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EMPIRICAL TUFF EQUATION-OF-STATE MODELS

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EMPIRICAL TUFF EQUATION-OF-STATE MODELS

ABSTRACT

We compare two empirical pressure-specific volume (P-v) tuff equation-of-state models with bulk density and grain density P-v data for 27 NTS tuffs. We propose combining these models to obtain a single superior model. We suggest that modeling could be improved by accounting for tuff-water-chemical interaction and by obtaining more grain density data.

INTRODUCTION

Since a variety of low-pressure (0 - 4.0 GPa*) rock equation-of-state (EOS) models are currently being developed,¹⁻⁴ it is useful to report some calculations and comparisons we recently performed. Our comparisons are between two empirically derived models:

- the Butkovitch model,¹ and
- the Moreland-Hastings model,² and our extension of this model.

These models are potentially valuable to the containment community because they provide convenient and economic input to containment calculations. The models also have scientific value in that successful modeling provides potential insight into the physics of phenomena such as pore collapse. We limit ourselves to P-v (pressure-specific volume) models because they are the simplest (due to the absence of deviatoric stresses) and, fortuitously, the most frequently required. We further limit ourselves to NTS tuffs. The methods, however, apply equally well to other porous media and more complex stress states.

A reasonable starting point for P-v modeling of any medium is to ignore the fine structure of the bulk loading curve and use only the gross response. This has been the approach of both models we consider; the form assumed for their P-v bulk loading curves is given in Fig. 1. The initial loading up to P_1 , where the pores begin to collapse, is assumed to be elastic. Pore collapse continues from P_1 to P_2 where the loading curve becomes tangent to the appropriately saturated grain density loading curve. At higher pressures, the bulk loading coincides with the grain density loading, consistent with the assumption that all the pores have been compressed out. The minimum input required to define this P-v loading curve is the

- initial bulk density
- initial grain density
- water content.

* 40 kbar.

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Fig. 1. Assumed form of the loading curves.

In addition, techniques must be available to describe the initial elastic loading, calculate P_1 and P_2 , describe the pore collapse, and generate the grain density loading curve, at least for pressures greater than P_2 . To be programmatically viable, the basis of these techniques must be simple and readily available.

We start by establishing a notation for our discussion and then briefly review each model. We then discuss the suite of rocks used in our comparison and, finally, we present our results.

NOTATION

$\rho_r(P) = \frac{1}{v_r(P)}$	Grain density loading path
$\rho_{r0} = \rho_r(0) = \frac{1}{v_{r0}}$	Initial grain density
$\rho_w(P) = \frac{1}{v_w(P)}$	Water loading path
$\psi(P)$	Pore collapse relation
$\rho(P) = \frac{1}{v(P)}$	Bulk (rock grains, pores, and water) loading path
$\rho_d(P) = \frac{1}{v_d(P)}$	Dry bulk (rock grains and pores) loading path
$\rho_0 = \rho(0)$	Initial bulk density
Z	wt% water content
ϕ	Volume fraction porosity

Due to physical constraints, these rock properties are interrelated. We derive below one particularly useful relation interconnecting five of these properties. This relation is explicitly or implicitly used as a basis for both of the models we discuss.

If

V = volume of rock, water, gas composite

V_r = volume of rock

V_w = volume of water

V_g = volume of gas

at a given pressure, then

$$Z = \frac{\rho_w V_w}{\rho V} \quad (1)$$

$$\psi = \frac{V_g}{V} \quad (2)$$

and

$$V = V_r + V_w + V_g \quad (3)$$

$$\begin{aligned} \rho V &= \rho_r V_r + \rho_w V_w + \rho_g V_g \\ &\approx \rho_r V_r + \rho_w V_w \end{aligned} \quad (4)$$

Combining these definitions

$$\rho = \frac{\rho_r (1 - \psi)}{\left[1 - Z + \frac{\rho_r Z}{\rho_w} \right]} \quad (5)$$

or, in terms of specific volumes,

$$v = \frac{v_r + Z (v_w - v_r)}{1 - \psi} \quad (6)$$

One common assumption applied to this expression is that Z be a constant, that is, independent of pressure. This is a more severe restriction than might be apparent because many tuffs display a pressure-dependent chemical interaction between the water and rock.⁵ Models based on the above assumptions therefore cannot directly capture this response. Nevertheless, Eq. (6) is a very interesting relationship for it shows how the pressure response of a rock-water-gas composite is defined in terms of the response of the components. To use this relationship for P - v models, we require:

- The water content, Z
- The grain density loading curve, $v_r(p)$
- The water loading curve $v_w(p)$
- A pore-collapse relation, $\psi(p)$
- A description of the initial elastic response up to P_1 .

THE MODELS

The Butkovich Model

The Butkovich^{*} model was developed as a tuff EOS generator for use in 1-d and 2-d stress wave codes.⁶ It calculates

- the bulk loading curve
- unloading characteristics
- the failure envelope

from input of the tuff initial bulk density, initial grain density, and water content (or input from which this can be derived). However, we discuss only the bulk loading portion of the model.

^{*} Referred to as TB for T. Butkovitch.

Butkovitch starts with the previously derived relation [Eq. (6)]

$$v = \frac{v_r + Z (v_r - v_w)}{1 - \psi}.$$

$v(p)$ and $v_w(p)$ are derived indirectly from Hugoniot information in the form of shock wave velocity (u_s)-particle velocity (u_p) data. If the u_p - u_s relation for the medium is known, then a $v(p)$ relation can be derived from the conservation of mass and momentum relations.

Figure 2a gives the rock u_p - u_s data used by Butkovitch. The scatter is associated with a dependence on the initial grain density and using hydrostatic P-v data he constructs a family of u_p - u_s curves depending on the grain density.

The $V_w(P)$ model is derived from the water u_p - u_s data (Fig. 2b). The fine scale variations in the data are attributed to the phase changes of water (Fig. 2b), and several options for treating these changes are presented.

Based on data from two tuffs (Scroll and Schooner) and an interpretation of an "average" tuff (Diamond Dust), the pore-collapse relation was taken to be

$$\psi = \psi_i \frac{\ln (P/P_2)}{\ln (P_1/P_2)}, \quad (7)$$

where ψ_i is the initial gas-filled porosity. Definition of the model is completed by correlations, obtained by trial and error, of P_2 and P_1 with the physical properties of the tuffs.

The Moreland-Hastings Model

Next we consider the P-v model for dry tuffs developed by Moreland and Hastings.² Again, the basis of the model is the relation [Eq.(6)]:

$$v = \frac{v_r + Z (v_r - v_w)}{1 - \psi},$$

which for dry tuffs reduces to

$$v_d = \frac{v_g}{1 - \psi}. \quad (8)$$

The Moreland-Hastings model of the grain density loading curve is based on a collection of Hugoniot P-v data for tuffs (Fig. 3).² They argue that the high-pressure data represent a typical grain density tuff with

- an initial grain density of 2.4 g/mm
- a mineralogy of glass, 80 wt%
quartz, 10 wt%
clay, 10 wt%
- a sound speed of 3.2 km/s

Fig. 2. Hugoniot equation-of-state data (from Ref. 1).
 (a) For near grain density rock used in analysis.
 (b) For water showing correction for phase transitions at 9.6 and 24.0 kbar.

Fig. 3. Hugoniot pressure-specific volume data for dry porous tuffs. Taken from Ref. 2.

These properties, combined with

- conservation of mass
- conservation of momentum
- the high-pressure Hugoniot data in Fig. 3
- the assumption that the Hugoniot data and 25°C isothermal P-V data coincide to at least 4 GPa,

yield the following grain density P-v model:

$$P = 245.8 \mu + 298.7 \mu^2 + 61.49 \mu^3, \quad (9)$$

where

$$\mu = \frac{\rho_r - \rho_{r0}}{\rho_{r0}}. \quad (10)$$

Here Moreland and Hastings have assumed that grain density P-v curves for tuffs with $\rho_{r0} \neq 2.4$ g/cc can be derived by substituting the appropriate value of ρ_{r0} in Eq. (10). Clearly, this method for generating grain density P-v curves differs only in detail from that developed by Butkovitch.

The Moreland-Hastings model of pore collapse is more interesting. The pore collapse relation was derived semi-empirically by comparing bulk loading P-v data for six dry tuffs* with their grain density loading curves as calculated above. In the interest of simplicity, P_1 was chosen to be negligibly small so that pore collapse begins immediately. Collapse continues until the bulk loading curve coincides with the grain density loading curve. We call the pressure at this point P_2 , but the authors define this point in terms of the density at this pressure, ρ_2 . The correlation of ρ_2 with the initial porosity and initial grain density of the rock completes the definition of the model.

An Extension of the Moreland-Hastings Model

We have extended the Moreland-Hastings model by including the effect of water on the loading curves. Note that if

V = volume of rock, water, and gas

V_d = volume of rock plus gas

V_w = volume of water

then, again by definition

$$Z = \frac{\rho_w V_w}{\rho V},$$

$$V = V_d + V_w,$$

and

$$\rho V = \rho_d V_d + \rho_w V_w. \quad (11)$$

* NTS Dry, 3 Schooner tuffs, and Stoddard (Table 2).

Combining, we obtain

$$v = v_d (1-Z) + Zv_w .$$

We use this relation to construct loading curves for wet tuffs from the loading curve of the corresponding dry tuff ($v_d(d)$). To minimize the variables in a comparison between models, we use the smoothed water model, $v_w(p)$, as developed by Butkovitch. We call this model the Extended Moreland-Hastings (EMH) model.

Note that input to this model is the same as is required by the TB model:

- initial bulk density
- initial grain density
- water content.

ROCK PROPERTIES

We consider two groups of tuffs; those for which grain density P-v data is available and those for which bulk P-v loading data is available (unfortunately these two groups do not overlap). For the grain density group, we give the core location of each sample, initial grain density, and references in Table 1.^{5,7,8} Similar information is given in Table 2^{5,9-14} for the bulk density samples along with notable features. We use Stephen's classification¹⁰ to define features: saturated ≥ 10 wt%, vitreous > 50 wt% glassy material, and crystalline < 50 wt% glassy material.

COMPARISON

Grain density samples

We now directly compare the TB model and the EMH model. We first present grain density P-V calculations and then consider the bulk loading P-v calculations.

In Fig. 4 through 8, we compare the two models and the grain density P-v data. The agreement in every case is acceptable, but we note that the errors associated with a particular model are related to the initial grain density; the TB model works best for grain densities over 2.57 g/cc, while the EMH model works best for lower grain densities. These biases are a direct result of the different Hugoniot data used in each model. Clearly, a judicious marriage of the Hugoniot data would result in a more versatile grain density model.

Bulk Density Samples

We present comparisons between the models and the bulk loading data in Figs. 9 through 29. The comparison in Fig. 9 through 12 is favorable to both models. Note in

Table 1. Grain density samples.

Tuff name	Hole No.	Depth(ft)	ρ_{r0} (g/cc)	Refs.
Benham	U20c	3706	2.57	7,8
Diamond Dust	U16a.05	Cavity	2.446	7,8
Mt. Helen	~70 mi NW of Mercury, Nevada	Surface	2.447	5,7,8
Schooner	Ue20u#3	150	2.635	7,8
Scroll	Ue19m	739	2.59	7,8

Table 2. Rock properties for tuffs for which bulk loading data is available.

Rock	Sample Location			P_0	P_{r0}	Z	ϕ_i	ψ	Comments	Refs.
	Hole No.	Depth(ft)	Refs.							
Scroll	Ue19m	862	10	1.406	2.37	0.004	0.409	0.4035	Vi	10,12
Schooner	Ue20u #1	304	9	1.604	2.656	.276	.5628	.12 ^a	Saturated	9,10
Schooner	Ue20u #3	154	9	1.766	2.689	.084	.3971	.25 ^a	Cr	9,10
Hudson Seal	U12r.04	18	9	1.679	2.462	.30	.5226	.0189	Saturated	9
Hudson Seal	U12n.04 Slifer No. 1	154,182	9	1.858	2.465	.205	.4008	.0199	Saturated	9
Hudson Seal	U12n.04 Slifer No. 1	53,129.5	9	1.977	2.459	.144	.3118	.0271	Saturated	9
Diamond Dust	Unit 3 U16a.05 inst 5	24	11	1.88	2.396	.158	.3336	.05 ^a	Zeolitic, nonliquid H ₂ O = 5% ± 1%	11
Diamond Dust	Unit 4a U16a.05 inst 8	138	11	1.79	2.266	.16	.3351	.05 ^a	Zeolitic, nonliquid H ₂ O = 5% ± 1%	11
Diamond Mine	U16a.06 PI-3	19	14	1.87	2.321	.144	.3190	.041 ^a	Similar to Diamond Dust	14
Jorum	Ue20e No. 1	3440	10	1.905	2.495	.194	.3846	.015	Saturated, 5% nonliquid H ₂ O = 5.3%	10
Jorum	Ue20e No. 1	2523	10	2.051	2.685	.147	.3484	.047	Saturated, 5% nonliquid H ₂ O = 4.5% anomalous data	10
Benham	U20c	4600	9	2.1	2.558	.134	.2924	.001	Saturated	9
Hardhat	U15a	740	12	2.648	2.70	.005	.0291	.0025	Cr	12
Jorum	Ue20e No. 1	1793	10	2.188	2.454	.025	.131	.0763	Cr	10
NTS, Dry	U12b07	75	13	2.24	2.31	0.0	≥ .027	≥ .027	Zeolitic	13
Schooner	Ue20u #3	41	9	2.356	2.41	.003	> .034	> .027	Cr	9
Schooner	Ue20u #3	398	9	2.306	2.431	.003	> .053	> .046	Cr, but mineralogically different from Schooner above	9
Schooner	Ue20u	150	10	1.661	2.3314	.005	> .27	> .261	Cr	9,10
Stoddard	Ue25	1648	10	1.466	2.275	0.0	> .34	> .34	Vi, no free water	9,10
Mt. Helen, 100%	Surface outcrops, ~70 mi NW of Mercury		5	1.86	2.32	.192	.387	.0295	Water-tuff chemical interaction	5
Mt. Helen, 50%				1.64	2.32	.096	.395	.237		
Mt. Helen, dry				1.48	2.32	0.0256	0.411	0.374		

^aFrom unloading at 3.0 GPa, otherwise calculated.

Fig. 4. Comparison of the models with Benham grain density loading data.

Fig. 5. Comparison of the models with Diamond Dust grain density loading data.

Fig. 6. Comparison of the models with Mt. Helen grain density loading data.

Fig. 7. Comparison of the models with Schooner grain density loading data.

Fig. 8. Comparison of the models with Scroll grain density loading data.

Specific volume — cc/g

Fig. 9. Comparison of the models with Hudson Seal bulk density loading data, $\rho_0 = 1.977$, $\rho_{r0} = 2.459$, $Z = 0.144$.

Fig. 11. Comparison of the models with Benham bulk density loading data, $\rho_0 = 2.099$, $\rho_{r0} = 2.558$, $Z = 0.134$.

Fig. 10. Comparison of the models with Hudson Seal bulk density loading data, $\rho_0 = 1.679$, $\rho_{r0} = 2.462$, $Z = 0.3$.

Fig. 12. Comparison of the models with Hudson Seal bulk density loading data, $\rho_0 = 1.858$, $\rho_{r0} = 2.465$, $Z = 0.205$.

Fig. 13. Comparison of the models with Jorum bulk density loading data, $\rho_0 = 2.051$, $\rho_{r0} = 2.685$, $Z = 0.147$.

Fig. 14. Comparison of the models with Jorum bulk density loading data, $\rho_0 = 1.905$, $\rho_{r0} = 2.495$, $Z = 0.194$.

Fig. 15. Comparison of the models with Diamond Dust bulk density loading data, $\rho_0 = 1.88$, $\rho_{r0} = 2.396$, $Z = 0.158$.

Fig. 16. Comparison of the models with Jorum bulk density loading data, $\rho_0 = 2.188$, $\rho_{r0} = 2.454$, $Z = 0.025$.

Fig. 17. Comparison of the models with Stoddard bulk density loading data, $\rho_0 = 1.466$, $\rho_{r0} = 2.275$, $Z = 0.0$.

Fig. 18. Comparison of the models with Schooner bulk density loading data, $\rho_0 = 1.661$, $\rho_{r0} = 2.331$, $Z = 0.005$.

Fig. 19. Comparison of the models with Schooner bulk density loading data, $\rho_0 = 1.604$, $\rho_{r0} = 2.656$, $Z = 0.276$.

Fig. 20. Comparison of the models with NTS Dry bulk density loading data, $\rho_0 = 2.24$, $\rho_{r0} = 2.31$, $Z = 0.0$.

Fig. 21. Comparison of the models with Schooner bulk density loading data, $\rho_0 = 2.306$, $\rho_{r0} = 2.431$, $Z = 0.003$.

Fig. 22. Comparison of the models with Schooner bulk density loading data, $\rho_0 = 2.356$, $\rho_{r0} = 2.41$, $Z = 0.003$.

Fig. 23. Comparison of the models with Diamond Mine bulk density loading data, $\rho_0 = 1.87$, $\rho_{r0} = 2.321$, $Z = 0.144$.

Fig. 24. Comparison of the models with Scroll bulk density loading data, $\rho_0 = 1.406$, $\rho_{r0} = 2.37$, $Z = 0.004$.

Fig. 29. Comparison of the models with Diamond Dust bulk density loading data, $\rho_0 = 1.79$, $\rho_{r0} = 2.266$, $Z = 0.16$.

Table 2 that each of these samples were saturated so that these data do not severely test the pore collapse model; the model response for these cases is governed completely by the compressibility of the rock matrix and water.

In Fig. 13 through 23 we give an interesting set of comparisons in which the TB model is consistently stiffer than the data at high pressures. We believe that this is largely a result of difficulties in the Butkovitch grain density model for low initial grain densities. This, as mentioned earlier, is an easily corrected deficiency. We also observe some low-pressure differences between the models and the data, particularly for the more porous rocks. For example, the EMH model is in significant low-pressure error for the Schooner ($\rho_0 = 1.604$) sample while the TB model is in good agreement. We believe this is because the TB pore collapse model is indirectly derived from this data, while the EMH model is not. Similarly we note that the EMH model is superior for Stoddard ($\rho_0 = 1.466$) and Schooner ($\rho_0 = 1.661$) data for the same reasons; the EMH pore collapse model was derived from these data. Finally, it is very interesting that the Jorum data ($\rho_0 = 2.188$) in Fig. 16 agrees so well with the EMH model. The data was considered to be in error by Butkovitch because of its poor agreement with his model, but this suggests that the problem is in the TB grain density model.

There are two comparisons (Fig. 24 and 25) for which the Butkovitch model is superior. The good agreement is to be expected since again the Butkovitch pore collapse model was derived from these data. It is, however, surprising to see the Scroll data fit the Butkovitch model so well, given its low initial grain density. We attribute this good agreement to the fact that the response is governed by pore collapse up to at least 3.0 GPa; above 3.0 GPa the Butkovitch model should diverge from the data as the influence of the grain density curve becomes increasingly important.

Finally, in Fig. 26 through 29, we give comparisons that are less favorable for both models. First, we present Mt. Helen tuff at three different saturations (0, 50, and 100%). The comparisons are generally unacceptable. Both models may be invalid for this tuff as there is an apparent interaction between the tuff and water.⁵ The data certainly appears to be anomalous, whether for this, or other, reasons. We observe that over ~ 2.0 GPa, the loading paths of the tuffs exactly superpose, independent of saturation. In any case, we do not feel at this time that the poor comparison negates either model. Finally, in Fig. 29, we present the comparison for Diamond Dust. Here the comparison is better than for Mt. Helen, but each model displays a deficiency at either low or high pressure.

CONCLUSIONS

There is very little conceptual difference between the Butkovitch model and our extended Moreland-Hastings model. In the detailed approach, however, there are significant differences.

First, the Moreland-Hastings model is built upon a larger and more relevant suite of grain density data. We saw several times in the comparisons how this superior grain density model better captured high-pressure data. Second, we believe that the Moreland-Hastings method of deriving a pore collapse model is superior to "cut and try" methods. The EMH model, however, could be significantly improved if the basis of their pore collapse model were enlarged to include all the tuff data presented in this report. We further suggest that these P-v models would be more versatile if they included a model for the chemical interaction between tuffs and water. Finally, it is urgent to obtain both grain density and bulk density loading paths for the same core in order that the pore collapse models can be quantitatively tested.

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