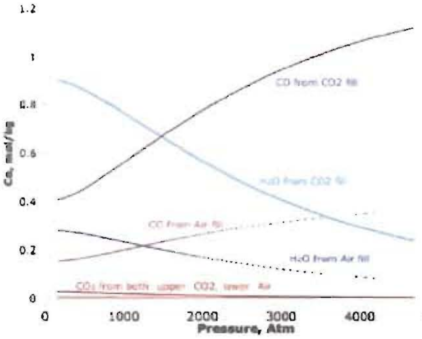

FIGURE 7. Change of pressure for products CO, CO_2, and H_2O produced by air and CO_2 initial gas fill.

The CO_2 is seen to react at high temperatures. While CO_2 produces more CO and H_2O than any other fill, (Figure 7,) these gases comprise a trivial fraction of the total product gases, and the pressure on the Hugnoiot is not elevated for PS with CO_2 fill. Emergence of CO appears to be responsible for the change in curvature of the PS/CO_2 products Hugoniot, seen in Figure 4. Concomitant increases in carbon in the PS/CO_2 products at high pressures are probably responsible for the similarity of CO_2 and argon solid and gaseous products at high pressures along the Hugoniot, as seen in Figure 5.

CONCLUSIONS

Foams blown with CO_2 or inert gases produce EOS upon reaction that are measurably different from those of foams blown with air. Reaction with air or O_2 increases the pressure of products, relative to CO_2 or inert gases. The differences between air and other gases can be seen in the variation of product species between air-filled foams and those filled with other gases. These effects decrease as the gas content of the polymer decreases, with dense air-filled PS resembling PS filled with Ar. Thus products vary somewhat with amount of fill gas.

Both air and CO_2 react at high temperature (T>2500) to produce CO and some water, products not seen for inert gases. While CO_2 reacts as readily as air at these temperatures, these minor products make a small contribution to total pressure for products of PS filled with CO_2.

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