An Analytic Investigation of "Hot-Spot" Formation in Compressible Energetic Materials

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Abstract: In this paper, the formation of the shock-induced "hot-spot" in compressible energetic materials has been analyzed. By applying the compressible elastic-viscoplastic material model to a hollow sphere, and solving the governing equations with the initial and boundary conditions, this paper proposes an analytic pore collapse model that is able to simulate the viscoplastic deformation which determines the formation of a "hot-spot". In this new model there are three mechanisms, of which instantaneous deformation and the subsequent quasi-static incompressible deformation dominate "hot-spot" formation, while quasi-static compressible deformation is of little effect. In comparison with the incompressible solution, this model demonstrates that the bulk compressibility has a great influence on "hot-spot" formation, as the degree of the "hot-spot" reaction is a positive quasi-linear function of Poisson's ratio *v*. An error in Kim's original pore collapse model has also been discussed.

Keywords: analytic model, bulk compressibility, pore collapse, "hot-spot" formation

1 Introduction

Shock ignition of heterogeneous solid energetic materials has been attributed to the chemical reaction of the "hot-spot", and in recent decades many researchers [1-12] have studied its generation mechanisms. Of the several mechanisms considered, the mechanism of pore collapse for the formation of the "hot-spot"

in a porous energetic material under shock has been investigated extensively. Numerous collapse models of the hollow sphere [13-19] have been established to simulate the pore collapse phenomenon, for they can concisely describe the key thermodynamic mechanisms which determine "hot-spot" ignition. In 1972, Carroll *et al*. [20] adopted a simple model of a ductile sphere containing a uniform pore in the center in order to discuss the motion of powdered materials and found that the "hot-spot" reaction may occur near the pore during pore collapse. In 1985, Kim *et al*. [21-23] proposed an analytic shock-induced ignition model based on the collapse of an elastic-viscoplastic hollow sphere and proved that the temperature due to viscoplastic heating is high enough to trigger the ignition of the "hot-spot" around the pore. From the 1990s until recently, a great deal of work has been done on the basis of the collapse of the hollow sphere. Whitworth [24], Massoni [25] and Kang [26] *et al*. studied the pore collapse of a visco-rigid plastic hollow sphere in a numerical way. In addition to the viscoplastic heating, they also studied the contributions of other mechanisms, such as the dynamic behaviour of the gas in the pore and heat exchange on the pore surface, *etc*., to "hot-spot" formation. Wen *et al*. [27] developed an elastic-viscoplastic collapse model of the double-layered hollow sphere to investigate the effect of binders on "hot-spot" ignition in PBX explosives. Li Xinghan *et al*. [30] evaluated the significant influences of the inertial effect on "hot-spot" formation by the collapse of the hollow sphere.

As the hypothesis of bulk compressibility would greatly complicate the analysis, the incompressibility assumption was used by almost all the previous pore collapse models. Little work has been done to examine the incompressibility assumption, except that Carroll *et al*. [20] have discussed preliminarily the small effect of elastic compressibility on pore collapse. However, for materials under a strong shock (several GPa), the Hugoniot curve [28, 29] shows that a large amount of the input energy is transformed into internal energy due to a great increase in density. Since the internal energy was neglected in the previous incompressible pore collapse models, most of the input energy was considered to be transformed into the dissipated viscoplastic energy, and the "hot-spot" due to the viscoplastic heating has been inevitably overestimated. Therefore, it was of great interest to investigate the impact of bulk compressibility on "hot-spot" formation.

The present study develops an analytic pore collapse model for a compressible elastic-viscoplastic hollow sphere to simulate the thermodynamic processes that determine "hot-spot" formation. The remainder of this paper is organized as follows: in Section 2, the governing equations, along with the initial and boundary conditions are solved analytically to describe the collapse of the compressible

hollow sphere; in Section 3, the analytic model is validated through a comparison with the incompressible model; in Section 4, the key mechanisms of the new model are examined; and in Section 5 the influence of bulk compressibility on the thermodynamic processes and the corresponding "hot-spot" formation during pore collapse are evaluated.

2   A Collapse Model of a Compressible Elastic-Viscoplastic Hollow Sphere

Having successfully approximated the overall compaction of powdered materials containing voids, a simple one-dimensional hollow sphere was applied in this study, as shown in Figure 1. Since the rise time of the shock is sufficiently short compared with the entire collapse time, this study assumes that the pressure is loaded symmetrically and instantaneously on the external surface of the hollow sphere.
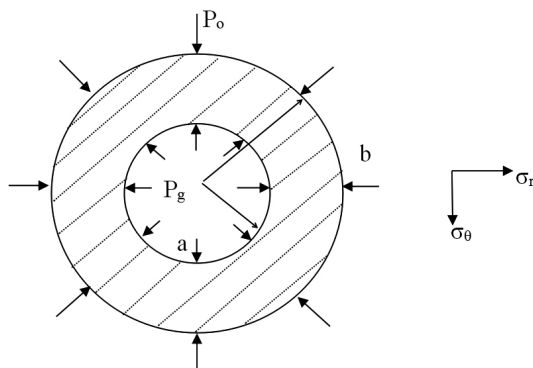

Figure 1.   A hollow spherical model; the shaded area represents the solid material, and the white area represents a uniform pore located in the center of the sphere

In Figure 1, b is the average size of the explosive particles, and a is the average size of the pores, which depends on the porosity of the explosive. P_g represents the value of the pressure in the pore and P_0 the value of the pressure on the external surface. The strains and stresses have the following definitions and relations in the spherical symmetric coordinates:

$$\varepsilon_r = \frac{\partial R(r,t)}{\partial r}, \quad \varepsilon_\theta = \varepsilon_\varphi = \frac{R(r,t)}{r}, \quad \sigma_\theta = \sigma_\varphi \tag{1}$$

where σ_r, $\sigma_\theta/\sigma_\varphi$, ε_r and $\varepsilon_\theta/\varepsilon_\varphi$ are the radial stress, the tangential stress, the radial strain and the tangential strain, respectively, while R and r are the radial displacement and the radial coordinate, respectively.

As indicated in the Kim model [21-23], the strain-rate dependent viscoplastic deformation could also describe the effects of shear banding and friction, which are possible formation mechanisms for a "hot-spot". So elastic-viscoplastic material with a useful constitutive relation was adopted in this work:

$$\frac{d\varepsilon}{dt} = \frac{\gamma}{\sigma_0}(\sigma - \sigma_0) + \frac{1}{E}\frac{d\sigma}{dt} \tag{2}$$

where ε is the strain, σ the stress, t the time, and σ_0, E, and γ represent the yield stress, the elastic module and the viscosity parameter, respectively.

For the motion of the compressible hollow sphere under shock, the partial differential equations that describe the deformation and the force balances in the spherical coordinates are:

$$\frac{\partial \sigma_r}{\partial r} + 2\frac{\sigma_r - \sigma_\theta}{r} = 0 \tag{3.1}$$

$$\frac{\partial v}{\partial r} - \frac{v}{r} = \frac{3}{2E}\frac{\partial}{\partial t}(\sigma_r - \sigma_\theta) + \frac{3\gamma}{2}\left[\frac{(\sigma_r - \sigma_\theta)}{\sigma_0} - 1\right] \tag{3.2}$$

$$\left(\frac{\partial v}{\partial r} + 2\frac{v}{r}\right)3K_V = \frac{\partial}{\partial t}(\sigma_r + 2\sigma_\theta) \tag{3.3}$$

$$\frac{\partial \rho}{\partial t} + \rho\left(\frac{\partial v}{\partial r} + 2\frac{v}{r}\right) = 0 \tag{3.4}$$

where v stands for the radial velocity, and ρ the density. K_V is the volume module with the definition of $E/3/(1-2v)$, and v is Poisson's ratio. Equation 3.1 describes the force balances within the hollow sphere; Equation 3.2 is the rewritten constitutive relation; Equation 3.3 represents the generalized Hooke's law, and Equation 3.4 defines the growth rate of density during pore collapse.

The boundary conditions of the pressures on the internal and external surfaces of the hollow sphere are:

$$\sigma_r(a,t) = -P_g, \quad \sigma_r(b,t) = -P_0 \tag{4}$$

where the negative signs in Equation 4 mean that σ_r and σ_θ are compressive stresses.

The initial conditions are given by:

$$\sigma_r(r,0) = 0, \quad \sigma_\theta(r,0) = 0 \tag{5}$$

The solution of the radial velocity v for Equation 3 can be achieved by the Laplace transformation method:

$$
\begin{aligned}
\mathrm{v} = \delta(t) &\left[\frac{3(P_0 - P_\mathrm{g})}{4E(b^{-3} - a^{-3})r^2} + \frac{\sqrt{3}(P_0 a^{-3} - P_\mathrm{g} b^{-3})}{6(b^{-3} - a^{-3})K_V} r \right] \\
&+ \frac{3\gamma}{4(b^{-3} - a^{-3})r^2 \sigma_0} \left(P_0 - P_\mathrm{g} - 2\sigma_0 \ln \frac{b}{a} \right) \\
&- \frac{6\gamma E e^{\xi t}}{(9K_V + 4E)} \left[\frac{a^3 \ln a - b^3 \ln b}{(b^3 - a^3)} r + \frac{\ln \frac{b}{a}}{(a^{-3} - b^{-3})r^2} \frac{1}{} + r \ln r \right]
\end{aligned} \tag{6}
$$

To express the solution concisely, a variable ξ is proposed as:

$$\xi = -\frac{9\gamma E K_V}{\sigma_0(9K_V + 4E)}$$

In Refs. [20-22], the radial velocity of the elastic-viscoplastic hollow sphere with the assumption of incompressibility is given by Kim (the original form):

$$(\mathrm{v_{KIM}})_O = \delta(t)\left[\frac{3(P_0 - P_\mathrm{g})}{4E(b^{-3} - a^{-3})r^2} \right] + \frac{\sqrt{3}}{2} \frac{\gamma}{(b^{-3} - a^{-3})r^2 \sigma_0} \left(P_0 - P_\mathrm{g} - 2\sigma_0 \ln \frac{b}{a} \right) \tag{7}$$

where the subscript O denotes the original expression. The definition of the Delta function is:

$$\delta(t) = \begin{cases} 0, (t \neq 0) \\ \infty, (t = 0) \end{cases}$$

The constitutive relation in Kim's model should be identical to Equation 3.2 as the same elastic-viscoplastic material is applied in his model. However, there is an error, *i.e.* the wrong expression of $\sqrt{3}\gamma$ is used instead of $3/2\,\gamma$ in Kim's constitutive relation. Therefore a correct solution can be obtained with the right

constitutive relation (the correct form):

$$(v_{KIM})_C = \delta(t)\left[\frac{3(P_0 - P_g)}{4E(b^{-3} - a^{-3})r^2}\right] + \frac{3}{4}\frac{\gamma}{(b^{-3} - a^{-3})r^2\sigma_0}\left(P_0 - P_g - 2\sigma_0 ln\frac{b}{a}\right) \quad (8)$$

where the subscript C denotes the correct function. Through a comparison of Equation 7 with Equation 8, it may be seen that the original solution overestimates the radial velocity, as the second term on the right has a larger coefficient.

3 Validation of the Compressible Pore Collapse Model

To validate the new model, under the condition of Poisson's ratio v=0.49, three radial velocity profiles of the specific radius and finally density ρ_{OA}, when the pore has completely collapsed, are compared with those of the incompressible models. The results are presented in Figures 2 and 3, respectively. In these simulations, P_0 remains constant while P_g varies following the law of $P_g(t)a^{3\beta} \equiv P_g(0)a_0^{3\beta}$, where β is the index of the perfect gas, and all of the parameters needed are listed in Table 1 for PBX-9404 [21-23]. From Figure 2, it may be concluded that the radial velocities of the compressible model under the condition of v=0.49, always reach perfect agreement with those of the correct incompressible form. The ratios of ρ_{OA} to ρ_0 in Figure 3 show that the increases in ρ_{OA} to the initial density ρ_0 along the radius are too small (approximately 1.14-1.16%) if the material is generally incompressible, which could validate the compressible model in another way.

In addition, the differences between the original incompressible solution and the correct solution are also shown in Figure 2. It is obvious that the radial velocities are generally overrated by the original solution and this validates the related discussion of error at the end of Section 2.

Table 1. Calculation parameters for PBX-9404 [a]

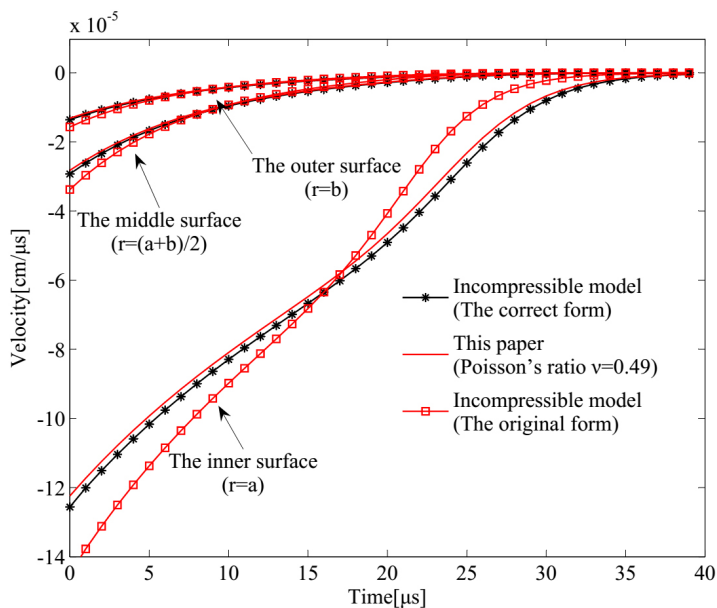| $P_g(0)$ [GPa]	ρ_0 [g·cm^{-3}]	σ_0 [GPa]	E [GPa]	β	C_p [J·g^{-1}·K^{-1}]	T_0 [K]	a_0 [cm]	b_0 [cm]	γ [s^{-1}]
1E-6	1.865	1.49E-2	12	9	1.368	300	0.0039	0.01	300

[a] From Refs. [21-23]

Figure 2. Three radial velocity profiles throughout pore collapse under a shock of 2.5 GPa
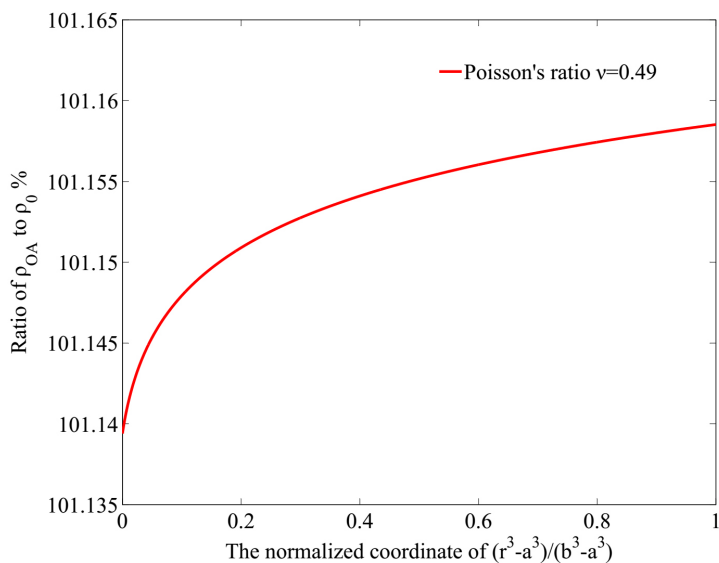

Figure 3. Overall ratio of the final density ρ_{OA} to the initial density ρ_0 under a shock of 2.5 GPa

4 Investigation of the Mechanisms within the Compressible Collapse Model

As shown in Equation 6, the radial velocity of the compressible hollow sphere is constructed by three functions. The first function on the right, which contains a δ(t) function, defines the instantaneous deformation due to the stress wave/shock wave propagation at the initial time. The remaining two functions work after the instantaneous influences have been eliminated. The second function stands for the quasi-static incompressible deformation; the last function, which contains a negative-index exponential function of time, represents the quasi-static compressible deformation during pore collapse. These mechanisms work together throughout the collapse of the compressible elastic-viscoplastic hollow sphere, and it is meaningful to evaluate their respective contributions.

4.1 Investigation of the incompressible and compressible deformations

It may be inferred from Equation 6 that the instantaneous deformation does not contribute directly to the collapse velocity for δ(t) = 0 during the entire pore collapse. So it is the quasi-static incompressible and compressible deformations that dominate the collapse velocity. The respective contributions of the incompressible and the compressible deformations to the radial velocities throughout the pore collapse are outlined in Figures 4 and 5.

Figures 4 and 5 show that at either the inner or the outer radius of the hollow sphere, the collapse velocity is almost completely determined by the quasi-static incompressible deformation regardless of Poisson's ratio, and that the quasi-static compressible mechanism contributes little to the velocity. It can thus be concluded that the quasi-static compressible mechanism has no influence on the collapse motion.

4.2 Investigation of the instantaneous deformation

In Equation 6, the function of the quasi-static incompressible deformation, which involves a factor of $1/r^2$, would induce the incompressible deformation. At the same time other functions that involve factors of r or ln$r$, are related to the compressible deformation. The density evolution throughout pore collapse occurs in the following way. In the first instance, the instantaneous deformation causes a uniform density increase along the radius r at time zero, and ρ_{IN} represents the density at this time. Subsequently, the density gradient emerges and grows due to quasi-static compressible deformation until collapse is completed. The results in Figure 3 demonstrate that the final density ρ_{OA} is an increasing function of the radius r.
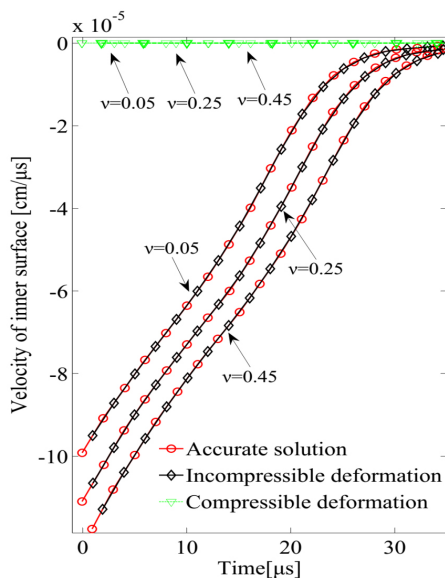
Figure 4. Radial velocity profiles at the inner radius for three values of Poisson's ratio *v* under a shock of 2.5 GPa
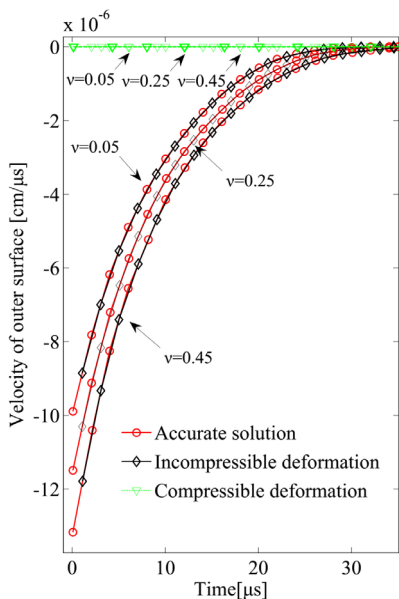

Figure 5. Radial velocity profiles at the outer radius for three values of Poisson's ratio *v* under a shock of 2.5 GPa

Although the quasi-static compressible mechanism has been proved to have little effect on the collapse velocity, it is still unclear whether it affects the density evolution significantly or not. The progress in studying the relation between ρ_{IN} and ρ_{OA} under different conditions of pressure and Poisson's ratio are shown in Figure 6.
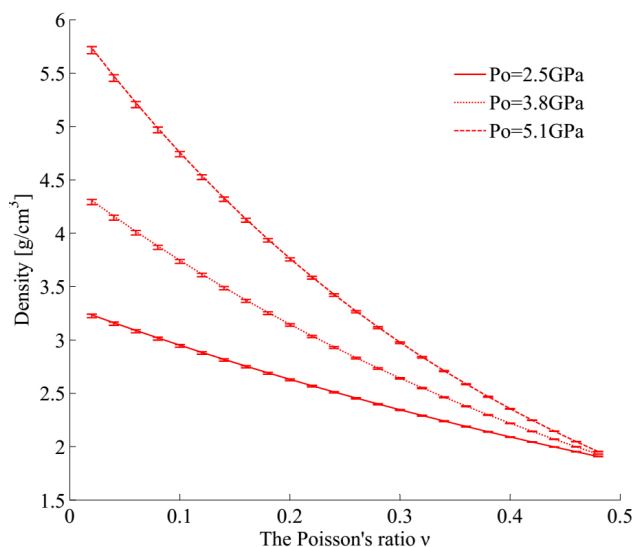

Figure 6. The relations between ρ_{IN} and ρ_{OA} under different Poisson's ratios v and pressures P_0. The lines represent ρ_{IN}, the upper error bars correspond to the maximum of ρ_{OA}, and the lower error bars correspond to the minimum of ρ_{OA}

Regardless of the variations of Poisson's ratio v and pressure P_0, the slight differences between the upper and lower error bars and the respective ρ_{IN} are outlined in Figure 6. The largest deviation of ρ_{OA} from ρ_{IN} is achieved under a P_0 of 5.1 GPa and v close to 0, and the value is from −0.23% to +0.94%, indicating that it is reasonable to equate ρ_{OA} with ρ_{IN} over a wide range. In another words, the instantaneous deformation generally determines the density evolution and the small impact of the quasi-static compressible deformation during the entire collapse may be ignored. Therefore, the elastic-viscoplastic hollow sphere suffers a shock compression in an extremely short time, and it is almost incompressible throughout the pore collapse.

When the bulk compressibility is taken into account, part of the input energy would be transformed into the inertial energy as the density increases, and this

transformation would become more important as Poisson's ratio v decreases. Therefore the bulk compressibility would greatly affect the dissipated viscoplastic energy during pore collapse.

Normally, the calculation of the dissipated viscoplastic energy is complicated by the compressibility assumption.

5   Influence of Poisson's Ratio v on "Hot-Spot" Formation

Normally, the calculation of the dissipated viscoplastic energy is complicated by the compressibility assumption, however, as the hollow sphere is generally incompressible during the collapse, the dissipated viscoplastic energy can be computed accurately in a simple way. When the material is incompressible, the heating rate due to the viscoplastic deformation is [21-23] (the original form):

$$(\frac{\mathrm{d}T}{\mathrm{d}t})_O = \frac{9\sqrt{3}\gamma}{4\sigma_0\rho C_p(b^{-3}-a^{-3})^2}\left(P_0 - P_g - 2\sigma_0\ln\frac{b}{a}\right)^2\frac{1}{r^6} \tag{9}$$

where C_p is the heat capacity and its value is shown in Table 1. Since the heating rate relies on the radial motion, the above function also suffers from an error due to the inaccuracy of Kim's original radial velocity. After a derivation based on the correct radial velocity, the viscoplastic heating rate is given by (the correct form):

$$(\frac{\mathrm{d}T}{\mathrm{d}t})_C = \frac{9\gamma}{4\sigma_0\rho C_p(b^{-3}-a^{-3})^2}\left(P_0 - P_g - 2\sigma_0\ln\frac{b}{a}\right)^2\frac{1}{r^6} \tag{10}$$

When the pore has completely collapsed, the relationship between the temperature rise of the hollow sphere and Poisson's ratio v is shown in Figure 7.

In Figure 7, the temperature in the new model is a monotonically decreasing function of the radius r, so the region concentrated around the inner radius ($r=a$) is hottest where the "hot-spots" should have been formed. Futhermore, the temperature is a decreasing function of Poisson's ratio v, which shows that less input energy is transformed into the dissipated viscoplastic energy with a smaller v. In Figure 7, compared with the correct solution, the results show that the temperature rise due to the viscoplastic heating has been largely overrated by the original form, and this error is most noticeable around the inner radius. So the development of the "hot-spot" would be overestimated by Kim's original model.
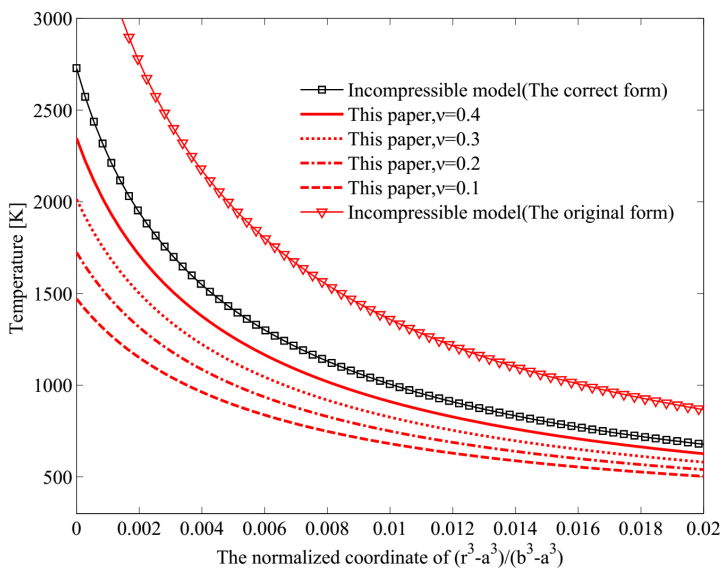
Figure 7. Temperature distribution of the hollow sphere when the pore has completely collapsed with a variety of Poisson's ratios *v* under a shock of 2.5 GPa

Since the chemical reaction rate of PBX-9404 is nearly infinite when the temperature approaches 1000 K, according to the Arrhenius reaction law [21-23], the reaction of PBX-9404 is recognized to be completed instantaneously when the temperature is above 1000 K. Accordingly, the "hot-spots" must form within a range of temperatures above 1000 K. When the pore has completely collapsed, a study of the relationship between the degree of the "hot-spot" reaction, *i.e.*, the mass fraction of the "hot-spot", and Poisson's ratio *v* under different pressures, is shown in Figure 8.

In Figure 8, when Poisson's ratio *v* is close to 0.5, the degree of "hot-spot" reaction at different pressures is of magnitude 1E-2 and is consistent with that of the incompressible model [21-23]. The results in Figure 8 show that the reaction degree of the "hot-spot" is an approximately positive linear function of Poisson's ratio *v*. Consequently an important conclusion may be drawn, that the bulk compressibility has a great impact on the "hot-spot" reaction due to viscoplastic heating. This conclusion validates the above analysis that a smaller *v* results in a reduction in the dissipated viscoplastic energy. In addition, the greater the pressure, the faster the reaction degree of the "hot-spot" decreases. For the previous ignition models, the degree of "hot-spot" reaction has been

overestimated due to the bulk incompressibility assumption, and the deviation becomes more obvious under a stronger shock.
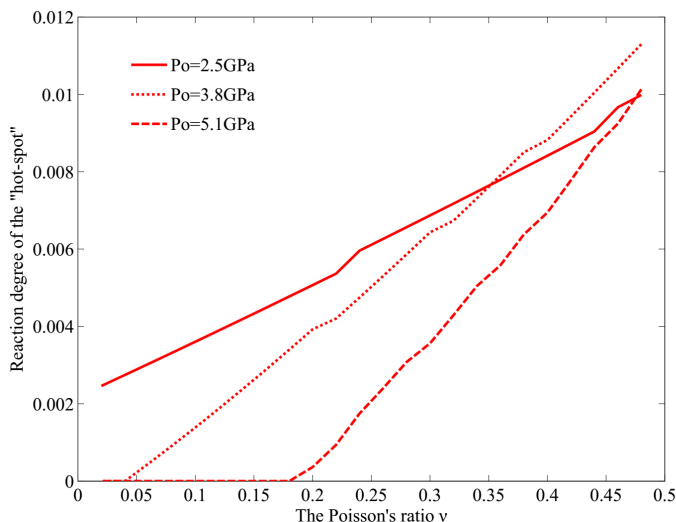

Figure 8.   Degree of "hot-spot" reaction for a variety of Poisson's ratios *v* under three values of pressure P_0

6   Conclusions

The collapse model of the hollow sphere has been the foundation for the analysis of the shock-induced "hot-spot" ignition of porous explosives. In order to investigate the impact of bulk compressibility on "hot-spot" formation, this work solves the compressible partial differential equations together with the initial and boundary conditions in an analytic way, and proposes a collapse model for a compressible elastic-viscoplastic hollow sphere. Within the new model, there are three mechanisms that work together throughout pore collapse. The results demonstrate that at time zero, the instantaneous deformation, which is attributed to the propagation of the stress wave/shock wave, causes an instantaneous increase for the radius and density of the hollow sphere. When the instantaneous effect disappears, it is the quasi-static incompressible deformation that dominates the pore collapse and the accompanying "hot-spot" formation, while the quasi-static compressible deformation has been proved to be insignificant. The calculated results show that there is a strong influence of bulk compressibility on the growth of the "hot-spot", and the reaction degree of the "hot-spot" is a positive, quasi-

linear function of Poisson's ratio v. Therefore the degree of the "hot-spot" reaction is generally overestimated by the previous incompressible ignition models, and the error increases with a stronger shock. In addition, since Kim's original pore collapse model suffers from an error, a correct solution is derived and the deviations between the two forms have been discussed. A comparison of the results indicates that the degree of "hot-spot" reaction is overestimated by Kim's original model.

Acknowledgments

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