

1 **Statistical rock physics inversion for assessing source rock properties from**
2 **seismic signatures: an application to the Canning Basin, Australia**

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9
10 ***Abstract***

11
12 Quantifying source rock properties is essential for subsurface characterization but remains a high-
13 dimensional and nonlinear inverse problem. A statistical rock physics inversion workflow is
14 implemented to efficiently estimate source rock properties from seismic and well-log data and
15 quantify associated uncertainty. A thermal-maturation-dependent rock physics model is calibrated
16 through Monte Carlo simulation to link source rock parameters with elastic properties. Weighted
17 Approximate Bayesian Computation (ABC) integrates prior petrophysical knowledge, model
18 calibration errors, and measured elastic data to estimate posterior distributions of source rock
19 properties. The workflow is first validated through well-log inversion, showing posterior updates
20 in source rock properties. Then the workflow is applied to seismic inversion after outlier detection
21 using a robust Mahalanobis distance method, generating spatially coherent 2D distributions of rock
22 properties in the Goldwyer III of the Canning Basin, consistent with well-log observations.

23 Sensitivity analysis identifies porosity, kerogen, and illite as the most influential parameters. The
24 workflow provides a robust, uncertainty-aware framework for source-rock property estimation.

25

26 **Keywords:** Statistical inversion; Uncertainty quantification; Rock physics modeling; Source
27 rock properties

28

29 **1. Introduction**

30 Understanding petrophysical properties such as porosity, total organic carbon (TOC), mineral
31 composition, and fluid saturation is fundamental to the exploration and production of hydrocarbons.

32 These properties play a crucial role in reservoir characterization, basin modeling, and production
33 forecasting in petroleum industry (Clarkson, 2013; Mukerji et al., 2001; Peters et al., 2017). Rock
34 physics provides a link between geological reservoir parameters (e.g., porosity, clay content,
35 sorting, lithology, saturation) and seismic properties (e.g., acoustic impedance, P-wave/S-wave
36 velocity ratio V_p/V_s , bulk density, and elastic moduli) (Avseth et al., 2010). Various rock physics
37 models, such as the Gassmann fluid substitution model (Gassmann, 1951), Hertz-Mindlin contact
38 theory (Hertz, 1882; Mindlin, 1949), inclusion models using self-consistent approximation and
39 differential effective medium (DEM) theory (Berryman, 1995), have been developed and widely
40 applied to different geological scenarios, each offering specific strengths depending on the
41 complexity of the reservoir condition and data availability.

42 For non-linear rock physics models, it is difficult to obtain the analytical formulation to estimate
43 petrophysical properties from elastic properties. Moreover, the rock physics models are often non-
44 unique mappings from petrophysical properties to elastic properties, i.e., different combinations

45 of petrophysical properties might give rise to very similar elastic properties. To address this
46 problem, various rock physics inversion methods have been widely employed. These methods
47 range from deterministic techniques that optimize an objective function to stochastic frameworks
48 that incorporate uncertainty in both data and models. Estimating subsurface properties from
49 geophysical measurements is inherently uncertain due to data errors and model approximations
50 (Bosch et al., 2010). Therefore, stochastic approaches are more practical for quantifying
51 uncertainty for risk analysis and optimal decision-making (Grana et al.,2022). Recently,
52 likelihood-free Bayesian methods have gained attention for highly non-linear inverse problems,
53 where the likelihood function is difficult or impossible to formulate. These approaches provide
54 flexible alternatives for uncertainty quantification without requiring explicit likelihood definitions
55 (Pradhan & Mukerji, 2020; Pacchiardi et al., 2021; Zeng et al., 2025).

56 Among likelihood-free methods, Approximate Bayesian Computation (ABC) provides an efficient
57 and flexible framework for probabilistic inversion when the likelihood is intractable (Rubin, 1984).
58 In geophysics, and specifically in rock physics inversion, complex forward models and uncertain
59 data distributions often make traditional Bayesian inference intractable. ABC circumvents the need
60 for explicit likelihood evaluation by relying on simulations and summary statistics to approximate
61 posterior distributions, making it particularly suitable for high-dimensional and nonlinear
62 problems. This approach is adopted in subsurface characterization in this study, where it enables
63 probabilistic assessment of rock properties while accounting for observational noise and modeling
64 uncertainties.

65 In this study, we propose a novel rock physics inversion workflow based on weighted ABC to
66 estimate petrophysical properties from elastic properties. The workflow begins with constructing

67 a rock physics model tailored to the geological setting of the study area, followed by Monte Carlo
68 sampling of mineral properties to calibrate the model using well-log data. To enhance inversion
69 reliability, model calibration errors and data correlations are incorporated as weights into the ABC
70 acceptance criteria. The weighted ABC framework is then employed to infer the posterior
71 distribution of petrophysical properties by comparing simulated and observed elastic properties.
72 We first do a sensitivity analysis of the rock physics model and test the workflow with a synthetic
73 dataset. Then, we apply the proposed workflow to an unconventional shale formation in the
74 Canning Basin, Australia, using well-log and seismically derived elastic properties. The results
75 demonstrate the efficacy of weighted ABC in improving subsurface characterization and
76 uncertainty quantification. The methods are described in the following section 2. This is followed
77 by a Monte Carlo sensitivity analysis (section 3) and test with synthetic data (section 4). Section 5
78 finally presents the field application, followed by discussion and conclusions in section 6.

79

80 **2. Methods**

81

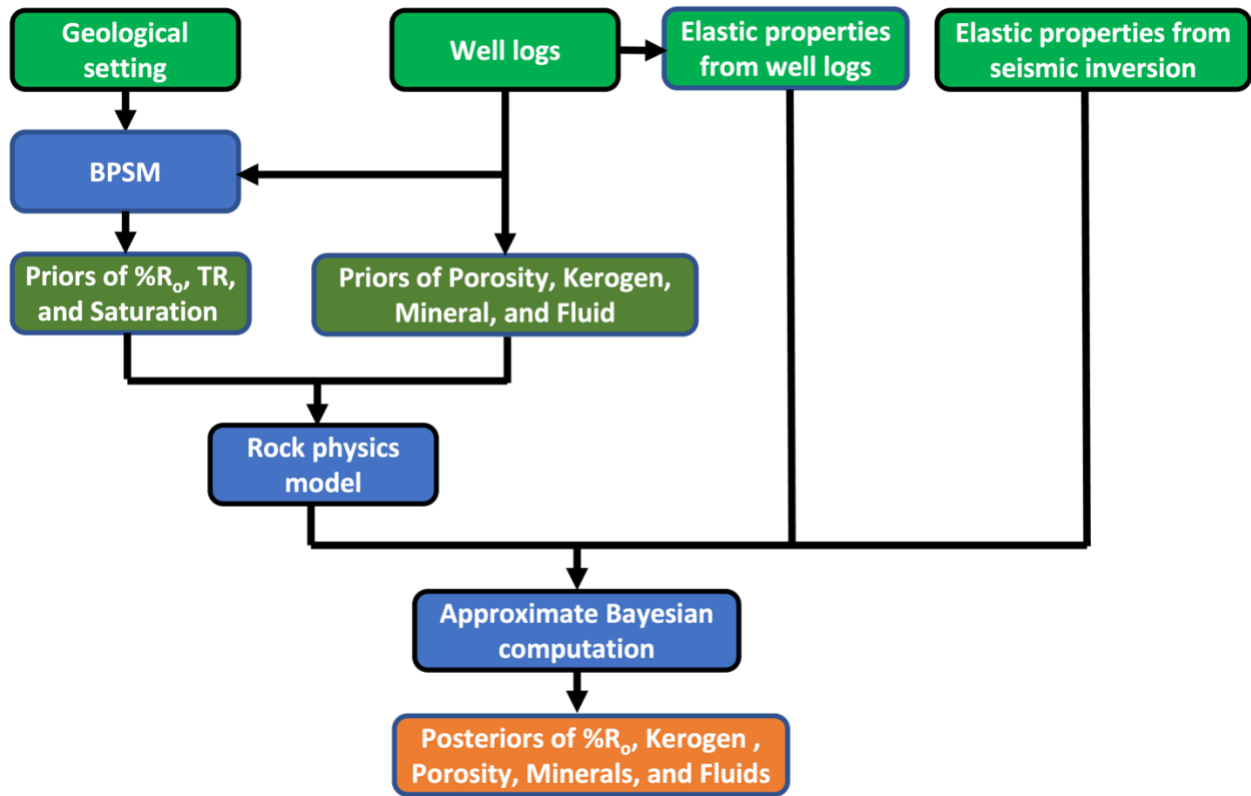
82 **2.1 Proposed workflow**

83

84 The goal of the proposed workflow is to quantify uncertainty of source rock properties, such as
85 vitrinite reflectance, porosity, and kerogen content in unconventional shale reservoir from elastic
86 properties, such as P- and S-wave velocities and impedances. In our workflow (Figure 1), Basin
87 and Petroleum System Modeling (BPSM) is applied to simulate vitrinite reflectance,
88 transformation ratio, and fluid saturation conditioned on basin geohistory and stratigraphy. The
89 simulated vitrinite reflectance, transformation ratio, and fluid saturation can be used as priors for

90 rock physics model inputs used for the inversion. Well logs are utilized to construct and calibrate
 91 the rock physics model and estimate prior distributions of kerogen, porosity, mineral, and fluid
 92 compositions. Finally, ABC is applied to invert the rock physics model using elastic properties
 93 obtained from either well logs or seismic inversions to estimate posterior distributions of vitrinite
 94 reflectance, kerogen, porosity, mineral, and fluid compositions.

95



96

97 Figure 1. Proposed workflow for rock physics model inversion. BPSM, % R_o , and TR refer to
 98 Basin and Petroleum System Modeling, vitrinite reflectance, and transformation ratio, respectively.

99

100 **2.2 Thermal-maturation dependent rock physics model for organic-rich mudrocks**

101

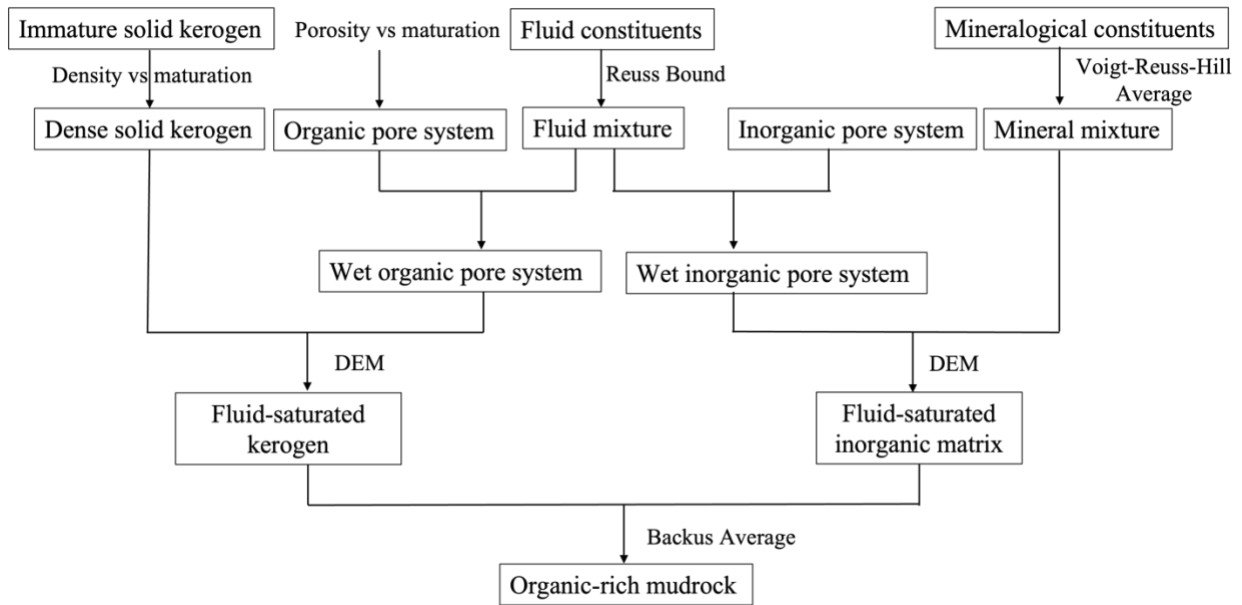
102 In this study, a thermal-maturation dependent rock physics model is applied to model
103 unconventional shale source rock (Figure 2) (Al Ibrahim et al., 2020). The rock physics model
104 separately considers the contributions from kerogen and inorganic matrix. For inorganic rock
105 component, elastic moduli of mineral mixture are modeled using Voigt-Reuss-Hill average, and
106 fluid mixture are modeled using Reuss lower bound, with a simplifying assumption that all fluids
107 coexist within the pore system and can be represented as a single effective phase. For organic rock
108 component, Vitrinite reflectance ($\%R_o$) is widely used as an indicator of kerogen thermal maturity
109 (Sweeney & Burnham, 1990). The organic porosity of kerogen is modeled as a function of vitrinite
110 reflectance and kerogen types, considering creation of organic pores and conversion of kerogen to
111 hydrocarbon fluids. The Easy $\%R_o$ (Sweeney & Burnham, 1990) is used to establish the
112 relationship between transformation ratio (TR) and vitrinite reflectance and a linear empirical
113 model is employed to model the evolution of pores in kerogen as a function of the TR (Galford et
114 al., 2013). Kerogen density is modeled using a non-linear empirical model based on vitrinite
115 reflectance and kerogen types (Alfred and Vernik, 2012).

116

117 Pore systems containing fluid mixtures are inserted into the kerogen and inorganic matrix using
118 the Differential Effective Medium (DEM) theory (Berryman, 1995). Although other effective
119 medium models (e.g., self-consistent approximations) can also be used when properly calibrated,
120 DEM provides a more realistic representation of sequential pore addition in source rocks. Finally,
121 the overall effective elastic properties are obtained by combining the porous kerogen and inorganic
122 matrices using the Backus average (Backus, 1962). This averaging process upscales the fine-scale
123 lamination of organic and inorganic layers into an equivalent long-wavelength elastic medium,
124 ensuring consistency between the modeled properties and the seismic and log measurement scales.

125 Although the Backus averaging process inherently produces a vertically transverse isotropic (VTI)
 126 medium due to fine-scale layering, only the equivalent isotropic moduli were used in this study to
 127 maintain consistency with the isotropic well-log and seismic data. The inputs for the models are:
 128 1) kerogen content, 2) porosity, 3) mineralogical constituents, 4) fluid saturations (bound water,
 129 free water, and oil in this study), 5) matrix aspect ratio, 6) vitrinite reflectance, and 7) kerogen type.
 130 The outputs from the model are 1) Bulk-modulus, 2) Shear-modulus, and 3) density from which
 131 we can calculate the P-wave velocity $V_P = \sqrt{\frac{K+4/3\mu}{\rho}}$ and S-wave velocity $V_S = \sqrt{\frac{\mu}{\rho}}$, where K , μ ,
 132 and ρ are bulk and shear moduli, and bulk density of the rock.

133



134

135 Figure 2. Workflow for constructing thermal-maturation dependent rock physics model for
 136 organic-rich mudrocks (modified from Al Ibrahim et al., 2020).

137

138 2.3 Approximate Bayesian Computation

139

140 ABC has been successfully applied in various scientific disciplines, including ecology (Beaumont,
 141 2010), epidemiology (Minter and Retkute, 2019), and genetics (Beaumont et al., 2002), but its
 142 application to rock physics inversion remains relatively unexplored.

143

144 The rock physics model inversion can be understood in a Bayesian framework (Eq. 1).

145

$$146 \quad p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \quad (1)$$

147

148 where $p(\theta|D)$ is the posterior distribution of source rock properties, $p(D|\theta)$ is the likelihood,
 149 $p(\theta)$ is the prior distribution of source rock properties, and $p(D)$ is the evidence or marginal
 150 likelihood derived from the observed data D (elastic properties obtained from well logs or seismic
 151 signatures). θ represents the vector of source rock properties (e.g., porosity, kerogen content,
 152 mineral composition, and vitrinite reflectance).

153 The likelihood function is of curial importance for all model-based statistical inference but might
 154 be computationally costly to evaluate for complex models (Sunnåker et al., 2013). ABC is a
 155 likelihood free inference method first proposed by Rubin (1984). ABC can approximate the
 156 likelihood function by Monte Carlo simulations of a large number of models and their associated
 157 synthetic data, and comparing them with the observed data. More precisely, parameter values θ
 158 are first sampled from the prior distributions. For each sampled parameter θ , a forward model M
 159 parameterized by θ is run to generate a dataset \hat{D} . The generated dataset \hat{D} is accepted if a
 160 statistical distance between the generated dataset \hat{D} and the observed dataset D is smaller than a
 161 predefined tolerance ε (Eq. 2).

$$162 \quad \rho(\hat{D}, D) \leq \varepsilon \quad (2)$$

163 where $\rho(\cdot)$ is a distance measurement between simulated \widehat{D} and observed D . If the data is high
164 dimensional, then using summary statistics can map high dimensional data to low dimensional
165 summaries of information which can improve computational efficiency (Eq. 3).

166

$$167 \quad \rho(S(\widehat{D}), S(D)) \leq \varepsilon \quad (3)$$

168 where $S(\cdot)$ is a summary statistics.

169

170 **2.4 Weighted Mahalanobis distance for ABC**

171

172 Weighting the distance between observed and simulated data in ABC is crucial for accurately
173 capturing differences within the dataset. For example, different features of the data may have
174 varying levels of importance, requiring tailored emphasis to reflect their impact accurately.
175 Additionally, features often vary on different scales, and without weighting, features with larger
176 scales could disproportionately influence the distance calculation. Furthermore, if a forward model
177 used in ABC for inversion performs well at predicting some output variables but poorly at others,
178 this can introduce bias or inconsistency in the inference process if we weight them equally in the
179 distance calculation. Therefore, we propose weighting the distances to account for differences in
180 feature scales, feature importance, correlations between features, and modeling errors, ensuring
181 more robust and reliable inference.

182

183 The concept of weighting involves combining the reciprocal of the mean squared error (MSE)
184 between the normalized measured and modeled elastic properties from the calibration well. The
185 reciprocal of the MSE highlights the significance of each elastic property. Consequently, variables

186 with lower MSEs have higher weights in the distance calculation, while those with higher MSEs
 187 are assigned lower weights. The Mahalanobis distance can accounts for correlations of variables
 188 within the dataset. The weighted Mahalanobis distance D is defined in Eq. 4. More specific steps
 189 to compute distances in this work are:

190

191 1. Normalize the elastic properties in prior, modeled, measured, and target datasets:

192

$$193 \quad y'_i = \frac{y_i - \mu_{prior}}{\sigma_{prior}}$$

194 Where y_i is the value of the variable (y are v_p , v_s , density ρ in this study and i is the index of
 195 value) from the prior, modeled, measured, and target datasets. y'_i is the normalized variable. μ_{prior}
 196 and σ_{prior} are the mean and the standard deviation of the variable across the prior dataset. The
 197 prior dataset is generated from the rock physics model using the prior petrophysical distributions.
 198 The modeled dataset is simulated by the rock physics model using the measured petrophysical
 199 properties from a calibration well. The measured dataset is actual elastic properties from the
 200 calibration well. The target dataset is the elastic properties from new well logs or seismic sections
 201 that we want to invert.

202

203 2. Calculate the covariance matrix S of the normalized prior dataset:

204

$$205 \quad S = \begin{bmatrix} 1 & Cov(v_{p'prior}, v_{s'prior}) & Cov(v_{p'prior}, \rho'_{prior}) \\ Cov(v_{s'prior}, v_{p'prior}) & 1 & Cov(v_{s'prior}, \rho'_{prior}) \\ Cov(\rho'_{prior}, v_{p'prior}) & Cov(\rho'_{prior}, v_{s'prior}) & 1 \end{bmatrix}$$

206

207 Where $Cov(a, b)$ represents the correlation coefficient between variables a and b .

208

209 3. Calculate the weight matrix:

210

$$211 \quad W = \begin{bmatrix} w_{v_p} & 0 & 0 \\ 0 & w_{v_s} & 0 \\ 0 & 0 & w_{\rho} \end{bmatrix}$$

212 Where $w = \frac{1}{MSE(y'_{modeled}, y'_{measured})}$, $y'_{modeled}$ is normalized modeled elastic properties using rock
213 physics model and petrophysical properties from the calibration well, $y'_{measured}$ is normalized
214 measured elastic properties from the calibration well, and $MSE(y'_{modeled}, y'_{measured})$ is the
215 mean-squared error between the normalized modeled and measured elastic properties.

216

217 4. Calculate the weighted Mahalanobis distance between all the elastic properties in the normalized
218 prior dataset and a single normalized target elastic property.

219

$$220 \quad D = \sqrt{(y'_{prior} - y'_{target})^T W S^{-1} W (y'_{prior} - y'_{target})} \quad (4)$$

221

222 Where $y' = \begin{bmatrix} v'_p \\ v'_s \\ \rho' \end{bmatrix}$, W is the weight matrix, and S is the covariance matrix.

223

224 5. Set a threshold to accept the weighted Mahalanobis distances. The threshold can be a tolerance
225 level or based on a specified number of accepted prior samples. In this work, we accept the nearest
226 N samples to the target elastic property.

227

228 6. Calculate the probability distributions of the petrophysical properties associated with the
229 accepted samples using kernel density estimation (KDE). These distributions represent the
230 posterior probabilities of the petrophysical properties.

231

232 7. Repeat steps 4 to 6 to obtain the posterior distributions of petrophysical properties along the
233 entire target well log or seismic section.

234

235 **3. Monte Carlo sensitivity analysis of the rock physics model**

236

237 **3.1 Monte Carlo simulation of trends with different ranges of inputs**

238

239 The constructed rock physics model is high-dimensional and non-linear. The inputs of the rock
240 physics model are listed in Table 1. Elastic properties of minerals like quartz, Calcite, Dolomite,
241 and Pyrite are relatively well known. However, elastic properties of clay minerals like illite and
242 chlorite have wide range of values in literature, the difference being related to different
243 experimental techniques as well as fine-grained nature and bound fluids of clay minerals (Mondol
244 et al., 2008). Elastic properties of kerogen are not well constrained (Vernik and Landis, 1996;
245 Mavko et al., 2020) Therefore, in this study, elastic properties of kerogen and clay minerals are
246 considered as uncertain rock physics model parameters. These properties are set in reasonable prior
247 ranges and later can be refined by rock physics model calibration using well logs.

248

249 To investigate the variations of output elastic properties, we randomly sample the input variables
 250 within different ranges. The mineral and fluid properties and the variable distributions used in
 251 Monte Carlo sampling are listed in Table 1 and Table 2, respectively. The Dirichlet distribution is
 252 used for volumetric quantities to ensure that they sum up to one. There are several observations in
 253 the cross plots for different types of kerogens (Figure 3): 1) Higher volumetric percentages of
 254 porosity and kerogen will lower P-wave impedance. 2) For all three types of kerogens, varying
 255 volumetric percentages of porosity and kerogen has limited impacts on V_P/V_S .

256

Component	K [GPa]	μ [GPa]	ρ [g/cc]	Reference
Kerogen	(2, 10)	(2, 5)	$f(\%R_0)$	(Vernik and Landis, 1996; Mavko et al., 2020; Al Ibrahim et al., 2020)
Quartz	37	44	2.65	(Carmichael, 2017)
Calcite	76.8	32	2.71	(Simmons, 1965)
Illite	(20, 60)	(5, 30)	(2.7, 2.9)	(Mondol et al., 2008; Wang et al., 2001)
Chlorite	(20, 60)	(5, 30)	(2.7, 3.0)	(Mondol et al., 2008; Wang et al., 2001)
Dolomite	94.9	45	2.87	(Humbert, 1972)
Pyrite	139	112.3	5.01	(Whitaker et al., 2010)
Bound water	2.2	0	1.0	(Mavko et al., 2020)
Free water	2.2	0	1.0	(Mavko et al., 2020)
Oil	1.02	0	0.8	(Batzie & Wang, 1992)

257

258 Table 1. Mineral properties used in rock physics modeling. Properties of kerogen, illite, and
 259 chlorite have uniform distributions. Deterministic values can be obtained by Monte Carlo rock

260 physics model calibration using well logs. Kerogen density is a function of vitrinite reflectance

261 % R_0 .

262

263

Input variable	Distribution	Range
Kerogen type	Categorical	(I, II, III)
Vitrinite reflectance	Uniform	(0.23, 1.6)
Kerogen	Uniform	(0, 0.2)
Porosity	Uniform	(0, 0.2)
Matrix aspect ratio	Uniform	(0.001, 0.2)
Quartz	Dirichlet	(0, 1)
Calcite	Dirichlet	(0, 1)
Illite	Dirichlet	(0, 1)
Chlorite	Dirichlet	(0, 1)
Dolomite	Dirichlet	(0, 1)
Pyrite	Dirichlet	(0, 1)
Bound water	Dirichlet	(0, 1)
Free water	Dirichlet	(0, 1)
Oil	Dirichlet	(0, 1)

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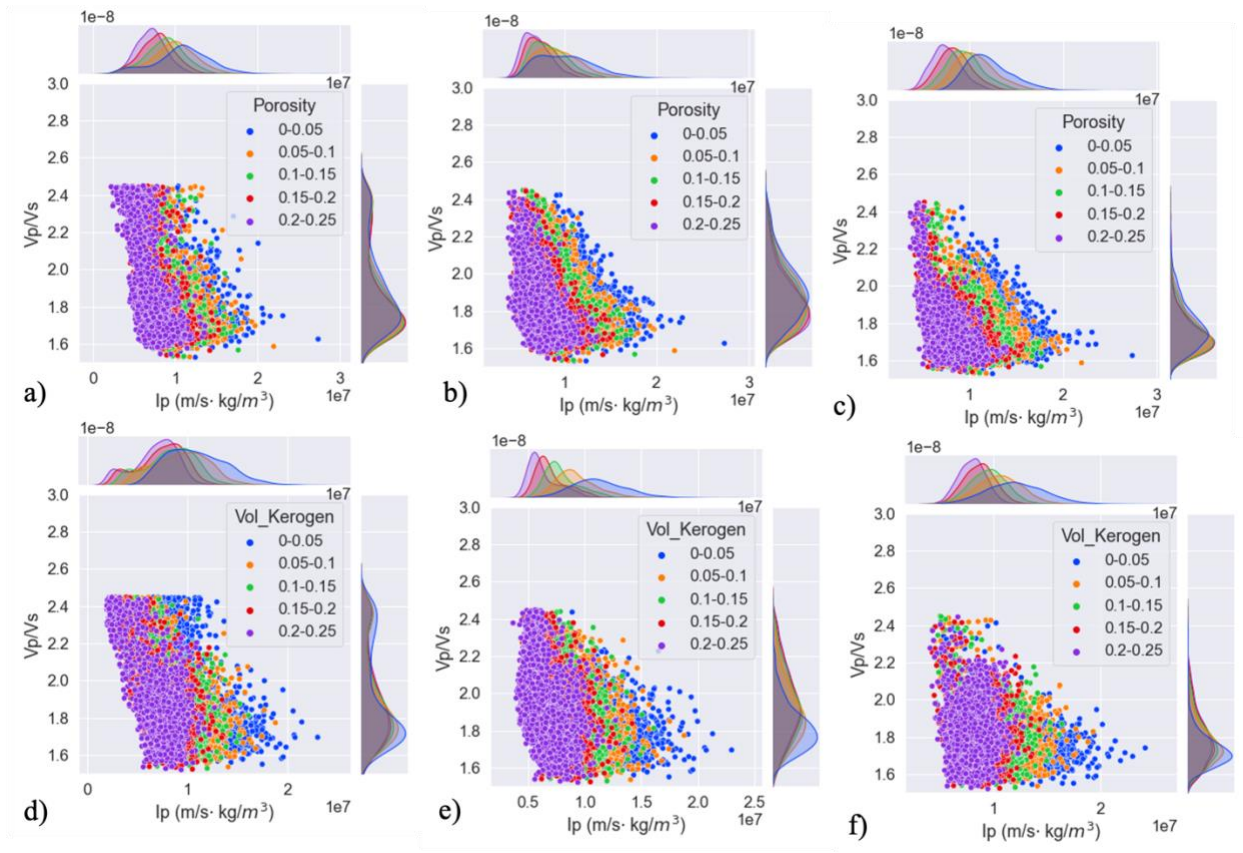
265 Table 2. Input variable distributions used in Monte Carlo sampling for elastic property trends

266 analysis and Monte Carlo sensitivity analysis. Kerogen, porosity, minerals, and fluids are

267 volumetric.

268

269



270

271

272 Figure 3. Crossplots of elastic properties (V_p/V_s and P-wave impedance) for Type I, Type II, and
273 Type III kerogen, showing different ranges of porosity and volumetric kerogen content. Each range
274 includes 2,000 realizations. (a), (b), and (c) illustrate the elastic properties trends by varying
275 porosity for Type I, Type II, and Type III kerogen, respectively. (d), (e), and (f) depict the elastic
276 properties trends by varying volumetric kerogen content for Type I, Type II, and Type III kerogen,
277 respectively.

278

279 3.2 Sensitivity analysis

280

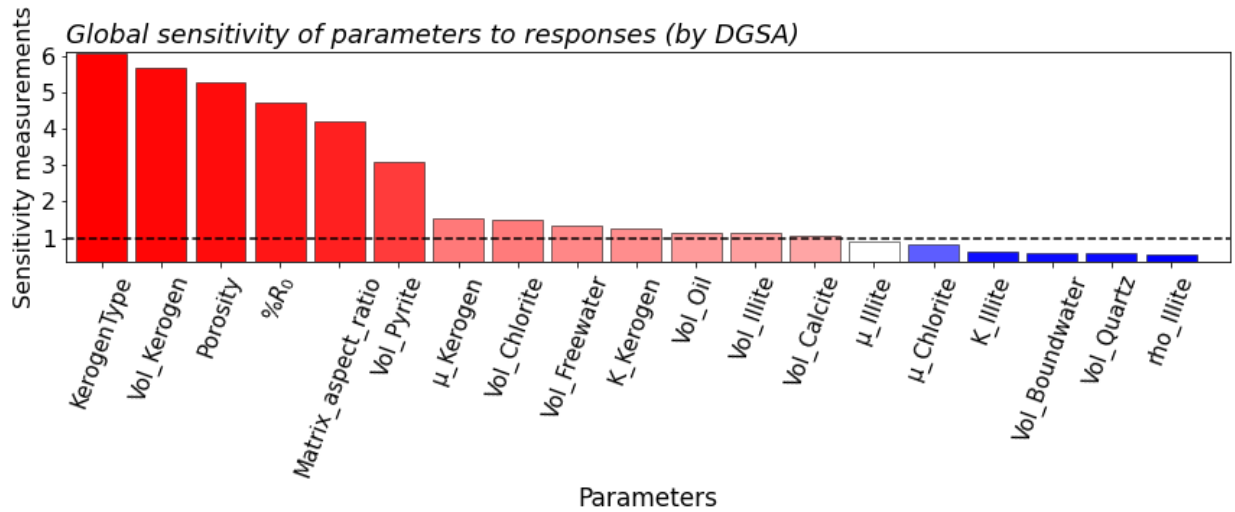
281 A global sensitivity analysis method, the Distance-based generalized sensitivity analysis (DGSA)
282 (Fenwick et al., 2014; Park et al., 2016) is applied to analyze the sensitivity of the output elastic
283 properties to the rock physics model input variables. Briefly the steps to implement DGSA are
284 (Fenwick et al., 2014): 1). Sample input variables from their prior distributions and run the forward
285 simulator (rock physics model) to get the response variables (elastic properties). 2). Classify and
286 group the response variables into predefined number of clusters using k-medoids clustering. 3).
287 Calculate the cumulative distribution function (CDF) of the input variables for each cluster and
288 the distance between the prior CDF of all the samples and conditional CDF of each cluster using
289 the L1 norm. 4). Test whether the distance is statistically significant using bootstrap resampling.
290 5). The CDF distance is standardized using the bootstrap results and is defined as a sensitivity
291 measure for each variable as explained in Eq.5 below. For more mathematical details of DGSA
292 please see Fenwick et al., 2014 and Park et al., 2016. The input variables include porosity, kerogen,
293 mineral fractions, fluid fractions, matrix aspect ratio, and vitrinite reflectance. The response
294 variables are I_p and I_s (P-wave and S-wave impedance). The variable distributions used in Monte
295 Carlo sampling are listed in Table 1 and Table 2. The sensitivity analysis result in Figure 4 shows
296 that the top 5 sensitive input variables are porosity, volume fraction of kerogen, kerogen type,
297 vitrinite reflectance, and matrix aspect ratio.

298

299 The DGSA sensitivity index $s(p_i)$ was calculated as the average normalized distance between
300 unconditional and class-conditional CDFs of each input parameter (Fenwick et al., 2014):

301
$$s(p_i) = \frac{1}{K} \sum_{k=1}^K \hat{d}_{k,i}^S \quad \text{with} \quad \hat{d}_{k,i}^S = \frac{\hat{d}_{k,i}}{\hat{d}_{k,i}^{(q)}} \quad (5)$$

302 Here, i denotes the parameter index, k represents the response cluster, and K is the total number
 303 of clusters in the model response space. $s(p_i)$ is a standardized sensitivity measure for parameter
 304 p_i on the response. $\hat{d}_{k,i}$ is the distance between the unconditional and cluster-conditional
 305 cumulative distributions of parameter p_i , and $\hat{d}_{k,i}^{(q)}$ is the corresponding quantile distance obtained
 306 from random sampling for normalization (e.g $q = 0.95$). Larger $s(p_i)$ values indicate stronger
 307 parameter influence on model responses



308
 309 Figure 4. Sensitivity analysis of the rock physics model output elastic properties (I_p and I_s) to the
 310 inputs using DGSA. The top 5 sensitive input variables are kerogen type, volume fraction of
 311 kerogen, porosity, vitrinite reflectance, and matrix aspect ratio.

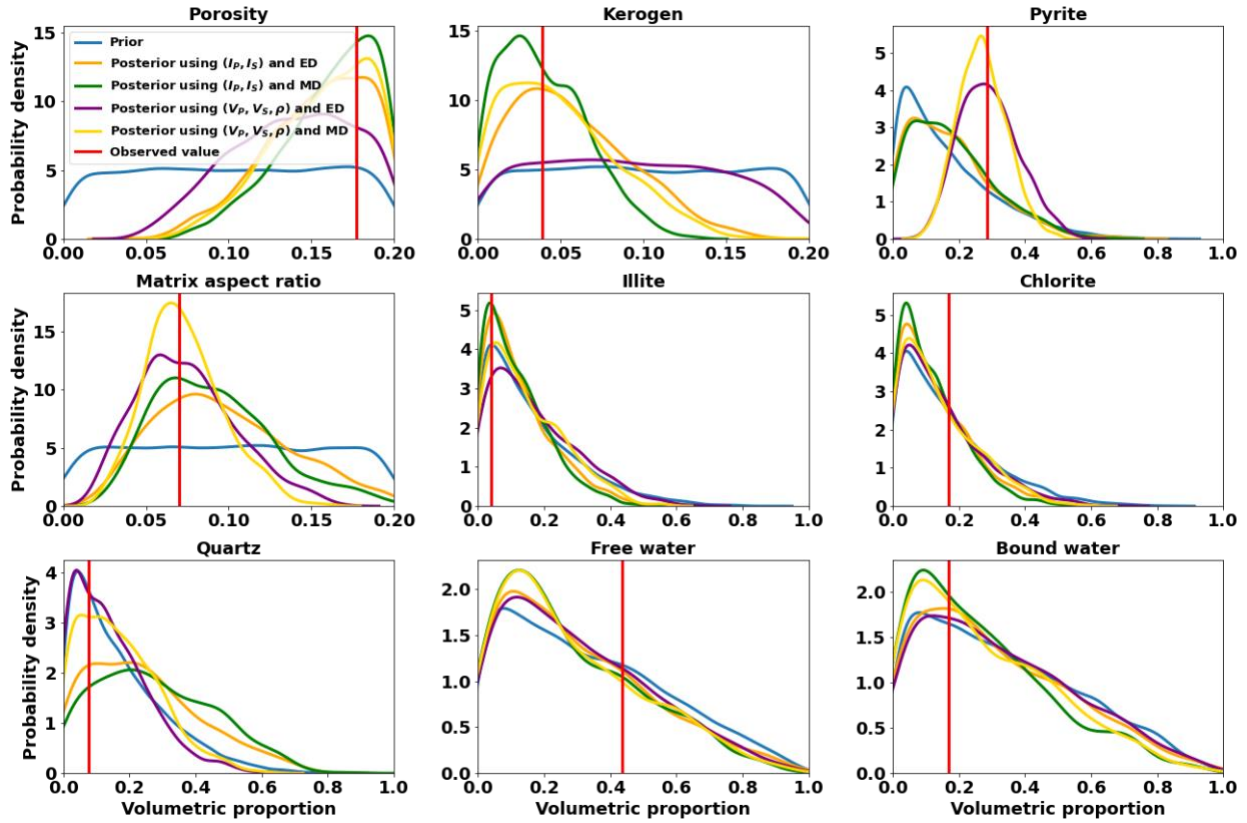
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313 4. Synthetic example of rock physics inversion using ABC

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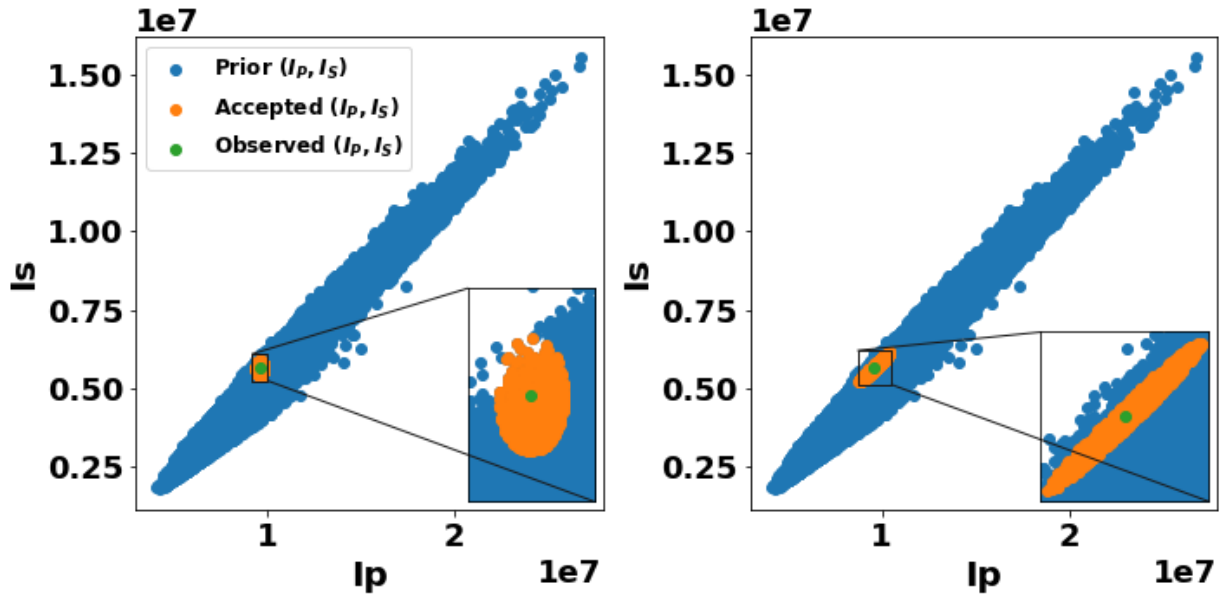
315 A synthetic case is experimented to test the feasibility of rock physics inversion workflow using
 316 ABC. Uncertain properties of kerogen, illite and chlorite are randomly sampled and fixed for the
 317 following Monte Carlo simulations. A set of input variables are randomly sampled from Table 2
 318 and the kerogen type is set as type III. This set of input variables represent the observed values in

319 Figure 5. Then sets of elastic properties (I_p, I_s) and (V_p, V_s, ρ) are calculated using the constructed
320 rock physics model. These sets of elastic properties (I_p, I_s) and (V_p, V_s, ρ) are used for inversion.
321 When applying ABC for inverting the elastic properties, we compare the results when inverting
322 elastic properties (I_p, I_s) versus inverting (V_p, V_s, ρ) . We also compare the results when using
323 Euclidean distance versus Mahalanobis distance as acceptance criteria. The ABC steps are as
324 follow: 1) Randomly generate a test set (100,000) of input variables from Table 2 and calculate
325 the corresponding sets of elastic properties (I_p, I_s) and (V_p, V_s, ρ) by the rock physics model. 2)
326 Calculate Euclidean distances and Mahalanobis distance between the sampled 100,000 sets of
327 elastic properties (I_p, I_s) and (V_p, V_s, ρ) and the set for inverting (i.e., corresponding to the
328 observed value). 3). Find the 1,000 samples that are nearest to the elastic properties that are being
329 used for the inversion. 4). Calculate Probability density functions (PDF) of the input variables of
330 the 1,000 nearest samples using kernel density estimation. The obtained PDFs are the posteriors
331 of input variables. An example of inverting observed elastic properties (I_p, I_s) and (V_p, V_s, ρ)
332 using ABC is shown in Figure 5. A comparison of prior (I_p, I_s) , accepted (I_p, I_s) , and observed
333 (I_p, I_s) when using Euclidean distance and Mahalanobis distance as acceptance criteria is in Figure
334 6. There are some observations in the inversion results: 1) For sensitive variables like porosity and
335 kerogen, there are more updates in their posteriors compared to insensitive variables like free water
336 and bound water. 2) Posteriors obtained by inverting (V_p, V_s, ρ) have less uncertainty than
337 inverting (I_p, I_s) . 3) In Figure 6, accepted (I_p, I_s) samples scatter around the observed (I_p, I_s)
338 when using Euclidean distance while accepted (I_p, I_s) samples using Mahalanobis distance have
339 strong correlation that is similar the prior correlation. 4) Overall, the posteriors obtained by
340 inverting (V_p, V_s, ρ) and incorporating the Mahalanobis distance yield the most accurate results.
341



343

344 Figure 5. An example of inversion results using ABC. The blue curves are prior, the orange curves
 345 are posteriors when inverting the observed (I_p, I_s) using Euclidean distance, the green curves are
 346 posteriors when inverting the observed (I_p, I_s) using Mahalanobis distance, the purple curves are
 347 posteriors when inverting the observed (V_p, V_s, ρ) using Euclidean distance, the yellow curves are
 348 posteriors when inverting the observed (V_p, V_s, ρ) using Mahalanobis distance, and the red
 349 vertical lines are the corresponding observed values. I_p is P-wave impedance, I_s is S-wave
 350 impedance, V_p is P-wave velocity, V_s is S-wave velocity, ρ is density. ED and MD refer to
 351 Euclidean distance and Mahalanobis distance, respectively.



352

353 Figure 6. Scatter plots of prior, accepted, and observed (I_p, I_S) using Euclidean distance and
 354 Mahalanobis distance. The blues dots are prior (I_p, I_S) , the orange dots are accepted (I_p, I_S) , and
 355 the green dots are the observed (I_p, I_S) for inverting.

356

357 5. Field example: Source rock potentials of Unconventional shale in the Canning Basin,

358 Australia

359

360 We apply the above workflow to a field data set from the Canning Basin, Australia. The Canning
 361 Basin is the largest sedimentary basin in Western Australia that has increasing unconventional
 362 resource potential (Alshakhs and Rezaee, 2019). The Goldwyer Formation of the Canning Basin
 363 has significant shale gas and oil potentials in the basin (U.S. Energy Information Administration,
 364 2015). The Goldwyer formation can be divided into three zones based on source rock lithofacies:
 365 upper shale (Goldwyer I), middle carbonates (Goldwyer II), and lower shale (Goldwyer III) (Foster

366 et al., 1986). The Goldwyer III has been proven to have unconventional hydrocarbon potential
367 (van Hattum et al., 2019). This field example focuses on the Goldwyer III unit.

368

369 **5.1 Introduction to the dataset**

370

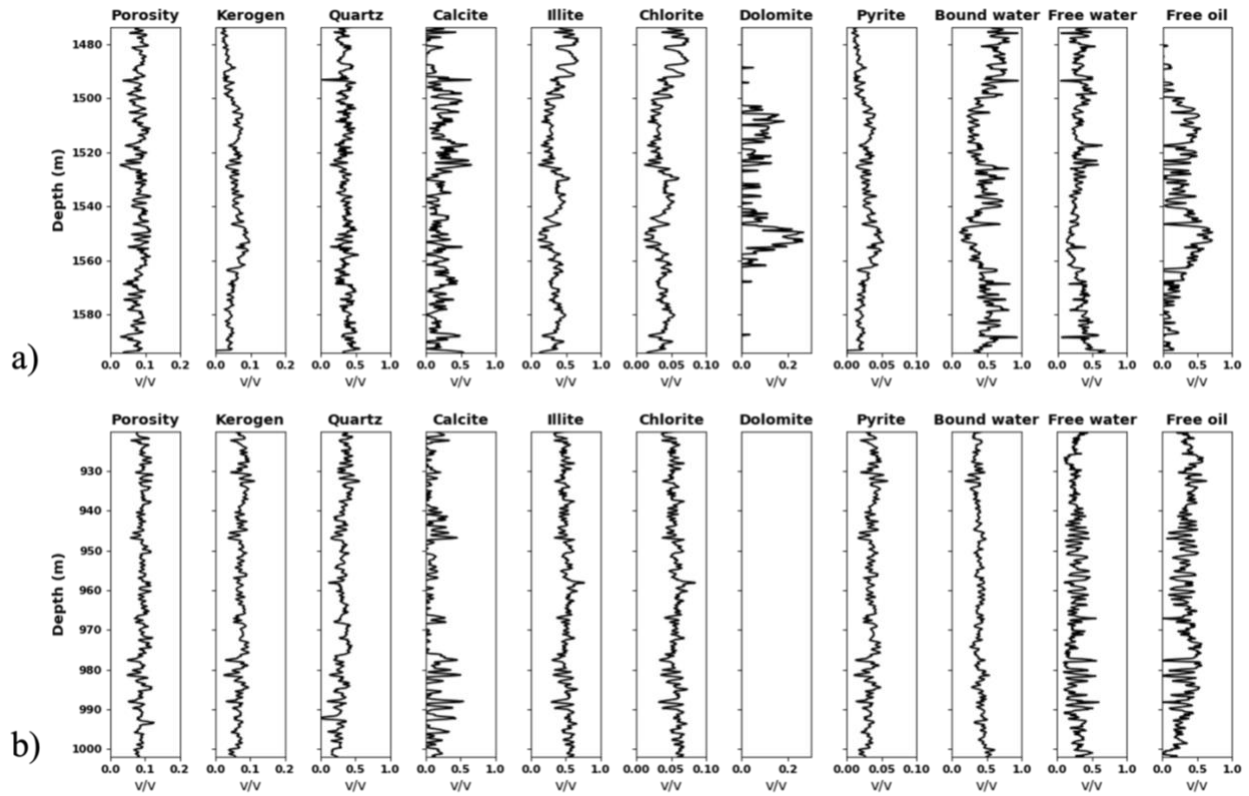
371 The study area includes two wells, Cyrene-1 and Theia-1, both of which penetrate the Goldwyer
372 formation (Figure 7). These wells provide geochemical, petrophysical, and sonic logs (Figure 8
373 and 9). Additionally, a 2D pre-stack seismic inversion section across the Theia-1 well is available,
374 containing P-wave impedance, density, and V_P/V_S which are then converted to V_P , V_S , and ρ for
375 rock physics inversion. A portion of the pre-stack seismic inversion section near the Theia-1 well
376 is used in the subsequent rock physics inversion (Figure 9). Vitrinite reflectance from a 3D basin
377 model is available in the study area and will be used to calibrate the rock physics model and
378 inversion (Finder Exploration, 2016) (Figure 10).

379

380

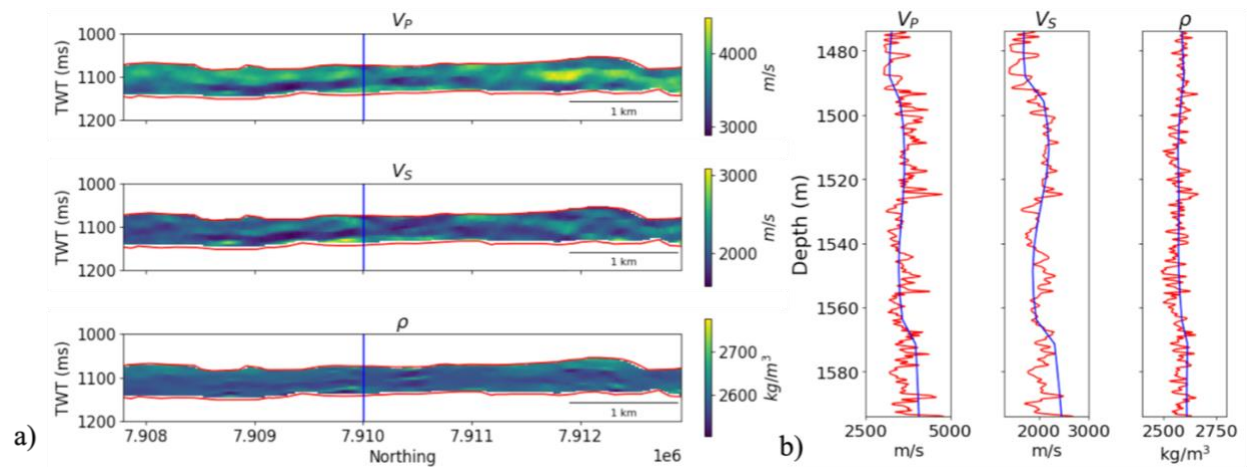


381 Figure 7. Locations of wells and seismic survey in the Canning Basin. Red dots indicate well
 382 locations, with an approximate spacing of 116 km, while the blue curve represents the seismic
 383 survey.
 384



385
 386 Figure 8. Well-log data, including porosity, kerogen, minerals, and fluids. The minerals form the
 387 matrix and are normalized to sum to 1. Fluid saturations, assumed to fill the pore system, are also
 388 normalized to sum to 1. The sum of porosity, kerogen, and matrix equals 1. (a) Theia-1 well. (b)
 389 Cyrene-1 well, where no dolomite is present.

390

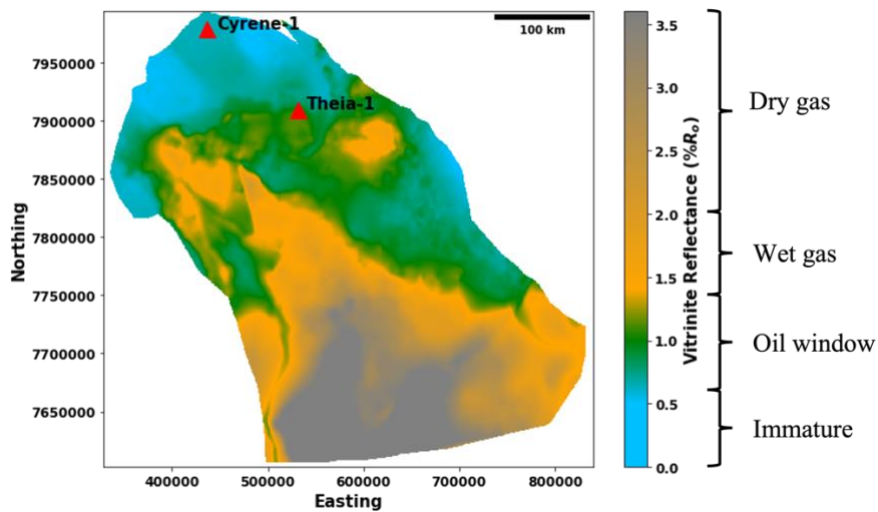


391

392 Figure 9. a) A portion of the pre-stack seismic inversion section near the Theia-1 well. The blue
 393 vertical line is the Theia-1 well, the red curves are the top and the bottom of the Goldwyer III unit.

394 b) Comparisons of V_p , V_s , ρ from well log and seismic inversion in the Goldwyer III unit in the
 395 Theia-1 well. The red curves are from well log, the blue curves are from seismic inversion.

396



397

398 Figure 10. Vitrinite Reflectance ($\%R_o$) modeling at 0 Ma in the Canning Basin and hydrocarbon
 399 generation windows (Finder Exploration, 2016; Egbobawaye, 2017). The red triangles indicate the
 400 well location. The $\%R_o$ of Cyrene-1 and Theia-1 are 0.63 and 1.04 separately.

401

402

403 **5.2 Monte Carlo rock physics model calibration by well logs**

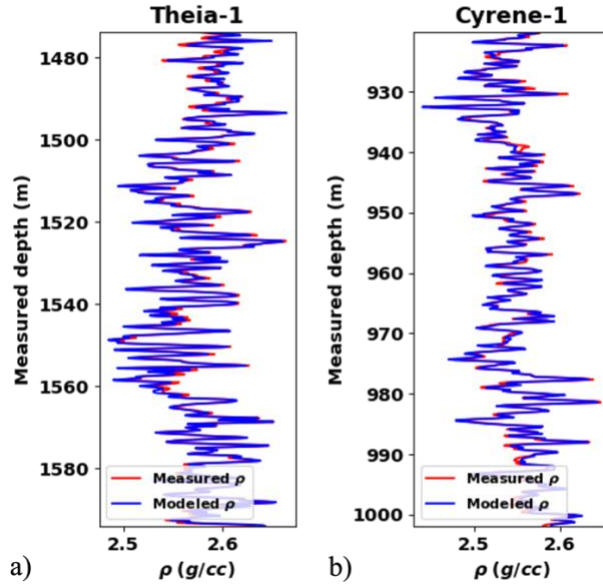
404

405 In Table 1, properties of clay minerals are uncertain. Therefore, Theia-1 well is used for calibrating
406 the uncertain properties of clay minerals before applying the model to rock physics inversion. It is
407 important to mention that matrix aspect ratio is a sensitive parameter in the rock physics model
408 but is not available in the well log. Varying the aspect ratio at each depth can address the complex
409 pore system and improve the accuracy of the rock physics model (Guo et al., 2021). Therefore,
410 instead of fixing the matrix aspect ratio for the whole well, we vary the matrix aspect ratio at each
411 depth when calibrating the moduli of clay minerals and kerogen. In the inversion process, the
412 matrix aspect ratio is one of the inverted properties.

413

414 For mineral density calibration, mineral volume fractions from geochemical log are input to the
415 rock physics model. A grid search method with interval of 0.01 g/cc is applied to minimize the
416 MSE between the modelled density and the measured density log. The accepted illite density is
417 2.84 g/cc and chlorite density is 2.71 g/cc. Then, the accepted densities are validated by Cyrene-1
418 (Figure 11).

419



420

421 Figure 11. Comparisons of the measured density logs and the modeled density logs with minimum
 422 MSE. a) Theia-1 well. b) Cyrene-1 well. The blue curves are modeled density logs and the red
 423 curves are measured density logs.

424

425 For mineral and kerogen moduli calibration, a Monte Carlo rock physics model calibration
 426 approach is applied to find optimal moduli of kerogen, illite, and chlorite. Bulk and shear modulus
 427 of kerogen, illite, and chlorite are assumed to be uniformly distributed and the ranges are specified
 428 in Table 1.

429

430 The steps of the moduli calibrations are:

431 1) Bulk modulus K and shear modulus μ of kerogen, illite, and chlorite are randomly sampled from
 432 Table 1.

433 2) Poisson's ratio ν is calculated by $\nu = \frac{3K-2\mu}{2(3K+\mu)}$. If ν of clay minerals is in the range of (0.1, 0.4)

434 (Wang et al., 2001; Mondol et al., 2008; Hedan et al., 2015) and ν of kerogen is in the range of

435 (0.2, 0.35) (Kashinath et al., 2019; Wu and Firoozabadi, 2020), the sampled bulk and shear
436 modulus are kept for next step. Otherwise, step 1 will be repeated until the Poisson's ratio is in the
437 reasonable range.

438

439 3) For each depth in Theia-1 well, volume fractions of minerals, kerogen, and fluids, vitrinite
440 reflectance, porosity from well logs are input to the rock physics model. Matrix aspect ratio is a
441 model parameter that cannot be obtained from well log. Therefore, a grid search method is applied
442 to find optimal matrix aspect ratio of each depth. More specifically, a reasonable range of aspect
443 ratios from 0.001 to 0.150 was defined, with increments of 0.001, and the optimal value was
444 selected by minimizing the the MSE between the measured (V_p, V_s) and the modeled (V_p, V_s) at
445 each depth.

446

447 4) After finding the optimal matrix aspect ratio of each depth, the MSE between the measured
448 (V_p, V_s) and the modeled (V_p, V_s) of the whole well is calculated.

449

450 5) Steps 1-4 are repeated N times, and the bulk modulus K and shear modulus μ of kerogen, illite,
451 and chlorite that have minimum MSE between the measured (V_p, V_s) and the modeled (V_p, V_s) of
452 the whole well are finally accepted.

453

454 6). The calibrated rock physics model is validated using the Cyrene-1 well. The same grid search
455 method in step 3 is applied here to optimize the matrix aspect ratio at each depth that can minimize
456 the MSE between the measured (V_p, V_s) and the modeled (V_p, V_s) at each depth.

457

458 In this case, 10,000 sets of properties are randomly generated. The accepted properties of kerogen
 459 and clay minerals with minimum MSE are list in Table 3. The cross-plots of measured and modeled
 460 (V_p, V_s, ρ) of Theia-1 and Cyrene-1 after calibration are shown in Figure 12.

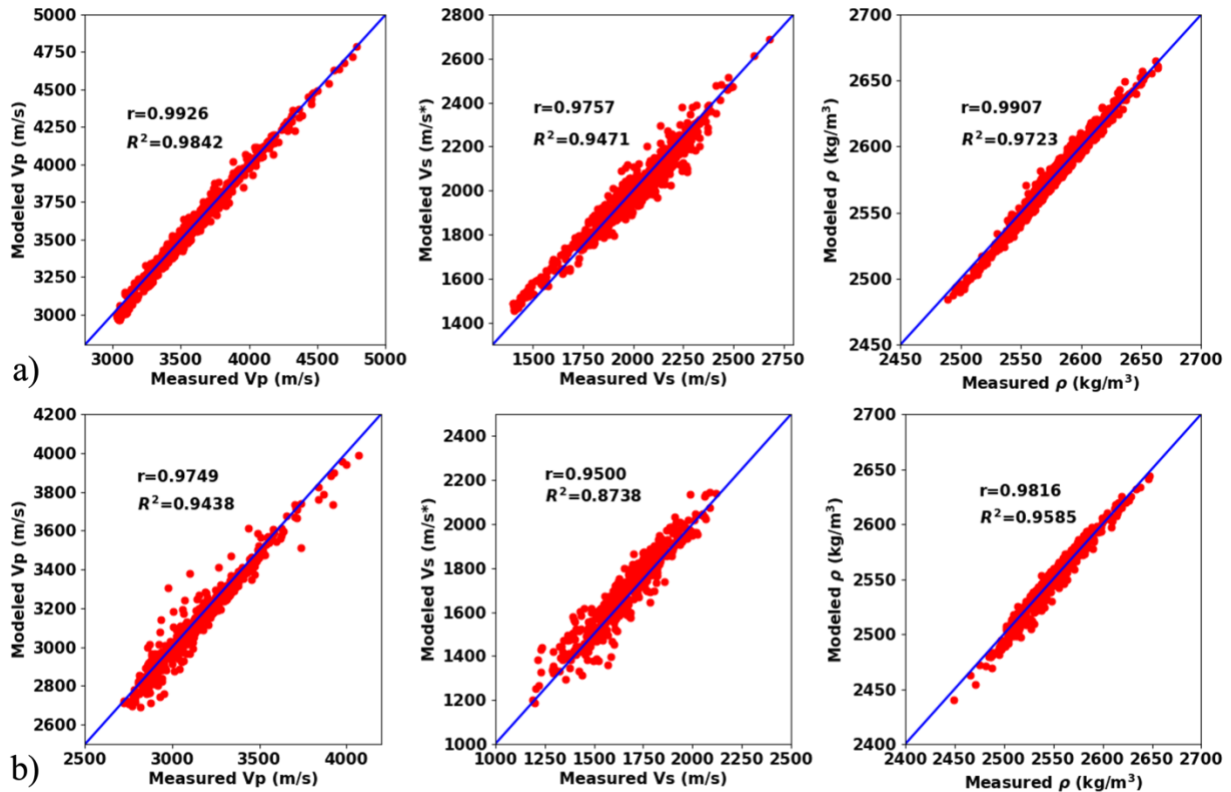
461

Component	K [GPa]	μ [GPa]	ρ [g/cc]
Kerogen	9.2	3.6	$f(\%R_0)$
Illite	28.2	6.1	2.84
Chlorite	39.2	8.8	2.71

462

463 Table 3. Accepted properties of kerogen and clay minerals from Monte Carlo rock physics model
 464 calibration. K is bulk modulus, μ is shear modulus, and ρ is density. $\%R_0$ is vitrinite reflectance.
 465 Density of kerogen is a function of vitrinite reflectance.

466



467

468 Figure 12. Crossplots of measured and modeled (V_p, V_s, ρ) of Theia-1 well. a) Theia-1 well. b)

469 Cyrene-1 well. V_p is compressional velocity, V_s is shear velocity, ρ is density, r is the Pearson

470 correlation coefficient, and R^2 is the coefficient of determination.

471

472 Prior falsification is performed to ensure consistency between modeled and real data (Scheidt et

473 al., 2018). The new priors are estimated from the Theia-1 well and are shown in Table 4.

474 Impedances (I_p, I_s) are modeled using the prior and calibrated rock physics model, then are

475 compared with real impedance data from sonic log in Figure 13. The real data are in the range of

476 the priors which means the rock physics model cannot be falsified.

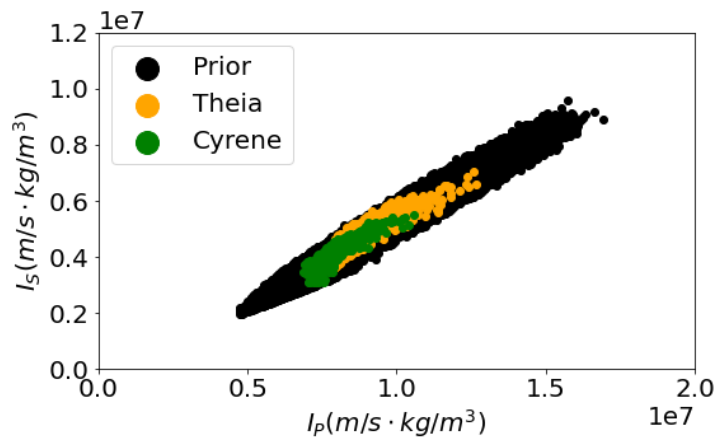
477

Input variable	Distribution	Range
----------------	--------------	-------

Kerogen type	Categorical	III (Iqbal et al., 2022)
Vitrinite reflectance	Uniform	(0.23, 1.6)
Kerogen	Uniform	(0, 0.15)
Porosity	Uniform	(0, 0.15)
Matrix aspect ratio	Uniform	(0.001, 0.2)
Quartz	Dirichlet	(0, 0.6)
Calcite	Dirichlet	(0, 0.8)
Illite	Dirichlet	(0, 0.8)
Chlorite	Dirichlet	(0, 0.1)
Dolomite	Dirichlet	(0, 0.1)
Pyrite	Dirichlet	(0, 0.06)
Bound water	Dirichlet	(0, 1)
Free water	Dirichlet	(0, 1)
Oil	Dirichlet	(0, 1)

478 Table 4. Prior distributions of input variables.

479



480

481 Figure 13. Consistency check between modeled impedances and real impedances from well logs.

482

483 5.3 Outlier detection for seismic inversion

484

485 Outliers in seismic inversion can result from various factors such as noise and errors in data
486 acquisition, geological anomalies, processing artifacts, and limitations of the inversion algorithm.

487 Removing these outliers is essential to improve the accuracy and reliability of the rock physics
488 inversion. Here, we detect and remove the outliers in the seismic inversion using the robust

489 Mahalanobis distance (RMD). The Minimum Covariance Determinant (MCD) estimator
490 (Rousseeuw, 1984) is used to estimate the covariance matrix of the seismic inversion as the MCD

491 is a statistically robust estimate of the covariance matrix. The RMD of each point in the seismic
492 inversion is then calculated in Eq. 6, and a threshold of ± 3 standard deviations is set to identify

493 and remove the outliers (Figure 14). The corresponding V_P , V_S , and ρ sections after outlier
494 removal are shown in Figure 15. Most of the removed outliers are located near the bottom of the

495 Goldwyer III unit, potentially caused by formation interpretation errors or changes in lithology.

496 The V_P , V_S , and ρ 2D sections will be used for rock physics inversion.

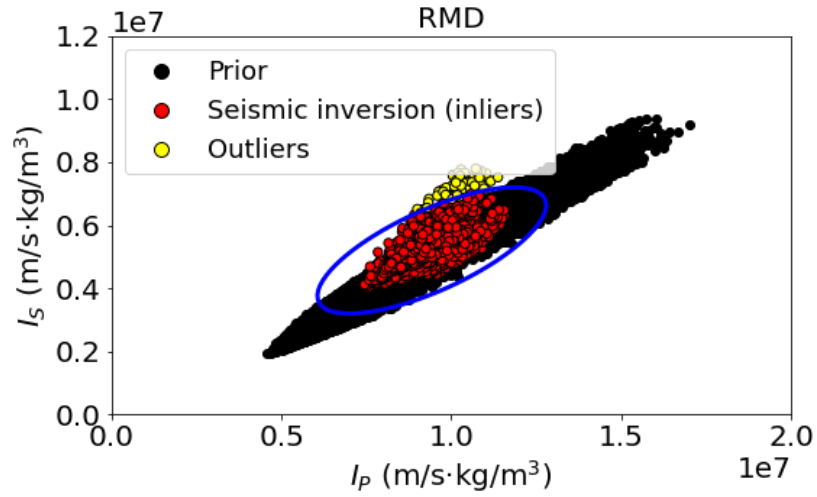
497

498 The RMD for each data point $x_i = (I_{P,i}, I_{S,i})$ is calculated as:

$$499 \quad D_{RMD,i} = \sqrt{(x_i - \mu_{MCD})^T \Sigma_{MCD}^{-1} (x_i - \mu_{MCD})} \quad (6)$$

500 Where μ_{MCD} and Σ_{MCD} are the robust mean vector and covariance matrix estimated using the MCD
501 method.

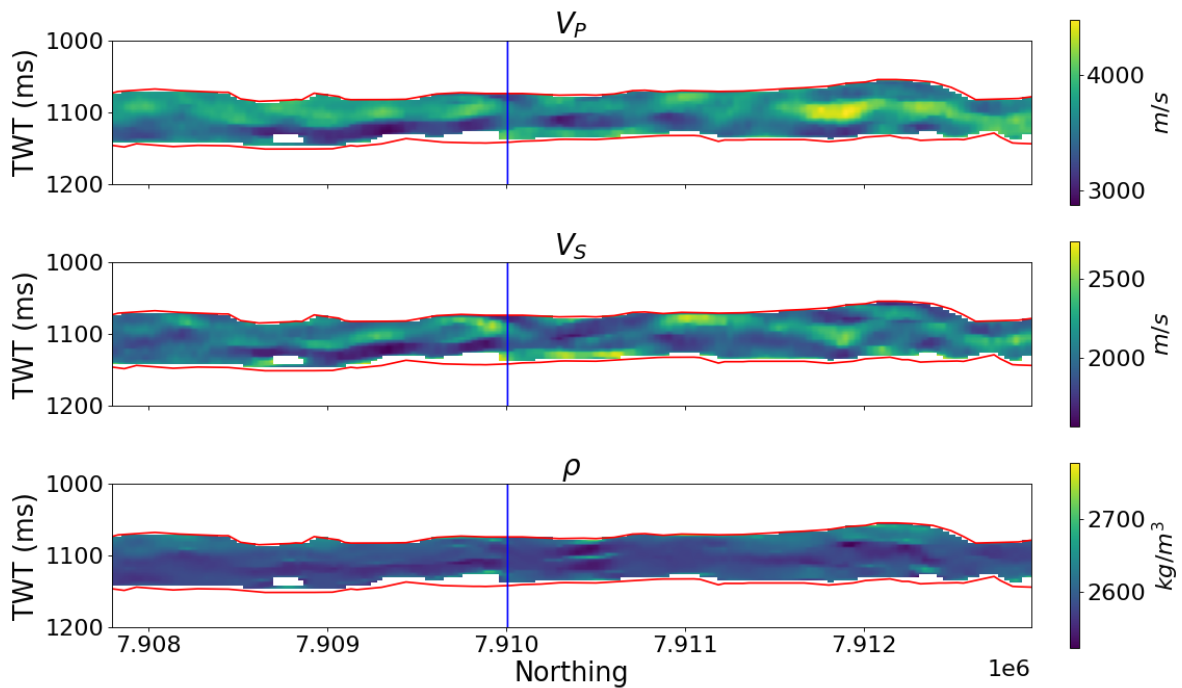
502



503

504 Figure 14. Seismic inversion outlier detection using robust Mahalanobis distance with threshold
 505 of ± 3 standard deviations. The blue ellipse represents the Mahalanobis distance contour
 506 corresponding to this threshold. Red points inside the ellipse are identified as inliers, while yellow
 507 points outside the ellipse are classified as outliers. Black points denote prior samples generated
 508 from the rock physics model.

509



510

511 Figure 15. V_p , V_s , and ρ sections after outlier removal. The blue line is Theia-1 well. The red
 512 curves are the top and bottom of the Goldywer III unit.

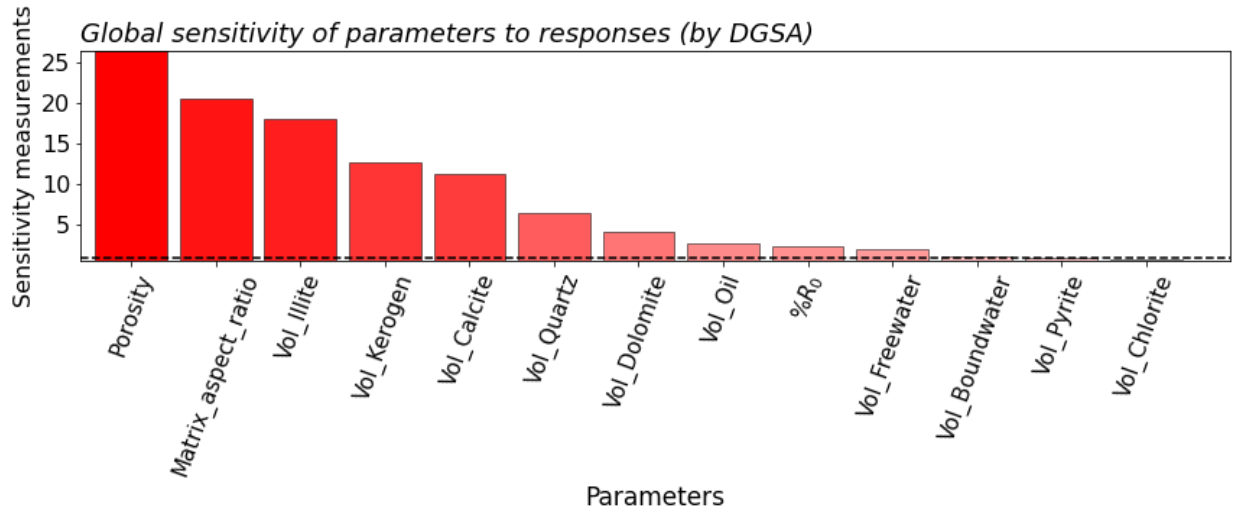
513

514 5.4 Sensitivity analysis of the calibrated model using the new priors

515

516 In Section 3.2, we investigated the sensitivity of the uncalibrated rock physics model using large
 517 priors. In the field study, the rock physics model is calibrated, and the new priors are estimated
 518 from well logs. Therefore, we need to analyze the sensitivity of the calibrated rock physics model
 519 again using the new priors in Table 4. The sensitivity analysis results are shown in Figure 16. The
 520 top four sensitive variables are porosity, matrix aspect ratio, volume fraction of illite, and volume
 521 fraction of kerogen. These results suggest that fixing the matrix aspect ratio in the well logs can
 522 potentially lead to inaccurate inversion results for other properties.

523



524

525 Figure 16. Sensitivity analysis of the calibrated rock physics model inputs to elastic properties (V_p ,
526 V_s , and ρ) using the new prior table. The top 4 input variables are porosity, matrix aspect ratio,
527 illite, and kerogen.

528

529 5.5 Weight calculations for ABC distance using the calibration well

530

531 The sensitivity analysis results indicate that the matrix aspect ratio is the second most sensitive
532 parameter in the rock physics model. As a model parameter, the matrix aspect ratio cannot be
533 directly obtained from well logs. It has a significant impact on velocity modeling but does not
534 influence density modeling. Therefore, it is necessary to account for this modeling error when
535 determining weights.

536

537 In the calibration well, all input variables except for the matrix aspect ratio are provided to the
538 calibrated rock physics model. To account for the effect of the matrix aspect ratio at each depth,
539 1,000 realizations of the matrix aspect ratio are randomly sampled from the prior distributions and

540 then input into the rock physics model. The modeled 1,000 realizations of V_P , V_S , and ρ are
 541 averaged at each depth. This process is repeated at each depth in the whole well log. Crossplots of
 542 the average modeled and measured V_P , V_S , and ρ in the whole well log are plot in Figure 17.
 543 Comparing the results in Figures 12 and 17, it is evident that the matrix aspect ratio significantly
 544 impacts the modeling of elastic properties. The weight matrix W and covariance matrix S for V_P ,
 545 V_S , and ρ are calculated and are listed below.

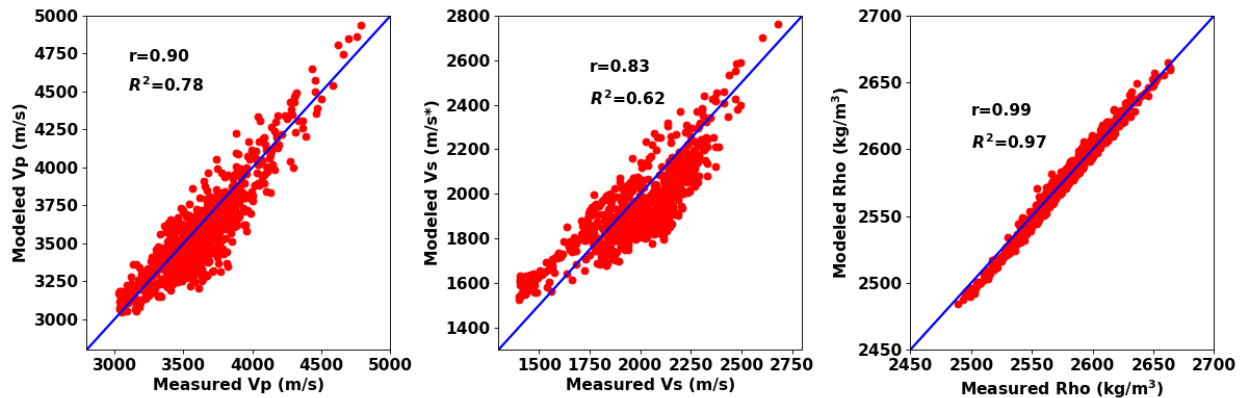
546

547
$$W = \begin{bmatrix} 16.97 & 0 & 0 \\ 0 & 7.47 & 0 \\ 0 & 0 & 405.26 \end{bmatrix}$$

548

549
$$S = \begin{bmatrix} 1 & 0.97 & 0.53 \\ 0.97 & 1 & 0.42 \\ 0.53 & 0.42 & 1 \end{bmatrix}$$

550



551

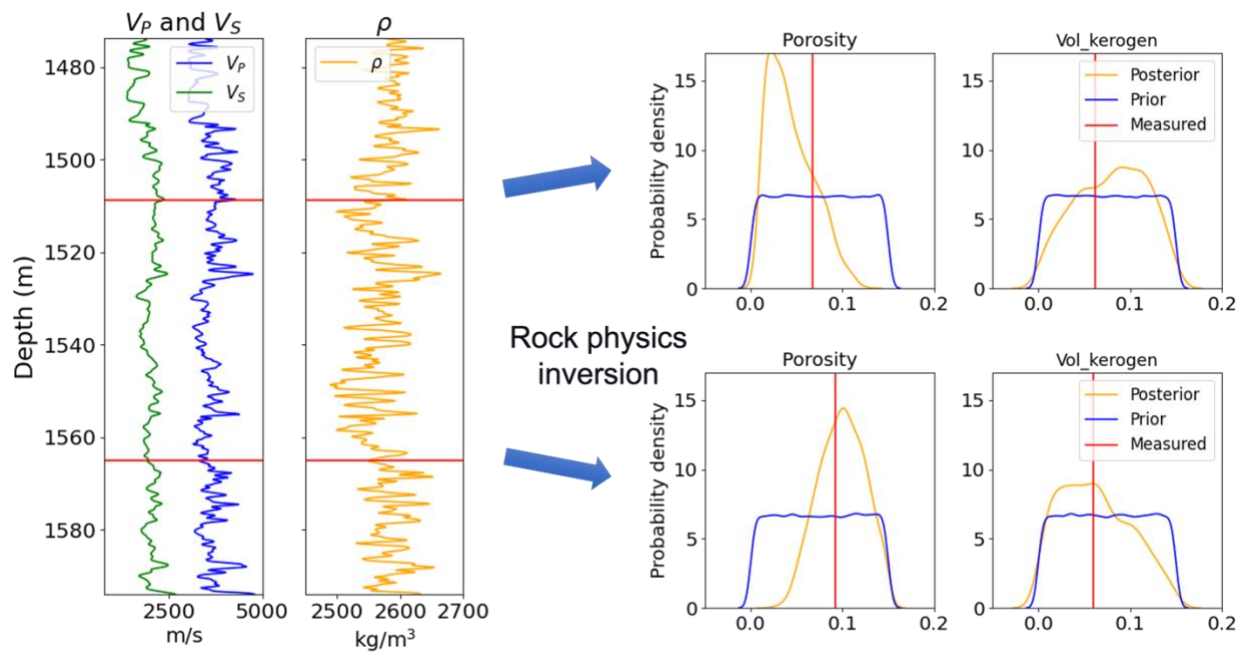
552 Figure 17. Crossplots of measured and average modeled (V_P , V_S , ρ) of Theia-1 well when varying
 553 matrix aspect ratio. V_P is compressional velocity, V_S is shear velocity, ρ is density, r is the Pearson
 554 correlation coefficient, and R^2 is the coefficient of determination.

555

556 **5.6 Rock physics model inversion using well logs**

557

558 The workflow of ABC is then applied to invert the source rock properties from well log ($V_p, V_s,$
559 ρ). The rock physics inversion is performed depth by depth in the well logs (Figure 18). 100,000
560 sets of prior (V_p, V_s, ρ) are generated. At each depth, the weighted Mahalanobis distances between
561 100,000 sets of prior (V_p, V_s, ρ) and the well log (V_p, V_s, ρ) are calculated. Based on the
562 weighted Mahalanobis distances, only the top 1% (V_p, V_s, ρ) that are nearest to the well log
563 (V_p, V_s, ρ) are accepted. The distributions of the accepted prior input variables are considered as
564 the posteriors of source rock properties at this depth. The rock physics inversion is performed at
565 each depth independently and therefore can be run in parallel to accelerate the inversion process.



566

567 Figure 18. Illustration of rock physics inversion using ABC applied to well log. The blue arrows
568 represent rock physics inversion with (V_p, V_s, ρ) depth by depth, at two specific depths shown by
569 the red horizontal lines on the well-log plots. The subplots on the right compare the posterior
570 distributions of rock properties with prior and measured values from well logs. The orange curves

571 are posterior distributions, the blue curves are prior distributions, and the red vertical lines are
572 measured values from well logs.

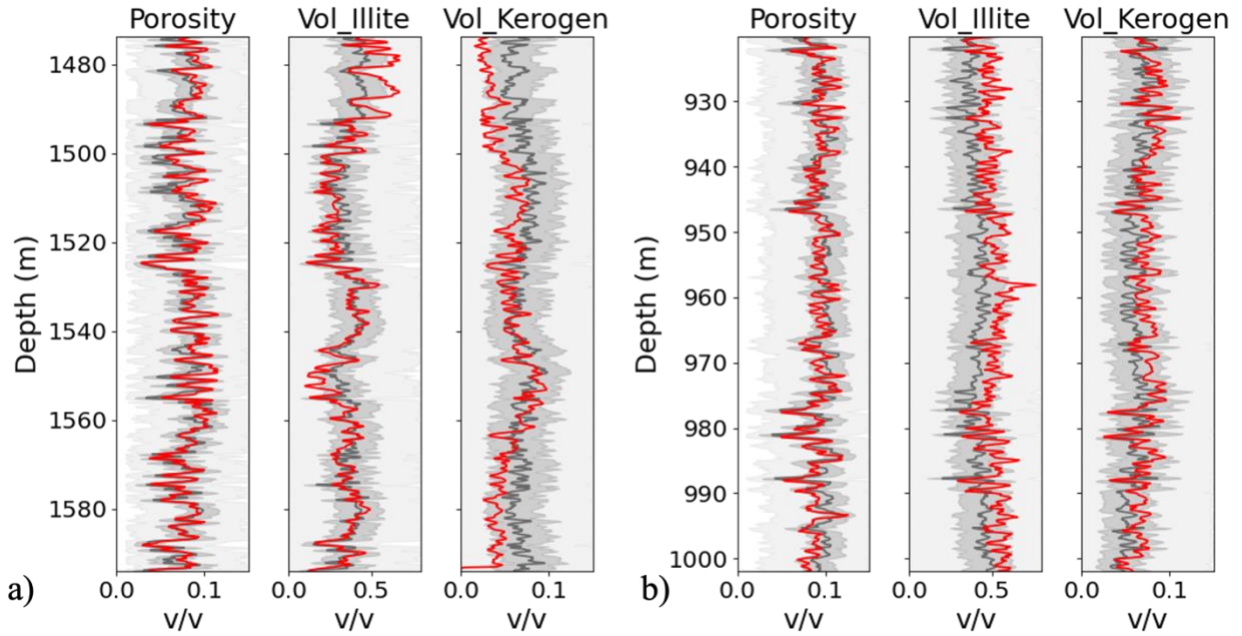
573

574 The inversion results for Theia-1 and Cyrene-1 are presented in Figure 19. The results show that
575 porosity, the volume fraction of kerogen, and the volume fraction of illite can be well estimated
576 compared to the well-log measurements, while the remaining volume fractions of mineral
577 compositions are less accurately estimated. This outcome is consistent with the sensitivity analysis,
578 which suggests that parameters with higher sensitivity are more accurately estimated, whereas
579 those with lower sensitivity are more difficult to constrain.

580

581 The accepted (V_p, V_s, ρ) are shown in Figure 20. The range of accepted ρ is very narrow, whereas
582 the range of V_p and V_s are broader. This is because the weight assigned to ρ is significantly higher
583 than the weights of V_p and V_s . More specifically, the modelling error for ρ is much smaller than
584 for V_p and V_s .

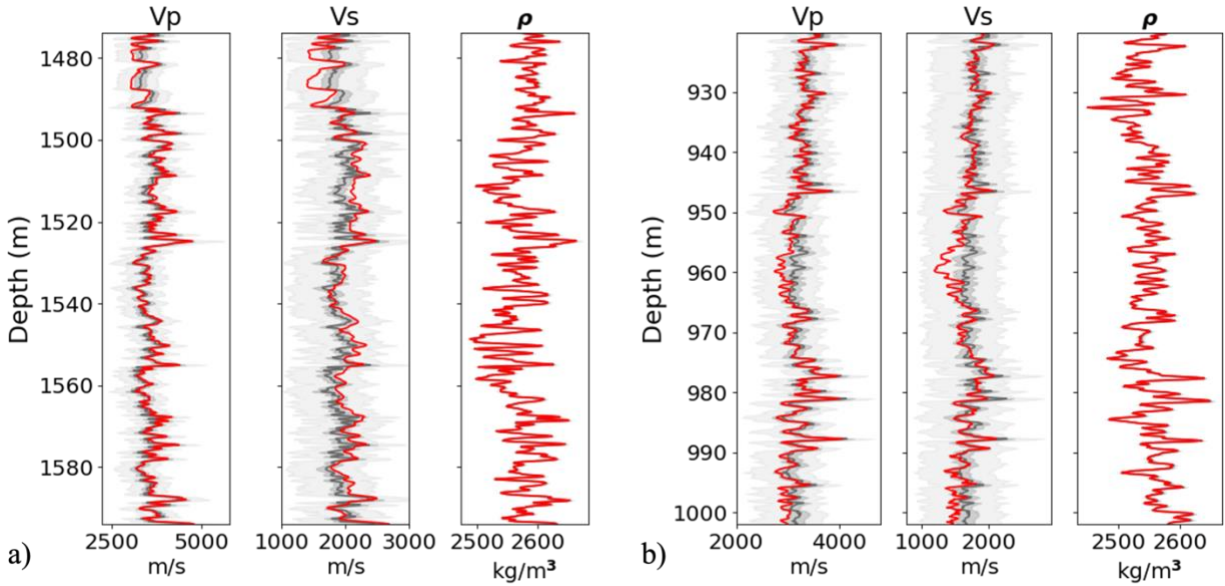
585



586

587 Figure 19. Inverted porosity, volume fraction of illite, volume fractions of kerogen from well-log
 588 elastic properties. a) inversion results of Theia-1 well. b) inversion results of Cyrene-1 well. The
 589 light grey areas are the ranges between minimum and maximum of the accepted samples. The dark
 590 grey areas are the ranges between 25th and 75th percentile of the accepted samples. The dark grey
 591 curves are the medians of the accepted samples. The red curves are the measured values from well
 592 logs.

593



594

595

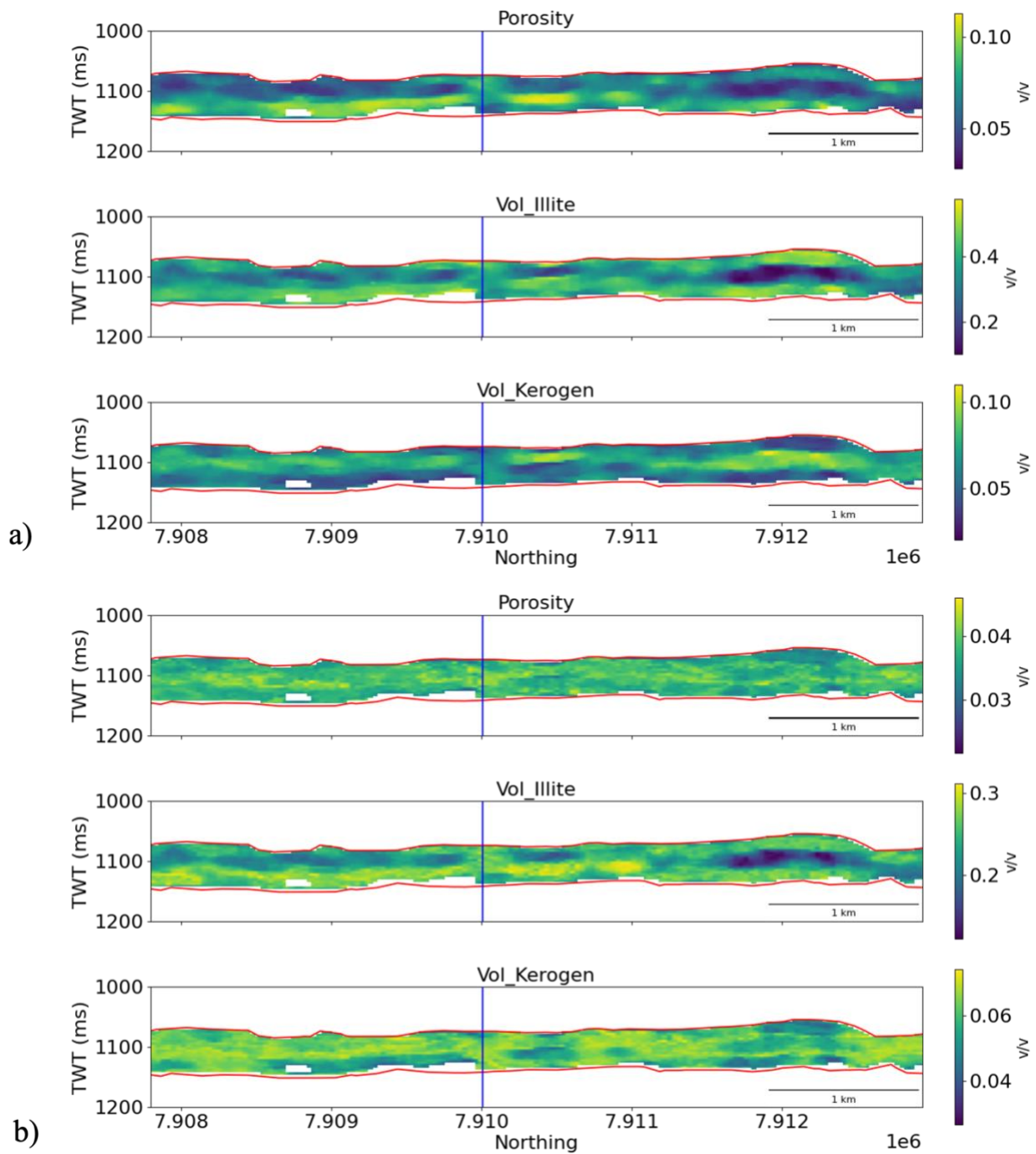
596 Figure 20. Accepted (V_p, V_s, ρ) using ABC. a) accepted samples from Theia-1. b) accepted
 597 samples from Cyrene-1. The light grey areas are the ranges between minimum and maximum of
 598 the accepted samples. The dark grey areas are the ranges between 25th and 75th percentile of the
 599 accepted samples. The dark grey curves are the medians of the accepted samples. The red curves
 600 are the measured values from well logs.

601

602 **5.7 Rock physics model inversion using seismic data**

603 The same workflow of ABC is applied to invert the source rock properties from 2D (V_p, V_s, ρ)
 604 sections obtained from seismic inversion. The rock physics inversion is performed point by point
 605 across the 2D sections. The means and interquartile ranges (IQR) of the inverted properties are
 606 presented in Figure 21. For porosity, the results indicate that the mean values are higher in the
 607 deeper areas of the Goldwyer III unit, with the IQR remaining relatively uniform throughout the
 608 formation. For the volume fraction of illite, the mean and IQR are higher in the deeper and

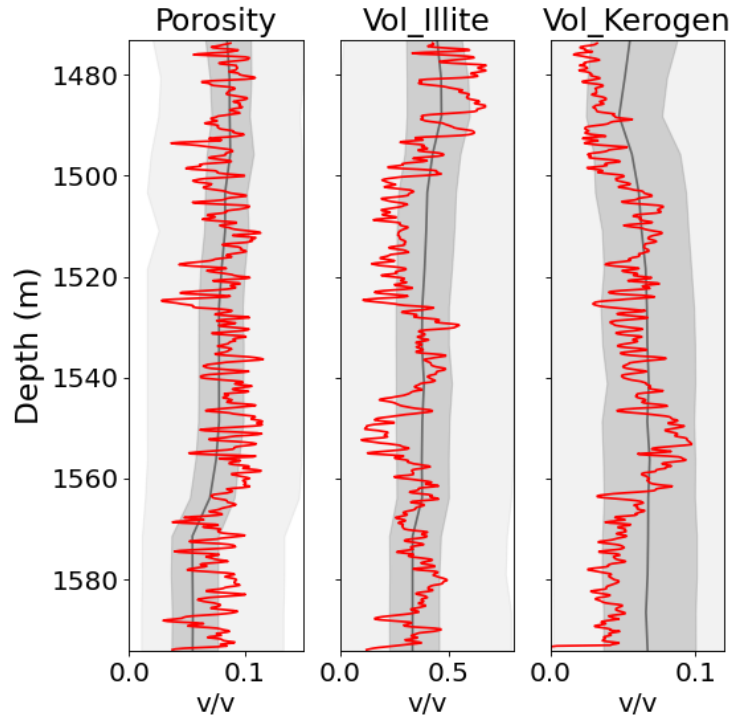
609 shallower areas of the formation. For the volume fraction of kerogen, the mean is higher in the
610 shallower and middle areas of the formation, and the IQR remains relatively uniform across the
611 entire formation. These inversion results can be used to identify sweet spots with high
612 unconventional source rock potentials. A comparison between inverted porosity, volume fraction
613 of illite, and volume fraction of kerogen derived from seismic elastic properties at the well location
614 and the corresponding measured values from well logs is shown in Figure 22, showing that the
615 inverted parameters successfully capture the main depth trends and magnitudes observed in the
616 well data.



617

618 Figure 21. Means and IQRs of the accepted porosity, volume fraction of illite, and volume fraction

619 of kerogen. The blue lines are the Theia-1 well. a) Means. b) IQRs.



620

621 Figure 22. Comparison between inverted porosity, volume fraction of illite, and volume fraction
 622 of kerogen derived from seismic elastic properties at the well location and the corresponding
 623 measured values from well logs. The light grey areas are the ranges between minimum and
 624 maximum of the accepted samples. The dark grey areas are the ranges between 25th and 75th
 625 percentile of the accepted samples. The dark grey curves are the medians of the accepted samples.
 626 The red curves are the measured values from well logs.

627

628 **6. Uncertainty and Limitations**

629 Several limitations exist in the proposed workflow. First, only the posteriors of the top sensitive
 630 variables can be updated significantly through the rock physics inversion, while insensitive but
 631 important parameters, such as thermal maturity and fluid saturations, have limited updates in the
 632 posteriors. Second, the rock physics inversion is sensitive to the prior distributions of input

633 variables. Therefore, inaccurate priors may lead to biased estimates, though this can be mitigated
634 to some extent if the priors are wide enough to assimilate the observed data. Third, the elastic
635 properties of kerogen and clay minerals may vary with depth, temperature, and compaction.
636 Consequently, if the rock physics model is calibrated using well logs from one formation and then
637 applied to the same formation at substantially different burial depths, it may lead to inaccurate
638 predictions.

639 To address these limitations, several improvements can be considered. Sensitivity analysis can be
640 further employed to identify whether limited posterior updates arise from data limitations or model
641 limitations. For poorly constrained properties, basin modeling can be reintroduced to incorporate
642 rock-physics inversion results together with basin burial history and boundary conditions, thereby
643 better constraining thermal maturity and related parameters. Finally, more sophisticated kerogen
644 and clay elastic models that account for variations with depth and temperature could enhance the
645 predictive capability of the workflow.

646

647 **7. Conclusion**

648 This study presents a statistical rock physics inversion workflow for efficiently estimating source
649 rock properties and quantifying their uncertainty using well logs and seismic signatures. A Monte
650 Carlo rock physics calibration approach is introduced to refine uncertain parameters, including the
651 elastic properties of kerogen and clay minerals. Weighted Approximate Bayesian Computation
652 (ABC) is applied to integrate prior petrophysical knowledge, model calibration errors, and
653 measured elastic property data from well logs and seismic data, enabling efficient estimation of

654 the posterior distributions of source rock properties. Sensitivity analysis of the rock physics model
655 provides insight into how well each input variable can be constrained through the inversion process.

656 The workflow is validated using well-log data, showing strong and accurate posterior updates. It
657 is then applied to seismic signatures from the Canning Basin to estimate the two-dimensional
658 distributions of rock properties. The seismic inversion yields spatially coherent trends that are
659 consistent with well-log observations, demonstrating the robustness of the proposed workflow for
660 field-scale characterization of source rocks.

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662

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666 Safety for providing the necessary data used in this study. We would also like to acknowledge
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668

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