Pore surface energy corrected $P - \alpha$ like models and the anomalous behaviour of porous materials

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Abstract. Accurate models for the description of porous materials are necessary in simulations of collisions between pre-planetesimals which are required to study the viability of collisional growth as a mechanism leading to the formation of planetesimals. We have compared two porosity models that have been used in the related field of impact cratering, and we have found that they suffer two problems when applied to high porosity materials that are likely to show the so called anomalous behaviour. To overcome the observed problems we have proposed a correction of the internal energy of the porous material considering the contribution of the surface energy of the pores.

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1. INTRODUCTION

The knowledge of the properties and of the mechanical behaviour of porous materials has recently became relevant in the collisional growth scenario proposed to explain the early stages of planet formation.

Planets are thought to form in protoplanetary discs made of gas and a component of dust grains of submicron size. The initial submicron dust grains are strongly coupled to the gas in the disc, therefore they move collectively at low relative velocities induced by Brownian motion and they can collide and stick due to van-der-Waals forces. Thus, fractal aggregates of the order of 100 μm in size are formed [e.g. 1, 2]. Such objects are less and less coupled to the gas the more their size increases. At the same time, turbulence, sedimentation, and radial drift [3, 4] become relevant and lead to an increase in relative velocity. The fractal aggregates then are restructured growing to non-fractal but highly porous bodies with size of the order of centimetres [5]. Experimental results [see 6, and references therein] show that the outcome of collisions between such bodies is not anymore dominated by sticking but that also bouncing or fracture become relevant. The outcome of collisions depends on impact speed and angle, objects size, and particularly on the internal structure of the bodies.

We do not have direct evidence of the structure and composition of pre-planetesimal matter, but some hints can be derived by the finding of very low densities in comets, from the order of 0.1 g/cm^3 to the order of 10 g/cm^3 [e.g., 7, 8]. Pre-planetesimals are then expected to be highly porous and because of this property they can potentially show the so called *anomalous behaviour*: under compressive shocks, the density of the body initially increases as observed in low porosity materials, but starts to decrease after a critical density has been reached [9, 10, 11].

Since laboratory experiments are limited to decimetre size, numerical simulations are necessary to study the problem at larger scales. Consequently, such simulations require detailed theoretical models to describe the complex physics involved in the description of the colliding solid bodies.

Porosity models. Here we focus on the choice of a porosity model with the aim of improving the description of pre-planetesimals. Such a porosity model is part of the constitutive equations adopted to describe the material properties of pre-planetesimals, such as elasticity/plasticity and damage. Our analysis is here restricted to a simple group of porosity models that we call *matrix based* or $P-\alpha$ like (from the name of the first of these models proposed by [12]) porosity models. In these kinds of models the properties of the porous material (density ρ, pressure P, internal energy U) are derived from those of the matrix (solid part of the body) througth the introduction of the new variable α, called *distension* and defined as the ratio of the matrix density to the density of the material $\alpha \equiv \rho_m/\rho$ [the subscript m refers to the quantities related to the matrix]. A *distension relation*, that connects the distension to the other thermodynamical quantities, has to be provided. The model is then determined by the following system of equations:

$$\begin{cases} U &= U(\rho, P) \\ \alpha &= \alpha(\ldots, A_i, \ldots) \\ P &= \frac{1}{\alpha} P_m(\alpha\rho, U) \end{cases} , \tag{1}$$

where the first equation identifies the thermodynamical path followed by the body during deformation (e.g. adiabatic, shock Hugoniot), the second is the distension relation with A_i identifying one or more generic thermodynamical quantities [see 13], and the third refers to the pressure of the porous material based on the equation of state (hereafter EOS) of the matrix. These models assume that the internal energy of the porous material is equal to that of the matrix, thus neglecting the effect of the surface energy of the pores. The consequences of this choice will be discussed in Sect. 3.

Two matrix based models have been recently used in the related field of impact cratering but only for low and intermediate porosity not higher than $\approx 60\%$. The original $P-\alpha$ model [12], where the distension depends only on the pressure $\alpha = \alpha(P)$, has been implemented by [14] in their hydrocode. The $\varepsilon-\alpha$ model, recently introduced by [15], is a modification of the $P-\alpha$ model and is characterised by a distension that depends on the volumetric strain, defined as $\varepsilon \equiv -\ln(\rho/\rho_0)$, where ρ_0 is the initial density. Here we want to determine if these models can also be used to describe pre-planetesimals, that are expected to reach a much higher degree of porosity.

2. DIFFERENCES BETWEEN $P-\alpha$ AND $\varepsilon-\alpha$ MODELS

We have compared $P-\alpha$ and $\varepsilon-\alpha$ models in the case of shock compression, expected as a consequence of collisions between pre-planetesimals and modelled by the Hugoniot relation (note that $\alpha_0 = 1/\hat{\rho}_0$):

$$\hat{U} = \hat{U}_0 + \frac{1}{2}(\hat{P} + \hat{P}_0)\left(\frac{1}{\hat{\rho}_0} - \frac{1}{\hat{\rho}}\right). \tag{2}$$

The hat identifies dimensionless quantities with respect to the following units: the matrix bulk modulus K_m for the pressure and the initial density of the matrix ρ_{m_0} for the density. It follows that the unit for the internal energy is K_m/ρ_{m_0}.

Two different EOS for the matrix are used. The first is a simplified version of the equation proposed by [16]: $\hat{P}_m(\hat{\rho}_m, \hat{U}_m) = c\hat{\rho}_m\hat{U}_m + A(\hat{\rho}_m - 1)$, where the pressure explicitely depends on the internal energy (U-dependent case) and c and A are two parameters. The second is the Murnaghan equation:$\hat{P}_m(\hat{\rho}_m, \hat{U}_m) = (\hat{\rho}_m^n - 1)/n$, where there is no explicit dependence on the internal energy (U-independent case) and n is a parameter.

In the case of shock Hugoniot, the porous EOS is identified by the general function:

$$F = F(\rho, P, \alpha; \alpha_0) \tag{3}$$

that has an explicit form only in a few cases.

The comparison has been performed for the two limiting cases of low ($\alpha_0 = 1.63$) and high initial porosity ($\alpha_0 = 22$). Results are presented in Fig. 1 where each plot has the same layout: the left and right columns refer to the U-dependent and U-independent EOS, respectively; the top, middle and bottom panels show the changes versus the pressure in, respectively, the density of the porous material ρ, the density of the matrix ρ_m, and the distension α. Solid lines refer to the $P-\alpha$ model and dashed lines to the $\varepsilon-\alpha$ model.

Low distension regime ($\alpha_0 = 1.63$). In this case, both models present the same qualitative features. They reach a full compaction state, where the distension becomes unity (bottom panels), characterised by a similar density (top panels). The density of the matrix at the full compaction state is larger than the initial value (middle panels), thus showing *normal* behaviour.

Only two differences are observed. First, when the U-dependent EOS is used, a characteristic bump is observed in the evolution of the density of the matrix. The bump becomes more and more pronounced with increasing porosity, leading to a qualitatively different behaviour at high porosity (see next paragraph). Second, the $\varepsilon-\alpha$ model shows a stronger dependence on the matrix EOS reaching full compaction at a smaller pressure when the U-independent EOS is used (see top right and bottom right panels).

High distension regime ($\alpha_0 = 22$). In this case the two models behave differently. The $\varepsilon-\alpha$ model is not physically acceptable (Unphy.) because of the presence of a singularity in the density domain that prevents the material to become fully compacted. The bottom left panel shows that α smaller than 11 are not allowed because they lay beyond the singularity, as a consequence the density of the material remains almost unchanged during the whole compression (top left panel). In the U-independent case a more strange behaviour is observed: when $\alpha \approx 5$, pressure becomes smaller and smaller reaching negative values (see top right and bottom right panels). In contrast, the $P-\alpha$ model does not show any singularity and allows the material to be fully compacted (bottom panels). Here we can see the effect of the growing bump, already observed in the low porosity case, with increasing porosity: the density of the matrix at the full compaction state is smaller than its initial value (middle left panel), thus the model is able to describe *anomalous* behaviour, visible in the top left panel where the density of the porous material decreases after full compaction.

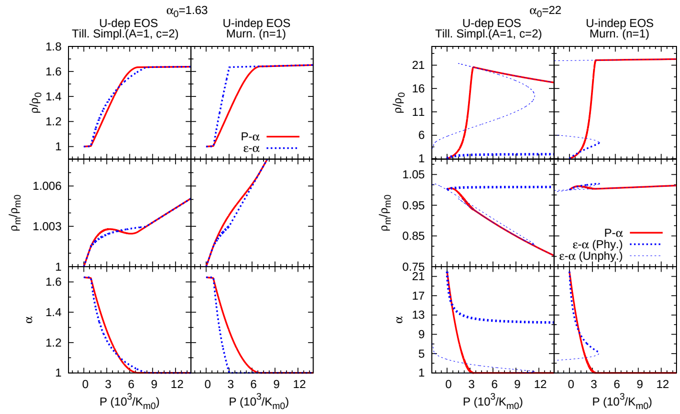

FIGURE 1. Differences between $P-\alpha$ (solid line) and $\varepsilon-\alpha$ (dashed line) model: low porosity (left panel), high porosity (right panel). The non physical and the physical branch of the $\varepsilon-\alpha$ model are represented with a thin and a thick dashed line, respectively.

A *critical initial distension* α_{0_c} is defined as that initial distension that at full compaction state, identified by the subscript fc, leads to a zero slope in the density-pressure relation: $\partial\rho/\partial P(\rho_{fc}, P_{fc}, \alpha_{fc}; \alpha_{0_c}) = 0$, where we have $\alpha_{fc} = 1$. The $P-\alpha$ model predicts normal behaviour for bodies starting with an initial distension below this critical value and anomalous behaviour for initial distension above it. A potential problem connect with the $P-\alpha$ model is that, for a given kind of matrix, the type of behaviour is determined only by the initial degree of porosity (identified by α_0, see Eq. 3). Since the evolution of a material under shock depends also on its internal structure, this model may have problems predicting anomalous instead of normal behaviour or vice versa. In the next section we propose a correction of both these models to overcome the observed problems.

3. EFFECT OF THE SURFACE ENERGY OF THE PORES

As mentioned in the introduction, standard $P-\alpha$ like models neglect the *surface energy of the pores* assuming that the porous material and its matrix have the same internal energy $U = U_m$. This approximation is valid for low porosity materials for which it was originally introduced by [12]. However it becomes less and less applicable the more the degree of porosity increases. In fact, for high porous materials the surface of the pores becomes so large that the associated energy cannot be neglected.

Here we propose a simple empirical relation between matrix and porous internal energy on the line of those relating density and pressure in the standard formulations presented in the previous section: $\hat{U}_m = \hat{U} - d\left(\alpha_0^n - 1\right)\hat{U}^l$. The parameters n, d, and l collect our uncertain knowledge of the internal structure of the material. For $d = 0$ or $n = 0$ the relation reduces to the standard approximation where both internal energies have the same value. Otherwise, the internal energy of the porous material is always larger than that of the corresponding solid. The pressure of the porous material, i.e. the last equation of system (1), has to be replaced by: $\hat{P} = \hat{P}_m\left[\alpha\hat{\rho}, \hat{U} - d\left(\alpha_0^n - 1\right)\hat{U}^l\right]/\alpha$.

The modified porous EOS along Hugoniot assumes the form:

$$F = F(\rho, P, \alpha; \alpha_0, d, n, l). \tag{4}$$

We consider two specific values of the parameter l which lead to three interesting consequences. In the following, $\rho - \alpha$ identifies a collection of matrix based models with the same qualitative properties characterised by a distension relation depending only on the density $\alpha = \alpha(\rho)$ [see 13]. The $\varepsilon - \alpha$ model belongs to this class. Results are presented in Fig. 2 where each of the three plots has the same layout. The left column displays the changes versus the pressure in the density of the porous material (top panel), the density of the matrix (middle panel) and the distension (bottom panel). The right column shows the changes versus the internal energy in the density (top panel) and the pressure (middle panel) of the porous material and the distension (bottom panel).

Shift of the singularity. The singularity present in $\rho - \alpha$ models is shifted in the $l = 1$ case (see left plot in Fig. 2). In fact, the singularity depends not only on the parameters of the EOS but also on the initial porosity and on the contribution of the surface energy of the pores. In the case that the matrix EOS is given by the U-dependent EOS the singularity is located at:

$$\frac{\hat{\rho}}{\hat{\rho}_0} = 1 + \frac{2}{c\left[1 - d(\alpha_0^n - 1)\right]}. \tag{5}$$

As a consequence, some of the models that are not physical in the standard formulation are acceptable now. However, only *normal behaviour* can be described by such models.

Disappearance of the singularity. The singularity present in $\rho - \alpha$ models completely disappears in the $l = 2$ case (see middle plot in Fig. 2). However, full compaction usually is accomplished at unrealistically high pressure (note the logarithmic scale in the figure). As in the previous case only *normal behaviour* can be described by such models.

Material dependent critical distension. In standard models that are not affected by the singularity such as those belonging to the $P - \alpha$ subclass, the correction for the surface energy of the pores allows the models to be able to describe both *normal* and *anomalous* behaviour independently on the initial degree of porosity (see right plot in Fig. 2). In fact, the critical initial distension now depends also on the parameters regulating the contribution of the surface energy of the pore that is material dependent.

4. CONCLUSIONS AND PERSPECTIVES

For materials characterised by high porosity, the $\varepsilon - \alpha$ model and all $\rho - \alpha$ models are not suitable for the description of pre-planetesimal matter because they become non physical, due to the appearance of a singularity. The $P - \alpha$ model is more appropriate but may be unable to model some materials. We proposed a correction to the internal energy of the porous material and of its matrix that considers the effect of the energy associated to the surface of the pores. These pore surface energy corrected models can

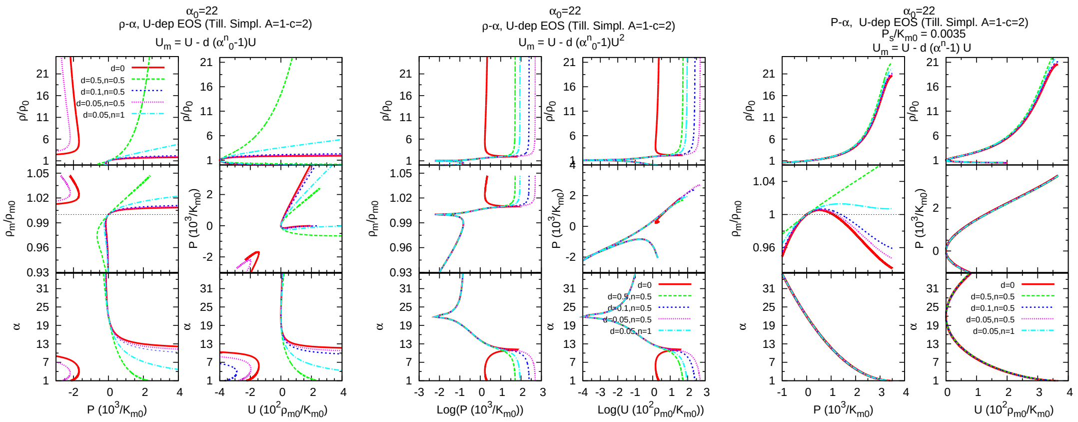

FIGURE 2. Effects of the surface energy of the pores. Shift of the singularity ($l = 1$, left plot), disappearance of the singularity ($l = 2$, middle plot) and material dependent critical distension ($l = 1$, right plot, the $l = 2$ case is qualitatively the same). The solid lines represent the standard model, the other type of lines represent the models corrected with different values of d and n.

overcome both of the problems observed in standard models. However, matrix based porosity models are empirical models with a weak physical foundation. Plasticity based models, which we have started to investigate, seem to give a more physically based description of the material in a thermodynamical context.

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