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On the use of rock physics models for studying the critical zone

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Key Points:

- Rock physics model performance depends on sediment age
- Jenkins, followed by Walton, and Hertz-Mindlin models perform best in cementless critical zone sands
- Rock physics models remain non-unique primarily because of a lack of constraint on how grain-contact forces are distributed in sands

ABSTRACT

How effective are rock physics models for relating seismic velocities to the physical properties of sediments, fluids, and cement within the critical zone, and what factors most substantially influence the models' accuracies? We answer these questions by testing and analyzing the accuracies of seven rock physics models (Hertz-Mindlin, Walton, Jenkins, Digby, stiff sand, soft sand, and contact cement) for estimating seismic velocities of vadose zone sands at Port Royal Beach in Jamaica. These sands are clean, well-rounded, and highly-spherical, which are ideal for rock physics model testing. Measured velocities and model input parameters (e.g., porosity, density, grain size, and fluid saturation percentage) derive from seismic refraction surveys and sidewall sediment cores, respectively. We find that, in their current forms, all seven rock physics models overpredict seismic velocities for sands deposited within the last forty-three years. Misfits between measured and predicted velocities reduce with time since deposition, with all but one (Digby) cementless models accurately predicting the seismic velocities for sands older than ninety-five years. Jenkins, followed by Walton, Hertz-Mindlin, and soft sand models are generally most accurate (i.e., have the lowest misfits), possibly because high porosity sands are more susceptible to tangential slip during seismic wave propagation. We conclude that the models will most substantially improve when the effects of the existence and locations of strong versus weak force-chain links are included in their respective equations.

1 1 Introduction

2 The critical zone is the shallow section of the earth's crust, where living organisms, 3 porous sediments, and fluids interact. There is an ongoing need to understand this section of 4 earth's crust better, partly because of its importance for combatting the adverse effects of climate change as well as its role in water conservation (e.g., Anderson et al., 2007; Parsekian et al., 5 6 2015). Researchers often characterize the critical zone using above-ground geophysical surveys, 7 which can be cheaper and more feasible than direct sampling methods such as drilling (Parsekian 8 et al., 2015). Common surface-based geophysical studies include electromagnetic, ground-9 penetrating radar, nuclear magnetic resonance, electrical resistivity, magnetotelluric, and seismic 10 refraction surveys (e.g., Selker et al., 2006; Rodell et al., 2007; Rabbel, 2010). Measured 11 geophysical observables from these surveys (e.g., seismic velocities) are often integrated with 12 empirical and theoretical models (e.g., empirical porosity-velocity curves and rock physics models) to provide quantitative links between the surveyed properties (e.g., seismic velocities) 13 and the physical properties of buried sediments and fluids (Day-Lewis et al., 2005; Parsekian et 14 al., 2015). Studying the critical zone in this way relies on the accuracy of empirical and 15 theoretical models. 16

The integration of seismic velocities and rock physics models represents a promising method for constraining critical zone sediments, fluids, grain microstructure, and cement (Holbrook et al., 2014; Shen et al., 2016; Flinchum et al., 2018). Methods for deriving seismic velocities from refraction surveys (e.g., first-break geometric, tau-p, and seismic tomography) are well-known and reasonably advanced but sometimes produce inconsistent results owing to variations in first-arrival picks, velocity averaging, and/or tradeoffs between velocity and layer thickness, and the inherent non-uniqueness in the geophysical inverse methods used to constrain

24	velocity profiles (e.g., Mota, 1954; Stephenson et al., 2005). Rock physics models predict
25	seismic velocities by integrating estimates for porosity, bulk density, grain size, coordination
26	number, effective pressure, cement fraction, grain friction, and mineral Poisson's ratio (Mavko et
27	al., 2020). Their use in critical zone studies remains contentious primarily because (1) the models
28	produce non-unique solutions due to a large number of variables, (2) model constraints often
29	lack ground-truthing in the critical zone that reduces model uncertainty, and (3) different models
30	use different physical approaches or assumptions to estimate seismic velocity (Day-Lewis et al.,
31	2005). An open question is whether improvements to the models are needed before they are
32	widely used in the critical zone.
33	The seven most commonly used rock physics models are Hertz-Mindlin, Digby, Walton,
34	Jenkins, contact cement, stiff sand, and soft sand (Mindlin, 1949; Digby, 1981; Walton, 1987;
35	Dvorkin & Nur, 1996; Jenkins et al., 2005; Mavko et al., 2020). Hertz-Mindlin is the only model
36	that has been tested in multiple deep-marine and shallow critical zone sands (Bachrach et al.,
37	2000; Bachrach & Avseth, 2008; Andersen & Johansen, 2010). Hertz-Mindlin performs best for
38	compressional wave velocities Vp in deep-buried (>400 km) sands but overpredicts shear wave
39	velocities Vs at similar depths (Bachrach et al., 2000; Andersen & Johansson, 2010).
40	Specifically, Hertz-Mindlin overpredicts Vp and Vs in vadose zone sands, assuming average sand
41	properties (Bachrach et al., 2000; Andersen & Johansson, 2010). Wright & Hornbach (submitted,
42	JGR: Solid Earth) tested the accuracy of Hertz-Mindlin with constraints on all model parameters
43	except coordination number, which they derived from Murphy (1982) 's empirical relationship
44	(Figure 2). They showed that Hertz-Mindlin accurately predicts seismic velocities for vadose

45 sands older than ninety-five years but overpredicts velocities for vadose sands younger than

46 forty-three years. The enigmatic results from these field, numerical, and theoretical studies are an

47 impetus for additional studies of the effectiveness of the other six rock physics models and the48 influences of microscale grain processes on the models' seismic velocity predictions.

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This study assesses the accuracies of the seven abovementioned rock physics models. We 49 discuss the sediment property insights that can be gained from model tests and the best ways to 50 51 improve and use the models for critical zone studies. Our study area consists of nearly pure 52 vadose zone sand at four sites at Port Royal Beach, Jamaica – i.e., the same sands studied by Wright & Hornbach (submitted, JGR: Solid Earth) (Figure 1). These sands are clean (contain <5 53 % fines), well-rounded, and highly-spherical (Figure 2), which makes them ideal for rock 54 55 physics model testing. Furthermore, the site has been trenched, cored, and surveyed with a 56 seismic refraction study so that the greatest uncertainties in physical properties are minimized.

The results show that Jenkins, followed by Walton and Hertz-Mindlin, most accurately predict measured seismic velocities in this study area. We conclude that predictions from these models will further improve when effects of the existence, locations, and strengths of force-chain links are accounted for in the models. Currently, there remains a significant risk of using rock physics models to infer that seismic velocity changes are related to changes to porosity, water saturation, and pore space cement, when instead, the observed velocity changes are caused by changes to grain-contact force distribution.

64 2 Background

65 The rock physics models approximate sand as a collection of randomly organized 66 identical spheres subjected to Hertzian contact forces (Hertz, 1881). In the same sand (i.e., same 67 porosity, lithology, and effective stress), differences between model predictions solely arise from 68 how the models treat cementation, grain friction, grain size, and slip at grain contacts (Mindlin, 69 1949; Digby, 1981; Walton, 1987; Dvorkin & Nur, 1996; Jenkins et al., 2005). We discuss these
70 differences below.

Hertz-Mindlin, Walton, Jenkins, and Digby assume that sands are cementless (Mindlin, 71 72 1949; Digby, 1981; Walton, 1987; Jenkins et al., 2005). Contact cement, soft sand, and stiff sand 73 are modified versions of Hertz-Mindlin with the caveat that cement is present within the sand's 74 matrix, reduces porosity, and/or increases grain-grain adhesion (Dvorkin & Nur, 1996). Contact 75 cement assumes that cement is only present at contacts or surrounds the grains (Dvorkin & Nur, 1996). Soft and stiff sand models assume that cement is deposited on the surface of the grains, 76 77 away from grain contacts (Dvorkin & Nur, 1996). Soft and stiff sand also respectively assume 78 that grains are organized in the weakest and strongest possible configurations, as constrained by 79 the Hashin-Shtrikman bounds (Hashin & Shtrikman, 1963).

80 The models differ based on assumptions for if, how, and why seismic waves induce microscale grain-contact slip. Hertz-Mindlin, and by extension stiff sand, soft sand, and contact 81 82 cement, assume that slip occurs after the tangential stresses exceed interparticle grain-contact 83 normal forces (Mindlin, 1949; Dvorkin & Nur, 1996). Walton assumes that normal and tangential slip co-occurs (Walton, 1987). Jenkins approaches slip from a force balance 84 85 perspective, arguing that grain-contact slip is nonlinear and depends on the force exerted on 86 neighboring grains (Jenkins et al., 2005). Digby assumes that grains are initially bonded across 87 their effective contact radius, and, away from there, grain-contact slip occurs without resistance 88 whenever grain-contact normal forces are exceeded (Digby, 1981). All models (except for Digby) could be modified to assume that grain-contact friction is infinite (rough-grained) or non-89 90 existent (smooth-grained) (Mindlin, 1949; Digby, 1981; Walton, 1987; Dvorkin & Nur, 1996; 91 Jenkins et al., 2005). Jenkins and Digby are the only models that parametrize grain size (Digby,

92 1981; Jenkins et al., 2005). Once all model parameters are constrained, comparisons between
93 modeled and measured velocities could provide insights into which unmeasured model
94 assumptions (e.g., slip mechanism) are poor approximations of real systems and or what
95 additional model parameterizations are needed to represent sands better.

96 **3 Methods**

We assess the models' accuracies by comparing modeled versus measured seismic
velocities at study sites 1-4 at Port Royal Beach (see Figure 1). Modeling *Vp* and *Vs* require
constraints on bulk density ρ_b, effective bulk modulus *K_{eff}* and effective shear modulus
μ_{eff} (equations 1-2). Rock physics models and Gassmann-Biot theory provide constraints on *K_{eff}* and μ_{eff}, whereas ρ_b derives from sidewall cores (Wright & Hornbach, submitted, JGR:
Solid Earth).

$$Vp = \sqrt{\frac{\frac{4}{3} K_{eff} + \mu_{eff}}{\rho_b}}$$
(1)
$$Vs = \sqrt{\frac{\mu_{eff}}{\rho_b}}$$
(2)

103 The rock physics equations for the dry-frame elastic moduli are in the appendix. For104 each model, we constrain:

105 (A) porosity ϕ using sidewall cores (Wright & Hornbach, submitted, JGR: Solid Earth),

106 (B) effective hydrostatic pressure P_{eff} using equation 3, where g, W_d, S_w , and Y_w

107 respectively represent gravitational acceleration, water table depth, fluid saturation

108 percentage, and unit weight of water,

$$P_{eff} = g \int_{0}^{z} \rho_{b}(z) dz - [z - W_{d}] S_{w} Y_{w}$$
(3)

109 (C) mineral bulk K_m and shear μ_m moduli using the Hashin-Shtrikman bounds (equations

110 4-5), where K_f , K_s , μ_f , and μ_s represent fluid bulk modulus, mineral bulk modulus, fluid

shear modulus, and mineral shear modulus (Hashin & Shtrikman, 1963),

$$K_m = K_s + \frac{\phi}{\left(K_f - K_s\right)^{-1} + (1 - \phi)(K_s + \frac{4}{3}\mu_s)^{-1}}$$
(4)

$$\mu_m = \mu_s + \frac{\phi}{\left(\mu_f - \mu_s\right)^{-1} + \frac{2(1-\phi)(K_s + 2\mu_s)}{5\mu_s\left(K_s + \frac{4}{3}\mu_s\right)}}$$
(5)

112

113 (D) Voigt M_v and Reuss M_R bounds for k_m and μ_m using equation 6-7, where f_i

114 represents the fractional proportion of the elastic moduli m_i of the i^{th} mineral (Hill,

115 1952),

$$M_{\nu} = \sum_{i=1}^{N} f_i m_i \tag{6}$$

$$\frac{1}{M_R} = \sum_{i=1}^N \frac{f_i}{m_i} \tag{7}$$

116 (E) mineral Poison's ratio η_m using equation 8,

$$\eta_m = \frac{3k_m - 2\mu_m}{6k_m + 2\mu_m}$$
(8)

(F) and coordination number *c* using equation 9 (Murphy, 1982).

$$c = 20 - 34\phi + 14\phi^2 \tag{9}$$

118 We use Gassmann-Biot's formula (equation 10) to estimate the effects of fluid saturation

on dry-frame bulk moduli K_{dry} estimated from rock physics models (Gassmann, 1951; Biot,

- 120 1956). There, K_{air} and K_{f2} represent the bulk modulus of air at constant temperature (101 kPa)
- and the bulk modulus of the fluid (i.e., seawater, 2.3 GPa), respectively.

$$\frac{K_{eff}}{K_m - K_{eff}} - \frac{K_{f2}}{\phi(K_m - K_{f2})} = \frac{K_{dry}}{K_m - K_{dry}} + \frac{K_{air}}{\phi(K_m - K_{air})}$$
(10)

With K_{eff} constrained, we use equations 1-2 to predict seismic velocities under three 122 scenarios that investigate the models' uncertainties. In scenario one, we empirically constrain 123 124 coordination numbers with Murphy (1982) 's relationship (equation 9) and predict velocities 125 10,000 times, each time inputting different groups of model parameters that we randomly select from a uniform distribution of numbers within each parameter's numerical range. This method 126 127 ensures that uncertainties associated with the measured input model parameters and effective 128 medium bounds (e.g., Hashin-Shtrikman and Voigt-Reuss) are reflected within seismic velocities 129 predictions. In scenario two, we constrain uncertainties in the same way, assume that Murphy 130 (1982) 's coordination number relationship may be erroneous, and instead calculate the 131 coordination number required to best predict seismic velocities. In scenario three, we predict seismic velocities assuming average sand properties (i.e., 100% quartz, $\phi_z = 0.4$, $\rho_b = 1.5$ g/cm³, 132 and mineral elastic moduli estimated from Voigt and Reuss bound averages). This scenario 133 134 assesses the importance of ground-truthing models with in-situ sediment property measurements. 135 4 Results 136 Misfits between modeled and predicted seismic velocities vary between the three 137 modeled scenarios, depth, and age (Figure 3-4). Models that use Murphy (1982) 's relationships 138 for coordination number and Monte-Carlo uncertainty analyses (i.e., scenario one models) overpredict seismic velocities at sites 1-2 below ~0.1 cm; misfits are lower for sites 3-4, with the 139 140 soft sand and all cementless models except Digby accurately predicting seismic velocities. For 141 scenario 2, we find that unrealistically low coordination numbers (1-2) are needed to predict

seismic velocities at sites 1-2, whereas the higher predictions from Murphy (1982) 's relationship

143 (4-8) are sufficient to predict velocities at sites 3-4, especially below 1 m depth (Figure 3-4).

Models assuming average sand properties (i.e., scenario three models) generally result in
mispredictions; these models perform best for sands deeper than 1 m at site 3.

Regardless of the scenarios, misfits for Vp (Figure 3-4) are generally lower than for Vs 146 147 (Figure 3-4). Smooth-grained and cementless models also generally result in lower misfits. Of 148 the cementless models, Jenkins, followed by Walton, Hertz-Mindlin, and Digby, has the lowest 149 mispredictions for Vp shallower than 1 m and all depths in Vs. Walton, followed by Hertz-150 Mindlin, Jenkins, and Digby, has the lowest mispredictions for Vp beneath 1 m. Of the cement 151 models, the soft sand, followed by the stiff sand and contact cement, results in the lowest misfits. 152 Soft sand is the only cement model that accurately predicts seismic velocities in sections of the 153 sand column with measured cement - i.e., between 0.8-2 m at site 3-4 under scenario one and all 154 depths at sites 1-2 under scenario two.

155 **5 Discussion**

Below, we use the results to discuss the significance of misfits between modeled and measured velocities, how to improve the models, and best practices for using the models for critical zone studies. We conclude that the models remain non-unique primarily because of a lack of understanding of how grain-contact forces are distributed.

160 5.1 Significance of misfits between modeled and predicted seismic velocities

Model comparisons provide insights into grain microstructure. Observations that (1) the models' accuracies improve with age without significant changes to the measured sand properties, (2) cement models more substantially overpredict velocities than cementless ones, and (3) that an unrealistically low coordination number [1-2 versus 4-8 as predicted by Murphy (1982) 's relationship] is needed to predict velocities in younger sands are instructive. The

166 observations further support Wright & Hornbach (submitted, JGR: Solid Earth) 's interpretation

167 that the main difference between sites 1-2 and 3-4 is likely an unmeasured physical property 168 relating to how grains and grain contact forces are distributed within the sand columns. One 169 interpretation to test is whether coordination numbers are similar across all sites [i.e., 4-8 as 170 predicted by Murphy (1982)'s relationship] but seismic velocities are greater in older sands 171 because the younger sands have less load-bearing grains (e.g., 1-3 of the 4-8 that are in contact) 172 that significantly participate in the transmission of seismic waves. Under these conditions, it is 173 not surprising that the lower coordination numbers produce better fits to the measured seismic 174 velocities. The above scenario highlights one of the major drawbacks of using rock physics to 175 study natural shallows sands – i.e., the models treat grains and grain-contact forces as being 176 identical even though these properties are almost certainly not identical.

177 The model comparisons provide insights into the micro-slip behaviors of vadose zone 178 sands. Observations that smooth-grained models perform better than rough-grained models 179 imply that propagating seismic waves induce microscale elastic grain-contact slip in these sands. 180 Observations that Jenkins generally performs best for scenario one models suggest that a 181 nonlinear grain-contact slip modeling approach may be best, especially in high porosity sands 182 (like we study) where tangential grain-contact slips can more freely occur. Jenkins, Hertz-183 Mindlin, and Walton do, however, predict velocities similarly (within 5 %) at sites 3-4, implying 184 that other factors are at play (e.g., grain-contact force distribution) and/or slip mechanism is of 185 second-order importance to seismic velocity predictions in the older sands. The most 186 straightforward interpretation is, therefore, that Port Royal Beach sands are generally susceptible to deformation (i.e., grain-contact slippage) during seismic wave propagation (including 187 188 earthquakes) and that the sands could increase grain-contact forces via grain reorganizing 189 processes such as compaction or contact creep.

190 The model comparison results suggest that cement most likely reduces porosity and is 191 unlikely to be present at grain contacts. When parameterized with cement fraction estimates 192 (i.e., between 0-3%; Figure 2), lower misfits by the soft sand (versus stiff sand and contact 193 cement) models (Figure 4) are consistent with an interpretation that the grains more probably 194 arrange in the softest configurations as well as that cement is most likely deposited on the grains, 195 but away from contacts. Observations that contact cement and stiff sand overpredict velocities by 196 at least ~500-1000 m/s in most cemented sections of the sand columns also imply that it is 197 unlikely that cement surrounds the grain and/or act as a grain adhesive. Moreover, better 198 predictions by Digby versus contact cement may suggest that any existing grain-grain adhesion 199 (by cement or capillary forces) is likely weaker than stresses induced by seismic wave 200 propagation. Cement, therefore, is unlikely to be the primary controlling factor for changes in 201 seismic velocities with sediment age.

202 5.2 Improvements needed for better rock physics modeling of the critical zone

203 Based on these observations, we suggest that rock physics models will most significantly 204 improve with a better understanding of how sands distribute overburden stresses (Makse et al., 205 1999; Makse et al., 2004; Majmudar & Behringer, 2005; Bachrach & Avseth, 2008). The need 206 for improved understanding of grain-contact force distribution is evidenced by observations that 207 modeled misfits primarily change as a function of coordination number, age, and depth, as 208 opposed to slipping mechanism or grain-contact friction (Figure 3-4). Previous studies' 209 observations that (1) overburden stresses within photoelastic beads become more uniformly 210 distributed (along grain force chain links) with increasing effective pressures (Majmudar & 211 Behringer, 2005), (2) sorting and angularity induced nonuniform grain-contact geometries can 212 cause Hertz-Mindlin to overpredict seismic velocities at 400-600 m depths (Bachrach & Avseth,

213 2008), and (3) beach, river, and dune sand porosities remain constant down to 17 m are 214 instructive. This, combined with results presented here, supports the hypothesis that, apart from 215 fluid saturation in Vp, changes to the seismic velocities of clean critical zone (upper 17 m) sands 216 are primarily controlled by variations in grain-contact force distributions as opposed to grain 217 contact number or porosity reduction alone. If true, we predict that there exists a transition zone 218 or set of conditions, whereby force distribution becomes homogenized within natural sands, and 219 rock physics models become appropriate for use. Testing these predictions will require directly 220 quantifying relationships between coordination number, porosity, sorting, angularity, effective 221 pressure, and force chain-link development within various critical zone depositional 222 environments, preferentially where seismicity is low.

223 5.3 Implementing rock physics models in future critical zone studies

224 Results and interpretations from this study highlight the major sources of non-uniqueness in rock physics model solutions. Incorrect model inferences would have likely occurred at one or 225 226 more of the study sites if we did not constrain all input model parameters (as is often done), used 227 empirically derived coordination number relationships, model velocities with Hertz-Mindlin 228 alone, assume average sand properties, and or did not account for all uncertainties in physical 229 properties and measured seismic velocities. Moreover, the models' relatively poor 230 representations of how overburden stresses are distributed in sands may lead scientists to 231 erroneously associate grain microstructure-induced seismic velocity changes to changes in 232 porosity, water saturation, and/or pore space cement. Along with modifying the models to account for force-chain distribution better, we recommend that future studies use direct 233 234 measurements to ground-truth and identify which models best predict seismic velocities at 235 multiple locations within each new critical zone environment. Future studies should also explore

the wide range of potential uncertainties discussed within this and other studies (e.g., Maske,
1999; Bachrach & Avseth, 2008).

238 6 Conclusions

239 Given the increasing use of rock physics models to explain changes to seismic velocities 240 within the critical zone, it is prudent that the community explores the effectiveness of rock 241 physics models, understand their limitations, and improve them where necessary. On this 242 backdrop, this paper discusses if, how, and under what conditions should critical zone scientists 243 use rock physics models to characterize the physical properties of sands, fluids, and cement 244 within the vadose zone and possibly down to at least 17 m. In their current form, each model 245 overpredicts seismic velocities for vadose sands younger than forty-three years. Their accuracies 246 improve for vadose sands older than ninety-four years, which we interpret to be the result of 247 microscale grain re-organizations that lead to a more uniform distribution of grain-contact forces 248 with time Jenkins, followed by Walton, Hertz-Mindlin, and soft sand results in the lowest 249 mispredictions. When combined with other studies, our results suggest that these rock physics 250 models will most substantially improve when they are modified to account for changes to the 251 existence, locations, and strengths of grain-grain force chain links as a function of age and 252 effective pressure. Until then, care should be taken when using rock physics models to study 253 critical zone sands - i.e., all uncertainties should be explored, and the models should be ground-254 truth in each new study area.

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FIGURE CAPTIONS

347	Figure 1. (A) Map [adapted from Wright & Hornbach (submitted, JGR: Solid Earth)] shows
348	Kington Jamaica. The red box highlights Port Royal, a town on the eastern terminus of a
349	complex sand spit. (B-C) Aerial images [also adapted from Wright & Hornbach (submitted,
350	JGR: Solid Earth)] show Port Royal Beach, the locations of beach's past shoreline positions, and
351	sites of refraction surveys and sediment sampling. The sands' ages [i.e., 1988-2016, 1956-1974,
352	1909-1923, and 1837-1862 at sites 1-4, respectively] derive from legacy maps of Port Royal
353	(Wright & Hornbach, submitted, JGR: Solid Earth).
354	
355	Figure 2. (A-J) Graphs [adapted from Wright & Hornbach (submitted, JGR: Solid Earth)] show
356	sediment physical properties results, which we use as inputs into the rock physics models. These
357	sediment physical properties derive from sidewall sediment coring analyses (Wright &
358	Hornbach, submitted, JGR: Solid Earth).
359	
360	Figure 3. Comparisons between measured and modeled seismic velocities for all four sites. Note
361	that the Jenkins produces imaginary solutions if coordination numbers are between 1-2 at Port
362	Royal Beach. The measured compressional wave velocities derive from the first-break geometric
363	and tau-p methods for estimating seismic velocities from refraction survey shot gathers; first-
364	break were picked by nine geophysicists (including the first author) and randomized (as a
365	function of geophone position) to create 100 different travel time curves used to create the
366	seismic velocity-depth profiles (Wright & Hornbach, submitted, JGR: Solid Earth). The shear
367	wave velocities derive from multichannel analyses of surface wave (MASW), with the selected

368 models being the 100 that have the lowest Akaike Information Criterion scores (Wright &

369 Hornbach, submitted, JGR: Solid Earth).

Figure 4. Comparisons between measured and modeled shear wave seismic velocities for all
four sites and models. Note that for model scenarios one and three, the contact-cement model
predicts that the *Vs* and *Vp* greater than 850 m/s for all depths. The caption for figure 3 explains
the methods used to calculate measured seismic velocities.















Figure 4.



APPENDIX

This appendix lists the equations for the dry-frame elastic moduli for each rock physics model. We refer the interested readers to the original papers for derivations of each equation and Mavko (2020) for briefer descriptions of the models' equations.

Nomenclature

K _{dry}	– dry-frame bulk modulus
μ_{eff}	– shear modulus (note: $\mu_{dry} = \mu_{eff}$ under hydrostatic pressure conditions)
ϕ	– measured porosity
P _{eff}	– effective hydrostatic pressure
K _m	– bulk modulus
μ_m	– shear modulus
η_m	– mineral Poison's ratio
С	– coordination number
f	– volume from of rough versus smooth grains (note: $f = 1$ for 100 % rough grains)
R	– average grain radius
K _{hm}	- dry-frame bulk modulus from Hertz-Mindlin
μ_{hm}	- dry-frame shear modulus result from Hertz-Mindlin
ξ	– cement fraction
ϕ_c	– critical porosity
K _c	– bulk moduli of the cement
μ_c	- shear moduli of the cement
η_c	- Poisson's ratio of the measured cement

Hertz-Mindlin

$$K_{dry} = \left[\frac{(1-\phi)^2 c^2 \mu_m^2 P_{eff}}{18\pi^2 (1-\eta_m)^2)}\right]^{\frac{1}{3}}$$

$$\mu_{eff} = \frac{2 + 3f - \eta_m (1 + 3f)}{5(2 - \eta_m)} \left[\frac{3(1 - \emptyset)^2 c^2 \mu_m^2 P_{eff}}{2\pi^2 (1 - \eta_m)^2} \right]$$

Walton

100 % rough-grained model

$$K_{dry} = \frac{1}{6} \left[\frac{3(1-\phi)^2 c^2 P_{eff}}{\pi^4 B^2} \right]^{\frac{1}{3}}$$

$$\mu_{eff} = \frac{3}{5} K_{eff} \frac{5B+A}{2B+A}$$

100 % smooth-grained model

$$K_{dry} = \frac{1}{10} \left[\frac{3(1-\phi)^2 c^2 P_{eff}}{\pi^4 B^2} \right]^{\frac{1}{3}}$$

$$\mu_{eff} = \frac{3}{5} K_{eff}$$

$$A = \frac{1}{4\pi} \left(\frac{1}{\mu_m} - \frac{1}{\mu_m + \lambda} \right)$$

$$B = \frac{1}{4\pi} \left(\frac{1}{\mu_m} + \frac{1}{\mu_m + \lambda} \right)$$

$$\lambda = k_m$$
$$-\frac{2}{3}\mu_m$$

Jenkins

$$\mu_{eff} = \left[\left(\frac{K_n c (1 - \phi)}{5\pi R^2} \right) \left(1 - 2(w_1 + 2w_2) \right) \left(\frac{c}{3} \right)^{-1} \right] - \left[(K_1 + 2K_2) \left(\frac{c}{3} \right)^{-2} \right] \\ + \left[(e_1 + 2e_2) \left(\frac{c}{3} \right)^{-3} \left(\frac{2 - \eta_m + 3f(1 - \eta_m)}{2 - \eta_m} \right) \right]$$

$$K_{dry} = \frac{2}{3}\mu_{eff} + \left[\left(\frac{K_n c(1-\phi)}{5\pi R^2} \right) (1-2\left(\frac{c}{3}\right)^{-1})(w_1+7w_2) \right] \\ + \left[2(K_1+2K_2+5K_3)\left(\frac{c}{3}\right)^{-2} \right] \\ - \left[(e_1+2e_2+5e_3)2\left(\frac{c}{3}\right)^{-3}\left(\frac{2-\eta_m-2f(1-\eta_m)}{2-\eta_m}\right) \right]$$

$$K_n = \left[\frac{\frac{3\mu_m \pi P_{eff}(1-\phi)}{1-\eta_m}}{2c\mu_m(1-\phi)}\right]^{\frac{1}{3}}$$

$$e_1 = n_1 w_1 + n_2 w_1 + 2n_2 w_2$$

$$e_2 = n_1 w_2$$

$$e_3 = n_2 w_2 + n_1 w_2$$

$$w_1 = \frac{166 - 11c}{128}$$

$$w_2 = -\frac{c+14}{128}$$

$$n_1 = b_1 - \alpha_1^2$$

$$n_2 = b_2 - (2\alpha_1\alpha_{2\prime} + \alpha_{2\prime}^2)$$

$$\alpha_1 = \frac{19c - 22}{48}$$

$$\alpha_{2\prime} = \frac{18 - 9c}{4}$$

$$b_1 = \psi_1 + \alpha_1$$

$$b_2 = \psi_2 + \alpha_2,$$

$$\psi_1 = \frac{1.96(c-2)(c-4) + 3.30c(c-2) + 0.49c(c-4) + 0.32c^2}{16\pi}$$

$$\psi_2 = -\frac{2.16 (c-2)(c-4) + 2.30c(c-2) + 0.54c(c-4) - 0.06c^2}{16\pi}$$

$$K_1 = a_1 - a_1 w_{1'} + w_{1'} \alpha_{2'} + 2 w_2 a \alpha_{2'}$$

$$K_2 = a_2 - w_2 \alpha_1$$

$$K_3 = a_3 - w_2 \alpha_{2'} + w_2 \alpha_1$$

$$w_{1\prime} = \frac{38 - 11c}{128}$$

$$a_1 = w_1, + g_1$$

$$a_2 = w_2 + g_2$$

$$a_3 = w_2 + g_3$$

$$g_1 = -\frac{0.52(c-2)(c-4) + 0.10c(c-2) - 0.13c(c-4) - 0.01c^2}{16\pi}$$

$$g_2 = \frac{0.44(c-2)(c-4) - 0.24c(c-2) - 0.11c(c-4) - 0.14c^2}{16\pi}$$

$$g_3 = -\frac{0.44(c-2)(c-4) - 0.42c(c-2) - 0.11c(c-4) + 0.04c^2}{16\pi}$$

Digby

$$K_{dry} = c(1-\phi) \frac{4\mu_m \left(\sqrt{d^2 + \left[\frac{a}{R}\right]^2}\right)}{\frac{1-\eta_m}{12\pi}}$$

$$\mu_{eff} = c(1-\phi) \frac{\frac{4\mu_m \sqrt{d^2 + \left[\frac{a}{R}\right]^2}}{1-\eta_m} + \frac{\frac{12\mu_m a}{R}}{2-\eta_m}}{20\pi}$$



$$a = \left[\frac{\frac{12\pi R^{3} P_{eff}}{2c(1-\phi)}}{\frac{4}{\frac{1-\eta_{m}^{2}}{K_{m}} + \frac{1-\eta_{m}^{2}}{\mu_{m}}}}\right]^{\frac{1}{3}}$$

$$d^{3} + \frac{3}{2} \left(\frac{a}{R}\right)^{2} d - \frac{3\pi (1 - \eta_{m}) P_{eff}}{2c(1 - \phi)\mu_{m}} = 0$$

Soft Sand

$$K_{dry} = -\frac{4}{3}\mu_{hm} + \left[\frac{\frac{\phi}{\phi_c}}{K_{hm} + 4\frac{4}{3}\mu_{hm}} + \frac{1 - \frac{\phi}{\phi_c}}{K_m + \frac{4}{3}\mu_{hm}}\right]^{-1}$$

$$\mu_{eff} = -A + \left[\frac{\frac{\phi}{\phi_c}}{\mu_{hm} + A} + \frac{1 - \frac{\phi}{\phi_c}}{\mu_m + A}\right]^{-1}$$

$$\phi_c = 1 - \left[(1 - \phi) - (1 - \phi) \frac{\xi}{100} \right]$$

$$A = \frac{\mu_{hm}}{6} \left[\frac{9K_{hm} + 8\,\mu_{hm}}{K_{hm} + 2\mu_{hm}} \right]$$

Stiff Sand Model

$$K_{dry} = -\frac{4}{3}\mu_m + \left[\frac{\frac{\phi}{\phi_c}}{K_{hm} + \frac{4}{3}\mu_m} + \frac{1 - \frac{\phi}{\phi_c}}{K_m + \frac{4}{3}\mu_m}\right]^{-1}$$

$$\mu_{eff} = -A + \left[\frac{\frac{\phi}{\phi_c}}{\mu_{hm} + A} + \frac{1 - \frac{\phi}{\phi_c}}{\mu_m + A}\right]^{-1}$$

$$\phi_c = 1 - \left[(1 - \phi) - (1 - \phi) \frac{\xi}{100} \right]$$

$$A = \frac{\mu_m}{6} \left[\frac{9K_m + 8\,\mu_m}{K_m + 2\mu_m} \right]$$

Contact Cement

Cement at grain contacts only

$$K_{dry} = \left(K_c + \frac{4\mu_c}{3}\right) \left(\frac{c(1 - \emptyset_c)}{6}\right) \left(-a_c^2 0.024153\lambda_a^{-1.3646} + a_c 0.20405\lambda_a^{-0.89008} + 0.00024649\lambda_a^{-1.9864}\right)$$

$$\mu_{eff} = K_{eff} + \frac{4}{3} \left[\frac{2}{3} K_{eff} + \left(\frac{3\mu_c c(1 - \emptyset_c)}{20} \right) \left(a_c^2 a_{1t} \lambda_\tau^{a_{2t}} + a_c b_{1t} \lambda_\tau^{b_{2t}} + C_{1t} \lambda_\tau^{C_{2t}} \right) \right]$$

Cement surrounds grains

$$K_{dry} = \left(K_c + \frac{4\mu_c}{3}\right) \left(\frac{c(1 - \phi_c)}{6}\right) \left(-a_s^2 0.024153\lambda_a^{-1.3646} + a_s 0.20405\lambda_a^{-0.89008} + 0.00024649\lambda_a^{-1.9864}\right)$$

$$\mu_{eff} = K_{eff} + \frac{4}{3} \left[\frac{2}{3} K_{eff} + \left(\frac{3\mu_c c(1 - \emptyset_c)}{20} \right) \left(a_s^2 a_{1t} \lambda_\tau^{a_{2t}} + a_s b_{1t} \lambda_\tau^{b_{2t}} + C_{1t} \lambda_\tau^{C_{2t}} \right) \right]$$

$$\phi_c = 1 - \left[(1 - \phi) - (1 - \phi) \frac{\xi}{100} \right]$$

$$a_c = 2 \sqrt{\frac{(\phi_c - Phi0)^{\frac{1}{4}}}{3c(1 - \phi_c)}}$$

$$a_s = \sqrt{\frac{2(\phi_c - Phi0)}{3(1 - \phi_c)}}$$

$$\lambda_a = \frac{2\mu_c(1-\eta_m)(1-\eta_c)}{\pi\mu_m(1-2\eta_c)}$$

$$\lambda_{\tau} = \frac{\mu_c}{\pi \mu_m}$$

$$a_{1t} = -0.01(2.2606\eta_m^2 + 2.0696\eta_m + 2.2952)$$

$$a_{2t} = 0.079011\eta_m^2 + 0.17539\eta_m - 1.3418$$

$$b_{1t} = 0.05728\eta_m^2 + 0.09367\eta_m + 0.20162$$

$$b_{2t} = 0.027425\eta_m^2 + 0.052859\eta_m - 0.87653$$

$$C_{1t} = 0.0001(9.6544\eta_m^2 + 4.9445\eta_m + 3.1008)$$

$$C_{2t} = 0.018667\eta_m^2 + 0.4011\eta_m - 1.8186$$