

1 **Full title:** Low computational cost stochastic Gassmann fluid substitution modelling of
2 hydrogen and carbon dioxide in clastic storage reservoirs

3 **Abbreviated title:** Seismic Response of H₂ & CO₂ in Clastic Reservoirs

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PREPRINT STATEMENT

14 This manuscript has not been peer-reviewed, it has been submitted to EarthArXiv
15 as a preprint. A subsequent version of this manuscript may have slight edits and
16 changes present. This manuscript has been submitted for publication in
17 Geoenergy. If accepted, the final version of this manuscript will be available via
18 the 'Peer-reviewed Publication DOI' link on the right-hand side of this webpage.

19

20 1.1 Abstract

21 The ability to safely store non-hydrocarbon fluids in the subsurface, such as carbon dioxide or
22 hydrogen, will likely be vital in all pathways to decarbonise global energy systems. Storage of
23 these fluids will require monitoring programmes to identify dynamic changes during the
24 injection and storage phases and to identify unintended migration. Seismic monitoring is
25 widely adopted in monitoring plans. We investigate the changes in seismic response for
26 different non-hydrocarbon fluids and different saturations.

27 The bulk elastic properties of subsurface rocks are influenced by the fluids present within the
28 pore space and impact the seismic response of the rock. We undertake fluid substitution
29 modelling, calculating new rheological properties of reservoir intervals after substituting brine
30 for either hydrogen or carbon dioxide, varying the water saturation from 100% to 0%, and
31 determining the new elastic properties. We investigate three proposed reservoirs for carbon
32 dioxide storage on the UKCS, the Triassic Bunter Sandstone Formation, the Permian Leman
33 Sandstone Formation and the Triassic Helsby (Ormskirk) Sandstone Formation. The workflow
34 is stochastic and as such allows for the investigation of the impact of geological uncertainty
35 on the results. The newly determined elastic properties are then used for modelling the
36 seismic response and wedge models.

37 1.2 Introduction

38 Pore-filling fluids within a reservoir modify the bulk elastic properties and consequently
39 impact the seismic response (Mavko et al., 2009). Forward modelling of the seismic response
40 of porous reservoirs with different pore-filling fluids is commonplace within hydrocarbon
41 exploration and production workflows where it is used to understand the expected seismic
42 response of the subsurface (Avseth et al., 2005). In recent years these methods have been
43 used to model carbon dioxide with respect to carbon capture storage (CCS) projects (Dupuy
44 et al., 2017; Carpentier et al., 2021; Harvey et al., 2022b), and can be considered applicable
45 to hydrogen storage also.

46 The seismic response of a geological boundary can be described by the reflection coefficient
47 of the interface, which is determined by the acoustic impedance of the two layers, defined
48 as: (Bacon et al., 2003);

$$49 \quad RC = \frac{Ai_2 - Ai_1}{Ai_2 + Ai_1} \quad \text{EQUATION 1}$$

$$50 \quad Ai = \rho_{\text{bulk}} * v_p \quad \text{EQUATION 2}$$

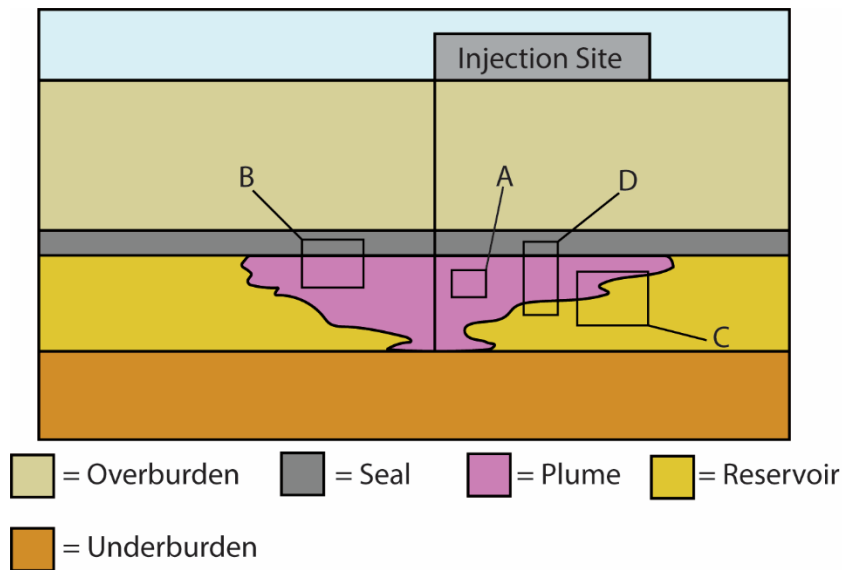
51 Where Ai_1 and Ai_2 are the acoustic impedance values for the reservoir layers above and below
52 the geological boundary, and where ρ_{bulk} is the bulk density of the reservoir layer and v_p is
53 the compressional velocity. Both the bulk density and compressional velocity of a reservoir is

54 modified by the pore-filling fluid. As different fluids have different properties, the extent to
55 which the bulk density and compressional velocity of a reservoir are modified depends on the
56 constituent properties of the filling liquid (Batzle and Wang, 1992). Forward modelling the
57 seismic response and comparing it with the actual seismic response allows for the prediction
58 of the fluid or fluid mixture present within the pore space at the time of acquisition (Ahmed
59 et al., 2015). The change in pore filling fluid will impact the amplitude of seismic response at
60 different seismic wave offsets. Changes in elastic properties hence modify the reflection
61 response, which can be interpreted to identify changes in fluid saturation (Wandler et al.,
62 2007). These approaches are used for both hydrocarbon exploration and production, where
63 changes in fluid distribution as a result of production can be detected, and for subsurface
64 storage, where, changes in fluid distribution due to injection can be detected (Chadwick et
65 al., 2005; Singer et al., 2018). In recent years there have been numerous studies that extend
66 conventional fluid prediction methods to make use of computationally more complex
67 methods, such as Bayesian inversion (e.g. and Pradhan et al. (2020)). While these methods
68 can be valuable, computationally low-cost Monte Carlo methods allow for rapid and easy
69 hypothesis testing and do not require *a priors*, instead relying on observed data to determine
70 the input parameters (Mosegaard, 2023). As such stochastic models can be used to distinguish
71 between differing geological models (Ringrose and Bentley, 2021).

72 In this paper, we use a stochastic implementation of the Gassmann equations to undertake
73 fluid substitutions in three reservoir intervals on the United Kingdom Continental Shelf
74 (UKCS). We consider both carbon dioxide and hydrogen, determine the new elastic properties
75 and model the expected seismic responses for different component parts of a storage
76 complex (Figure 1).

77 Throughout this work we implement low computational cost techniques focussing on:
78 Resource-Efficiency, where computational methods are designed and implemented to
79 minimise resource usage. Approximate technique utilisation, where precision within
80 calculations is traded for speed by using approximations. Data minimisation, only undertaking
81 calculations on the data of interest.

82



83

84 *FIGURE 1. SCHEMATIC SUBSURFACE DIAGRAM OF A FLUID STORAGE SITE IN A POROUS RESERVOIR (NOT TO SCALE). BLACK*
 85 *BOXES REPRESENT AREAS WHICH ARE FORWARD MODELLED, A) RESERVOIR PROPERTIES B) SEAL - RESERVOIR INTERFACE,*
 86 *C) RESERVOIR (INJECTED FLUID SATURATED) – RESERVOIR (BRINE SATURATED) INTERFACE, D) WHOLE RESERVOIR COLUMN.*
 87 *PLUME TRACED FROM QUEST CCS FACILITY 2050 MODEL (HARVEY ET AL., 2022A).*

88

89 1.3 Geological Setting

90 We undertake seismic modelling of three discrete reservoir – seal pairs from the UKCS. The
 91 chosen reservoir-seal pairs are located within two separate basins. The pairs from the
 92 Southern North Sea, the Bunter and Leman Sandstone, are located within the UK sector of
 93 the South Permian Basin, while the Helsby Sandstone is located within the Foryd-Gograth sub-
 94 basin of the East Irish Sea Basin (Ziegler, 1990; Jack et al., 1995). The South Permian Basin is
 95 an east-west trending basin, stretching from the eastern coast of the United Kingdom across
 96 Northern Europe to western Poland. Its formation is primarily attributed to mid-to-late
 97 Permian rifting events with modification from later phases of rifting and thermal subsidence.
 98 Its structural configuration was significantly influenced by the pre-existing tectonic
 99 framework established during the early Palaeozoic (Ziegler, 1992; Glennie, 1998; Glennie and
 100 Underhill, 1998). The East Irish Sea Basin is part of a Permo-Triassic rift system, consisting of
 101 northwest-southeast trending normal faults which control the basin architecture. A east-west
 102 trending horst graben system is responsible for the many sub-basins within the area including

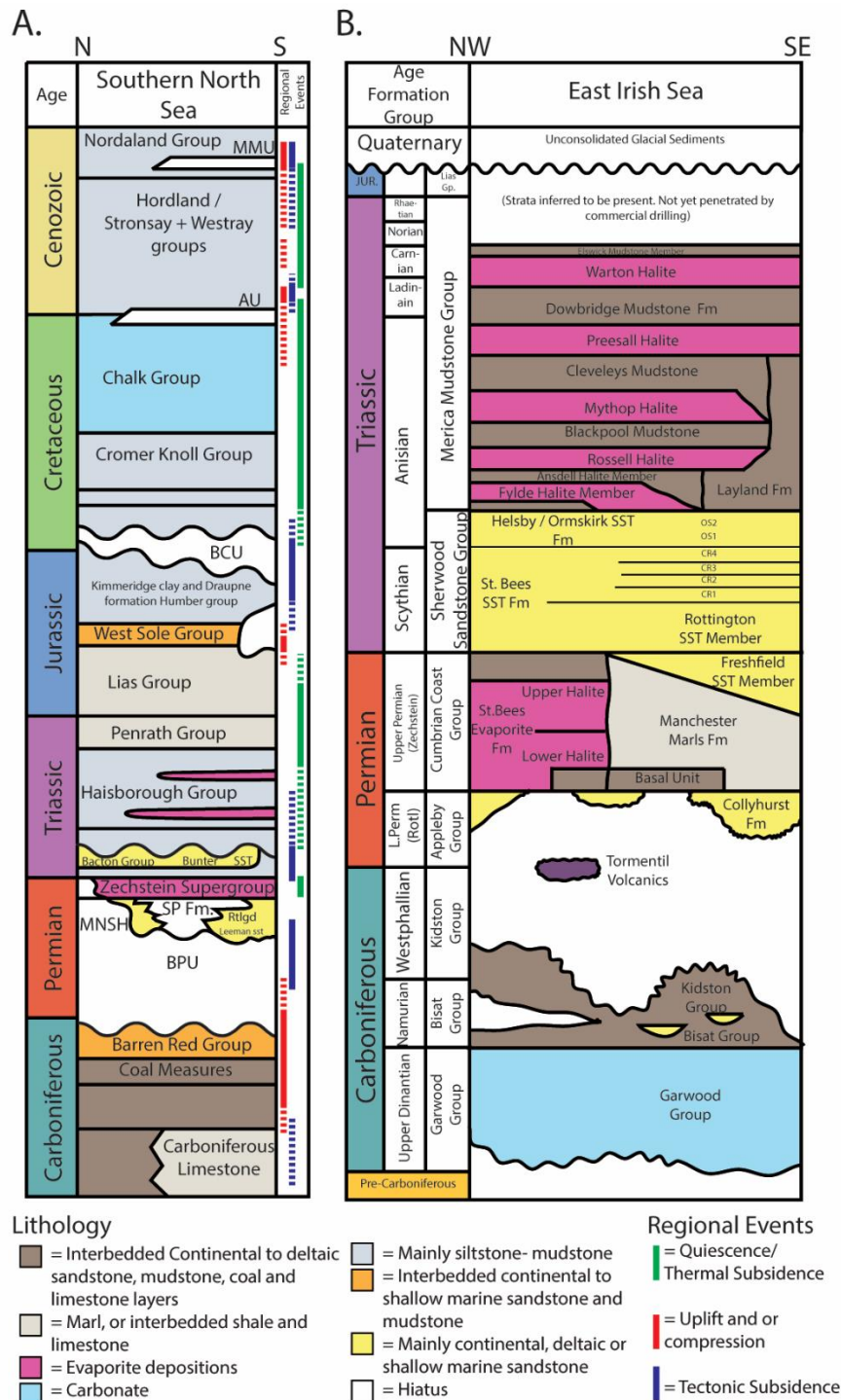
103 the Foryd-Gograth sub basin (Jack et al., 1995). Each of the reservoir intervals modelled has
104 an associated planned CCS project (Gluyas and Bagudu, 2020; Clery and Gough, 2022; de
105 Jonge-Anderson and Underhill, 2022; Gibson-Poole et al., 2024).

106 The Bunter Sandstone Formation is part of the Sherwood Sandstone Group and was deposited
107 during the Olenekian of the Lower Triassic (Figure 2) (Bachmann et al., 2010). It consists of
108 coarse-grained sandstones deposited in alluvial fan and fluvial environments in arid and semi-
109 arid environments (Brook et al., 2003). It is overlain by the Haisborough group, which consists
110 of a number of sealing formations, including claystone intervals and the Röt Halite (Bentham
111 et al., 2013). The Zechstein supergroup, which the Sherwood Sandstone Group overlies, has
112 undergone significant halokinesis, forming numerous salt domes and diapirs (Peryt et al.,
113 2010). The mobilisation of the underlying Zechstein has caused several trap geometries to
114 form within the Sherwood Sandstone Group of the Southern Permian Basin, one of which,
115 known as the Endurance structure, was awarded the first UK carbon storage permit in
116 December 2024 (James et al., 2016a; Gibson-Poole et al., 2024; UK Government, 2024).

117 The Helsby Sandstone Formation is part of the Sherwood Sandstone Group (Figure 2), it is
118 also known as the Ormskirk Sandstone Formation depending on the nomenclature used. It is
119 encountered throughout the East Irish Sea Basin (Kirk, 2005). It is early Triassic in age, having
120 been deposited during the Anisian (Howard et al., 2008). It was deposited in a fluvial
121 environment setting with aeolian influences, with facies of aeolian dunes and sandsheets
122 present (Yaliz and Taylor, 2003; Scorgie et al., 2021). It is a reservoir for a number of gas fields
123 within the East Irish Sea, with notable inclusions being the Hamilton field and Calder field
124 (Yaliz and Taylor, 2003; Blow and Hardman, 2022).

125 The Leman Sandstone Formation is part of the Rotliegend group and is an Early Permian
126 (Guadalupian - Lopingian) aged sedimentary succession consisting mainly of Aeolian
127 sediments (Figure 2) (Gast et al., 2010). The Rotliegend group is found extensively throughout
128 the South Permian Basin of Northern Europe, stretching from the east coast of the United
129 Kingdom to the eastern edges of the Polish trough in Ukraine (Gast et al., 2010). It is the main
130 gas-bearing reservoir within the UK sector of the South Permian Basin, where it is sealed by
131 the Zechstein evaporite supergroup (Rouillard et al., 2020). The Rotliegend is also the
132 reservoir used for the Rough gas storage field, where 54 BCF of natural gas is stored (Stuart,
133 1991).

134 It should be noted that within literature the lithostratigraphic nomenclature of the UKCS for
 135 different geological intervals can be varied and confusing, with different names being used
 136 for the same intervals. As such, we have followed the nomenclature set out by the British
 137 Geological Survey (2020) lexicon for the naming of reservoir intervals investigated.



138

139 FIGURE 2 SOUTHERN NORTH SEA (A) AND EAST IRISH SEA (B) CHRONOSTRATIGRAPHIC DIAGRAM. A MODIFIED AFTER

140 PATRUNO ET AL. (2022), B MODIFIED AFTER PATRONI ZAVALA ET AL. (2020)

141 1.4 Methodology

142 1.4.1 Fluid substitution

143 Fluid substitution is the property modelling of a rock, with the pore-filling fluid having been
 144 replaced by a new fluid or new ratios of two or more different fluids (Dvorkin et al., 2007).
 145 Fluid substitution modelling is commonly used to understand how the constituent properties
 146 of the rock are modified when alternative fluids to the original fill the pore space (Nolen-
 147 Hoeksema, 2000). The Gassmann equations are the most commonly used methodology to for
 148 fluid substitution modelling (Gassmann, 1951; Smith et al., 2003). The equations relate the
 149 bulk modulus of the saturated rock, K_{sat} , the bulk modulus of the dry rock frame, K^* , the bulk
 150 modulus of the mineral matrix, K_o , the porosity of the rock, Φ , and pore filling fluids bulk
 151 modulus, K_{fl} (Smith et al., 2003);

152

$$K_{sat} = K^* + \frac{(1 - \frac{K^*}{K_o})^2}{\frac{\Phi}{K_{fl}} + \frac{(1 - \Phi)}{K_o} - \frac{K^*}{K_o^2}}$$

EQUATION 3 – GASSMANN EQUATION

153

154 1.4.1.1 Bulk elastic rock properties

155 The bulk modulus of a saturated rock can be calculated using the compressional velocity, V_p ,
 156 the shear velocity, V_s and the bulk density, ρ_{bulk} as;

$$K_{sat} = \rho_{bulk}(V_p^2 - \frac{4}{3}V_s^2)$$

EQUATION 4 – BULK MODULUS

157 Compressional velocity and shear velocity data can be obtained from either wireline logging
 158 or core measurements for a specific formation. We use data derived from well logs. Where
 159 the data are recorded as slowness (us/ft) a conversion into velocity is required;

$$V_p \left(\frac{m}{sec} \right) = 10^6 * 0.3048 * \text{Sonic Log(us/ft)}$$

*EQUATION 5 – VELOCITY COMPRESSIONAL
FROM SONIC COMPRESSIONAL LOG DATA*

$$V_s \left(\frac{m}{sec} \right) = 10^6 * 0.3048 * \text{Shear Log(us/ft)}$$

*EQUATION 6 – VELOCITY SHEAR FROM
SHEAR SLOWNESS LOG*

160 1.4.2 Fluid physical properties

161 Physical properties for pore filling fluids for substitution into the pore space may be
162 determined from laboratory experiments (Salemi et al., 2018) or calculated theoretically using
163 equations of state (EoS) (Danesh, 1998). In this study, the fluid's physical properties were
164 calculated using the EoS models in the NIST Chemistry WebBook (1997). NIST used the
165 following equations of state, carbon dioxide (Span and Wagner, 1996), hydrogen (Leachman
166 et al., 2009), methane (Setzmann and Wagner, 1991). Reservoir conditions for the Helsby
167 Sandstone reservoir were taken from Yaliz and Taylor (2003), conditions for the Lemau were
168 taken from Anston-Race and Ganesh (2020), and conditions for the Bunter Sandstone were
169 taken from Gluyas and Bagudu (2020) (**Error! Reference source not found.**).

170 We assume carbon dioxide and hydrogen are in the supercritical phase at the described
171 reservoir conditions (NIST Chemistry WebBook, 1997; Okere et al., 2024) (Table 1), for
172 methane we model a pure dry pure system.

173 The bulk modulus of a fluid was calculated using the bulk density and speed of sound through
174 the medium as;

175

$$K_{fl} = \rho * v^2 \quad \text{EQUATION 7 – BULK MODULUS OF FLUID}$$

176

177 1.4.2.1 The Gassmann Equations

178 The Gassmann equation related the bulk modulus of the dry rock frame to the properties of
179 rocks in given in situ conditions,

$$K^* = \frac{K_{sat} \left(\frac{\Phi K_o}{K_{fl}} + 1 - \Phi \right) - K_o}{\frac{\Phi K_o}{K_{fl}} + \frac{K_{sat}}{K_o} - 1 - \Phi} \quad \begin{array}{l} \text{EQUATION 8 – GASSMANN - DRY} \\ \text{ROCK FRAME BULK MODULUS} \\ \text{CALCULATION} \end{array}$$

180

181 To calculate the dry rock frame's bulk modulus, the following parameters of the rock are
182 required: the bulk modulus of the mineral matrix, porosity, and the bulk modulus of the pore

183 filling fluid. To calculate the bulk modulus of the mineral matrix we can use the Voight-Reuss-
 184 Hill method (Smith et al., 2003):

$$K_o = \frac{1}{2}((F_1K_1 + F_2K_2) + \left(\left(\frac{F_1}{K_1} + \frac{F_2}{K_2}\right)^{-1}\right)) \quad \text{EQUATION 9 - VOIGHT-REUSS-HILL.}$$

185

186 where F_n is the mineral fraction and K_n is mineral bulk modulus of the mineral. The above
 187 implementation accounts for a two-mineral system. The gamma-ray log was used to calculate
 188 shale volume, and the non-shale volume assumed to represent the quartz volume to assume
 189 a 2-mineral system of quartz and clay. Shale volume was calculated as follows;

$$V_{sh} = \frac{GR - GR_{Matrix}}{GR_{Shale} - GR_{matrix}} \quad \text{EQUATION 10 - VOLUME SHALE}$$

190 While the investigated reservoirs are more complex than a 2-mineral system, the constitute
 191 minerals have a bulk modulus of similar orders of magnitude. The similarity allows the use of
 192 a mixing law, which provides sufficient accuracy for the Gassmann equation. This is due to the
 193 bulk modulus of the mineral matrix only having a minor effect on the bulk modulus of the
 194 whole rock (Darling, 2005).

195 Porosity can be derived from well-log data; in this study we use the neutron-density
 196 methodology (Kennedy, 2015);

$$\Phi_\rho = \frac{\rho_{matrix} - \rho_{Bulk}}{\rho_{matrix} - \rho_{fluid}} \quad \text{EQUATION 11 - DENSITY POROSITY}$$

197 The bulk modulus of the fluid and ρ_{fl} , the bulk density of the fluid, can be derived for a single
 198 fluid or a fluid mixture. Either can be calculated via;

$$K_{fl} = \left[\frac{S_w}{K_w} + \frac{(1 - S_w)}{K_{fn}} \right]^{-1} \quad \text{EQUATION 12 - BULK MODULUS OF FLUID MIXTURE}$$

199 and;

$$\rho_{fl} = S_w * \rho_w + (1 - S_w)\rho_{fn} \quad \text{EQUATION 13 - DENSITY OF FLUID MIXTURE}$$

200 Once the bulk modulus of the pore filling fluid mixture has been determined, the bulk
201 modulus of the mineral rock frame can be derived. With all constituent parts of the Gassmann
202 equation established, the new elastic properties of the fluid-substituted rock can be
203 calculated.

204 Along with the new bulk modulus of the fluid-substituted rock having, the bulk density of the
205 rock with the substituted fluids can be calculated with;

$$\rho_{\text{new}} = \rho_{\text{matrix}} * (1 - \Phi) + (\rho_{\text{fl}} * \Phi) \quad \text{EQUATION 14 – DENSITY OF FLUID}$$

SUBSTITUTED ROCK

206 Once the new bulk modulus and bulk density of the rock have been calculated, the new
207 compressional and shear velocities of the rock can be calculated by rearranging the equations
208 for bulk modulus and G, the shear modulus. Note that the shear modulus of the rock remains
209 unchanged despite fluid substitution;

$$V_p = \sqrt{\frac{K + \frac{4}{3}G}{\rho_{\text{bulk}}}} \quad \text{EQUATION 15 – VELOCITY}$$

COMPRESSIONAL FROM BULK AND
SHEAR MODULUS

$$G = \rho_{\text{bulk}} * V_s^2 \quad \text{EQUATION 16 – SHEAR MODULUS}$$

210 The equations used do not account for the carbon dioxide or hydrogen having been absorbed
211 by residual water at non-end member water saturations. Our methodology also does not
212 account for pore pressure changes, which can have effects on seismic responses (Bahmaei
213 and Hosseini, 2020). We assume a uniform heterogeneous matrix and uniform liquid
214 pathways. We assume the stored fluid (carbon dioxide or hydrogen) is fills the pore space as
215 a fluid and do not consider the precipitation of any fluid into the mineral phase, or dissolution
216 into brine.

217 1.4.3 Determining net reservoir

218 Reservoir cut-offs were used to define reservoir intervals within wells. Shale volume (V_{shale}),
219 porosity and bulk density were the chosen factors in determining which areas of the reservoir
220 were suitable (Table 2). A shale volume value of 30% was selected as the cutoff volume. The
221 bulk density values were chosen, as outside these ranges typically consisted of either A)

222 interbeds of low-density evaporites such as halite or B) interbeds of high-density evaporites
223 such as anhydrites or carbonates. A minimum porosity of 5% was chosen.

224 1.4.4 Stochastic modelling

225 A stochastic approach to implementing the Gassmann equations was adopted to quantify the
226 impact of the uncertainty in reservoir and fluid properties. This approach was implemented
227 using Python 3.10.13. In uncertainty quantification Monte Carlo methods have become
228 common place as they allow for the examination of a wide parameter space, can incorporate
229 different distributions for different parameters and outputs are probabilistic with a
230 quantification of uncertainties (Zhang, 2020). In the method developed the input properties
231 are derived from well logs. The elastic property inputs of the Gassmann equations were
232 defined as distributions derived from well data. The elastic properties of porous material can
233 be correlated (Appendix 1); hence, a multi-variate distribution was derived from the
234 properties (Castagna et al., 1993). Distributions were determined for defined porosity
235 intervals (Table 3). For a valid distribution to be defined, a minimum of 25 data points was
236 required, ensuring the shape of the distribution to be suitably characterised, and for the
237 avoidance of edge cases. The compressional velocity, shear velocity, porosity, bulk modulus
238 and shale volume were the required parameters to be derived from porosity-separated
239 distributions for the Gassmann equations. For each porosity of each formation investigated
240 (Table 3) there were 1,500 iterations of the model run. Our 'computationally low'
241 methodology takes ≈ 15 seconds to compute 1500 iterations of the Gassmann equations.
242 Multi-variate distributions were also created for the seal paired with the reservoir intervals.
243 The distribution for these was used within the AVO analysis, so the well data was used to
244 derive distributions for shear/compressional velocity and bulk density of the seals. Alongside
245 stochastic modelling we use the UQ(Py)Lab package for Python to undertake a sensitivity
246 analysis using the Solbol methods (Sobol', 1993; Marelli and Sudret, 2014). The output chosen
247 to investigate the sensitivity of the Gassmann equation was the new acoustic impedance of
248 the fluid-substituted rock. The use of sensitivity modelling allows for understanding which
249 parameters within the Gassmann equation have the most significant effect on the resultant
250 acoustic impedance.

251 1.4.4.1 Validation of parameters for stochastic modelling

252 While compressional and shear velocity and, bulk density, can be directly derived from the
253 data taken from the well logs, other parameters, notably porosity and bulk modulus of the
254 mineral matrix, must be calculated using transforms that relate to theoretical relationships.
255 Calculated porosity values for the Bunter Sandstone were checked against those from
256 measured core plug values (Appendix 11). 10 porosity measurements from core were
257 randomly sampled and compared with the calculate porosity at the same depth. The average
258 difference between the measured values and calculated values was found to be 11% (e.g. 20%
259 vs 22.2% porosity), which was determined to be reasonable.

260 To validate the calculated values for the mineral matrix bulk modulus, due to lack of other
261 independent data from which to compare, we used literature to determine typical mineral
262 percentages for the matrix and check against our shale volume and quartz volume estimates
263 (Howard et al., 2008; Scorgie et al., 2021; Qin et al., 2022). We assume a 2-mineral system, as
264 the only other main mineral within the system (apart from clays) is likely to be feldspar. The
265 average value for feldspars' bulk modulus is similar to that of quartz (37.5 vs 37), thus for this
266 use it was deemed suitable (Smith et al., 2003). We do not attempt to verify calculated bulk
267 modulus of the mineral matrix, K_0 , as even if exact values for the mineral matrix components
268 were available, there are high levels of variability between the two parameters, as shown by
269 Qin et al. (2022).

270 1.4.5 Seismic responses

271 Once the new elastic properties are calculated, the seismic response can be calculated. The
272 new reservoir elastic properties and associated seismic response of the fluid-substituted
273 reservoirs were calculated for water saturations from 100% to 0% in 10% increments. We
274 investigated the impact of hydrogen and carbon dioxide. We model methane (natural gas) as
275 a reference case.

276 1.4.5.1 Wedge modelling

277 Wedge models were created to model the seismic response at geological interfaces. The
278 wedge models were produced in Python using parts of the PySeisTuned 2.0 code base
279 (Dowdell, 2020). Two wedge models were created for each reservoir–seal pair investigated:
280 reservoir–reservoir interfaces and seal–reservoir interfaces. The wedge models used simple
281 three-layer geological models, which included an overburden, the reservoir wedge and the

282 underburden. The rock properties used in the wedge models were derived from the
 283 deterministic fluid substitution scenarios for the reservoir, and well logs for the original
 284 reservoir and seal properties. The acoustic impedance was calculated for each wedge section
 285 and, subsequently, the reflection coefficient at the wedge interfaces. A ricker wavelet with a
 286 frequency analogous to the seismic data that covers the area of the well data was used
 287 (Bunter formation = 35Hz, Helsby = 40Hz, Leman = 32 Hz). The wavelet was convolved with
 288 the reflection coefficient to generate a synthetic wedge model. The wedge models use the
 289 SEG standard polarity, where a negative reflection coefficient event shows a negative
 290 reflection event.

291 1.4.5.2 AVO Responses

292 Amplitude versus offset (AVO) analysis examines the change in reflection and transmission
 293 coefficient of an incident P-wave (compressional wave, V_p) as a function of the angle of
 294 incidence (Chopra and Castagna, 2014). For interface modelling and calculating the expected
 295 amplitude versus the offset of the seismic wave (AVO), the Zoeppritz's equations was used
 296 (Zoeppritz, 1919);

297

$$\begin{bmatrix} \cos\theta_{p1} & -\sin\theta_{s1} & \cos\theta_{p2} & \sin\theta_{s2} \\ \sin\theta_{p1} & \cos\theta_{s1} & -\sin\theta_{p2} & \cos\theta_{s2} \\ Z_1\cos 2\theta_{s1} & -W_1\sin 2\theta_{s1} & -Z_2\cos 2\theta_{s2} & -W_2\sin 2\theta_{s2} \\ \frac{V_{s1}^2}{V_{p1}}W_1\sin 2\theta_{p1} & W_1\cos 2\theta_{s1} & \frac{V_{s2}^2}{V_{p2}}W_2\sin 2\theta_{p2} & -W_2\cos 2\theta_{s2} \end{bmatrix} \begin{bmatrix} R_p \\ R_s \\ T_p \\ T_s \end{bmatrix} = \begin{bmatrix} \cos\theta_{p1} \\ -\sin\theta_{p1} \\ -Z_1\cos 2\theta_{s1} \\ \frac{V_{s1}^2}{V_{p1}}W_1\sin 2\theta_{p1} \end{bmatrix}$$

EQUATION 17 –THE ZOEPPRITZ (1919) EQUATIONS

298

299 The Zoeppritzs equations allow for the calculation of the reflected p-wave response at a
 300 geological interface with a set angle of incidence. For the application of the AVO equations to
 301 our data, we used the Python module Bruges by Agile-Scientific (2022) which is based on the
 302 methodology described by Dvorkin et al. (2014). Each generated value from the stochastic
 303 analysis of the reservoir response analysis (Section 1.4.4, 1500 values total) was used as an
 304 input into the Zoeppritz equations. Using the previously generated values, allowed for the
 305 range in possible AVO response values to be captured. Two separate geophysical responses
 306 were modelled, reservoir – reservoir contacts (water saturation 100% and water saturation

307 0%) and seal – reservoir contacts. The seal parameters used within the Zoeppritz were
308 generated from the seal multi-variate distributions (Section 1.4.4).

309 1.4.5.3 Timeshift analysis

310 As fluids within the pore-space affect the compressional and shear velocity properties of a
311 rock, they affect the travel time of seismic waves through the media and modify the recorded
312 responses in the seismic surveys (Dvorkin et al., 2014). Time-shift analysis involves identifying
313 the time variation between two seismic traces in the same location from different
314 acquisitions. These are typically taken pre-fluid injection/withdrawal (baseline) and after fluid
315 injection or withdrawal (monitor) (MacBeth et al., 2020). Two methods were used to
316 investigate the time shifts caused by fluid substitution, 1) Using a baseline and monitor
317 seismic trace generated from well data to measure the timeshift on actual geological data
318 and, 2) From stochastically generated compressional velocities for baseline and monitor
319 reservoir values to calculate Δt over various distances and water saturations.

$$\Delta t = z \left(\frac{1}{V'} - \frac{1}{V} \right)$$

EQUATION 18 TIME-SHIFT

ESTIMATION FROM MACBETH ET AL.

(2018)

320 1.5 Data

321 From the three chosen reservoir-seal pairs, the wells were selected based on the availability
322 of data. We prioritised wells that had bulk density, shear slowness, compressional slowness,
323 gamma ray and neutron porosity logs across reservoir intervals. This requirement for shear
324 slowness data limited well selection as it is not commonly acquired. The stratigraphic intervals
325 within the well logs were identified using the completion logs, which were available for each
326 well through the North Sea Transition Authority's National Data Repository
327 (<https://ndr.nstauthority.co.uk/>). For the wells used within this study, please view the
328 appendix.

329 Due to limited shear slowness data availability in wells from the Helsby and Bunter Sandstone
330 Formations, the parameter distributions are derived from a single well, whereas, for the
331 Leman, more wells had the required logs available, which allowed for distributions to be
332 derived from multiple wells. As the modelling of the Bunter Sandstone used a single well it
333 effectively investigates the vertical heterogeneity and uncertainty, while for the Leman

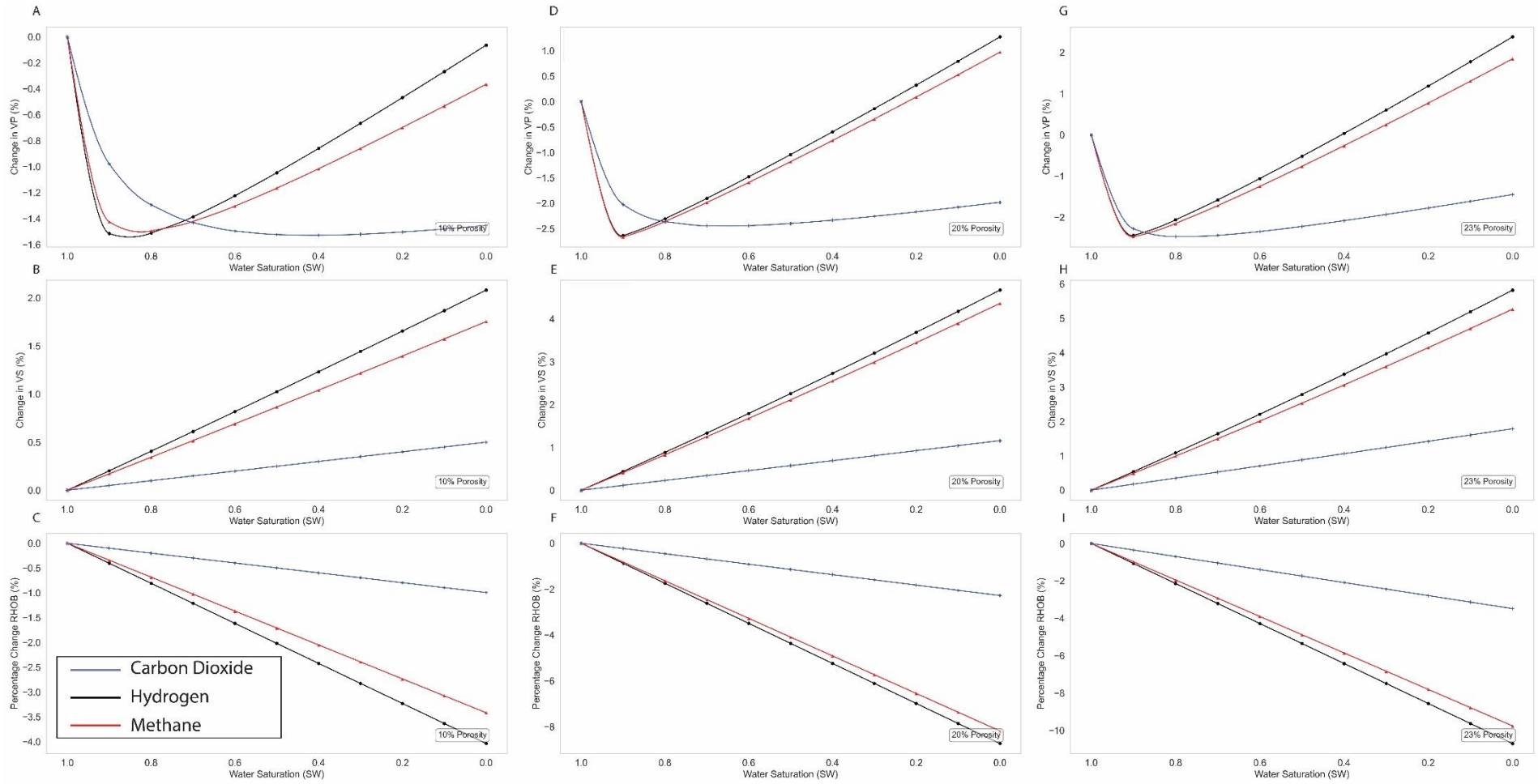
334 Sandstone that availability of data means the modelling effectively investigates the lateral
335 and vertical heterogeneity.

336 1.6 Results

337 1.6.1 Reservoir Responses

338 1.6.1.1 Response to different fluids (Deterministic)

339 The change in water saturation from 100% – 80% for all fluids and reservoirs shows a sharp
340 initial drop in compressional velocity, however, after this initial drop, compressional velocity
341 begins to increase (Figure 3). Hydrogen and methane in all reservoirs increase the
342 compressional velocity beyond the initial value at between 40% - 20% water saturation.
343 However, after an initial drop the compressional velocity due to carbon dioxide increases at
344 a proportionally slower rate than that of hydrogen and methane, in each scenario. The
345 compressional velocity for each reservoir never increases over the initial value for carbon
346 dioxide.



347

348 *FIGURE 3 DETERMINISTIC ELASTIC RESPONSES OF THE LEMAN (A-C), BUNTER (D-F), HELSBY (G-I). GRAPHS A,D,G SHOW % CHANGE IN COMPRESSION VELOCITY, B,E,H SHOW % CHANGE IN*

349 *SHEAR VELOCITY AND C,F,H SHOW % CHANGE IN BULK DENSITY*

350

351 The change in shear velocity for all reservoir fluid combinations is a positive linear increase
352 (Figure 3). There are differences amongst the fluids however. Hydrogen in all scenarios has
353 the greatest increase, with methane showing similar increases. Carbon dioxide has the lowest
354 increase in shear velocity overall for all scenarios. As the porosity of the reservoir has
355 increased so has the % increase of shear velocity (Figure 3).

356 Change in bulk density is a negative linear trend for all scenarios. This occurs as the substituted
357 fluids all have densities lower than water (Figure 3). Substitution of carbon dioxide into the
358 pore space causes a smaller percentage change to the bulk density than hydrogen, due
359 densities at reservoir conditions. The higher porosity reservoir undergoes the highest
360 percentage change to bulk density because there is more pore space for the less dense fluids
361 into which they can be substituted.

362 The sensitivity analysis of the Gassmann equation for calculating acoustic impedance shows
363 that it is most sensitive to a change in compressional velocity, with a first-order index value
364 of 78% and a total Sobol index of 53% (Figure 4). Moderate sensitivity to both porosity and
365 density is indicated, with first order results being 20.7 % and 20.4 % and total order indexes
366 being 4.9 % and 5.5 % respectively. The equation is not sensitive to shear velocity or the
367 mineral matrix composition.

368 1.6.1.2 Stochastic analysis of geophysical responses

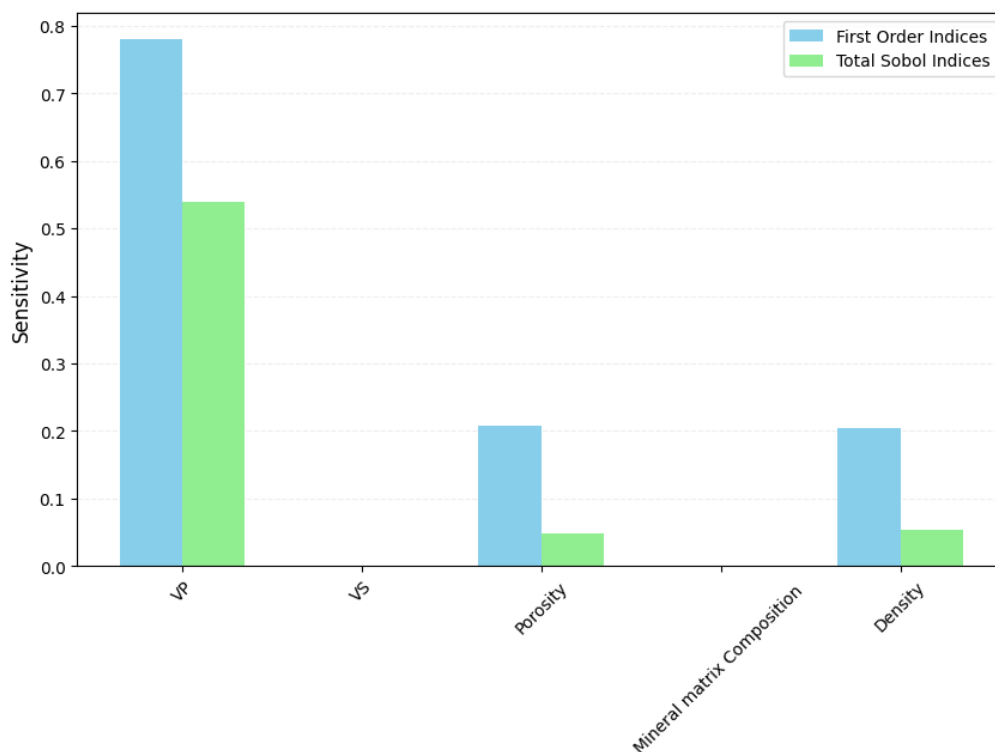
369 We concentrate on describing the results of the fluid substitution at 20% water saturation, as
370 this is likely the near maximum value possible for subsurface storage sites (Yan et al., 2018).
371 The Lemman data set was split into seven porosity groups with a 2% porosity interval from 7%
372 to 19% (Table 3). Increasing the proportion of hydrogen results in a greater acoustic
373 impedance change than for the equivalent carbon dioxide at each porosity interval. The
374 largest change in acoustic impedance for 20% water saturation for both hydrogen and carbon
375 dioxide occurred at 19% porosity, being -12.7% and -9.2% respectively (Figure 5). Hydrogen
376 has a much sharper initial decrease in acoustic impedance compared with carbon dioxide
377 (Figure 5).

378 For the Bunter Sandstone, the p50 results, hydrogen is shown to modify the acoustic
379 impedance a greater amount than carbon dioxide, at 27% porosity and 20% water saturation.
380 The effect change for these reservoir parameters on acoustic impedance for hydrogen is -9.8%

381 and for carbon dioxide it is -6.7%. The trend is the same as those in the deterministic reservoir
382 responses (Figure 6) with hydrogen having a sudden drop at 90% water saturation and then a
383 relatively continuous linear decrease, whereas carbon dioxide has a more pronounced curve
384 to its trend in decreasing acoustic impedance (Figure 6). The minimum response for hydrogen
385 and carbon dioxide in the p50 values is both at the lowest porosity, 19%, where at 20% water
386 saturation, hydrogen has an acoustic impedance change of -6.2% and carbon dioxide has a
387 negative change of -4.2%.

388 The results for the Helsby Sandstone follow the same trends as the Bunter data, with higher
389 porosities having a larger effect on acoustic impedance and hydrogen also having a larger
390 effect. At 26% porosity and 20% water saturation, hydrogen fluid substituted sample showed
391 a change in acoustic impedance of -10.4%, while carbon dioxide was -6.5%. At the lowest
392 porosity, 14%, the change in acoustic impedance at 20% water saturation was -2.8% for
393 hydrogen and -1% for carbon dioxide.

394

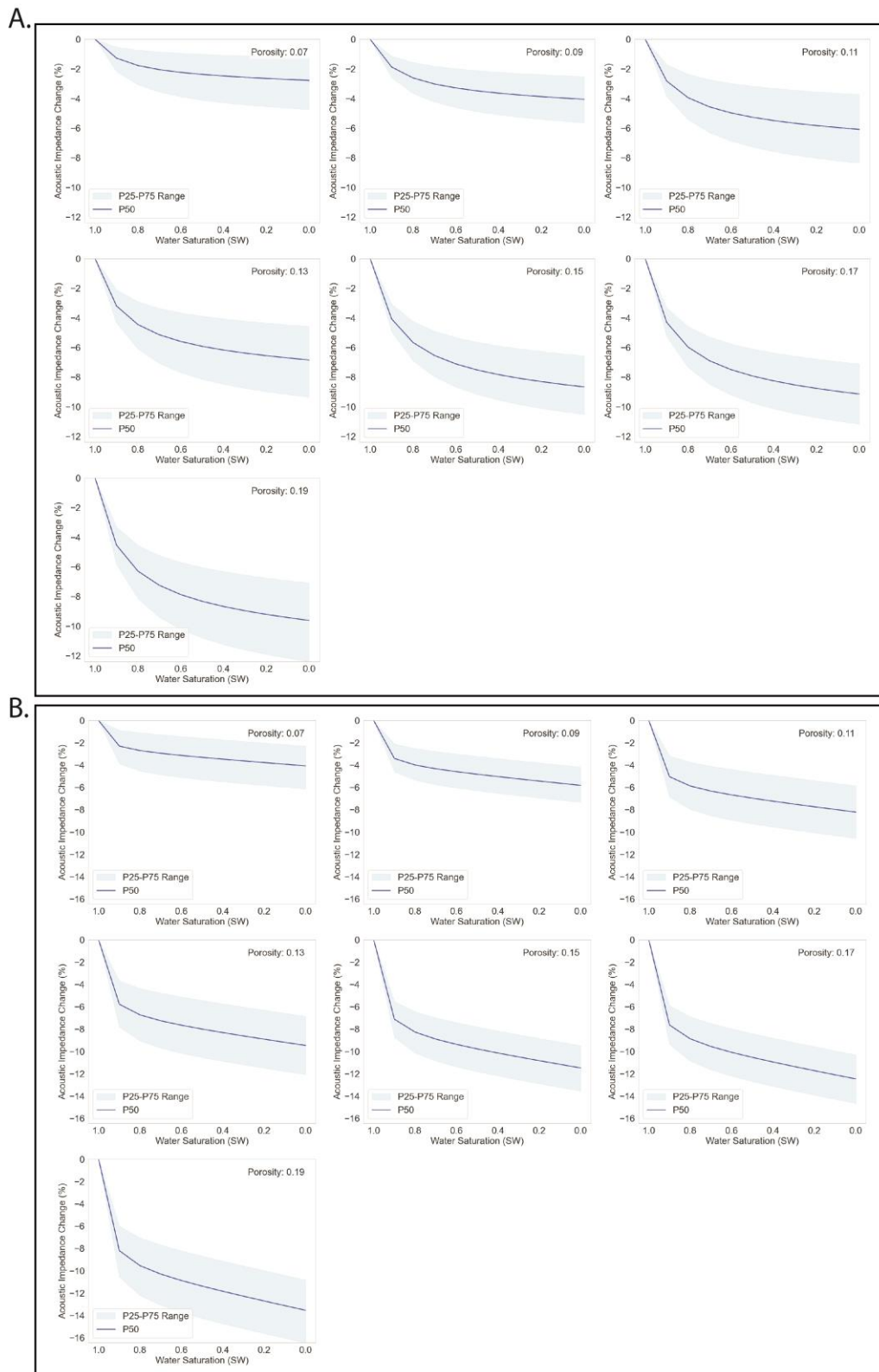


395

396 *FIGURE 4 SOBOL SENSITIVITY ANALYSIS RESULTS FOR THE PARAMETER INPUTS DERIVED FROM WELL LOG DATA ON THE*

397 *GASSMANN EQUATION FOR THE COMPUTATION OF THE ACOUSTIC IMPEDANCE.*

398



399

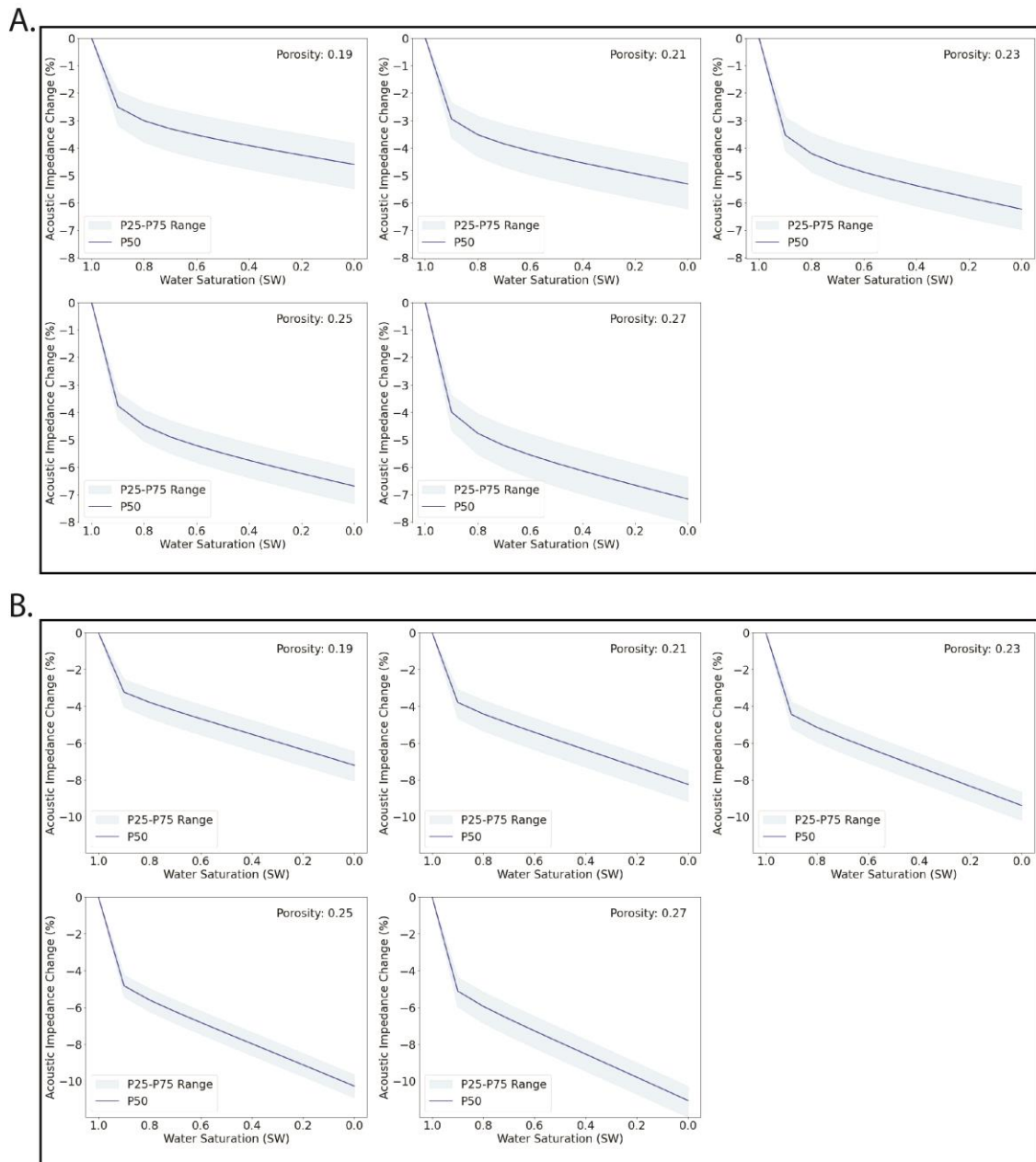
400 FIGURE 5 LEMAN STOCHASTIC ACOUSTIC IMPEDANCE MODELS FOR VARYING POROSITY VALUES AFTER FLUID SUBSTITUTION

401 FOR FLUIDS. A) CARBON DIOXIDE, B) HYDROGEN

402

403

404



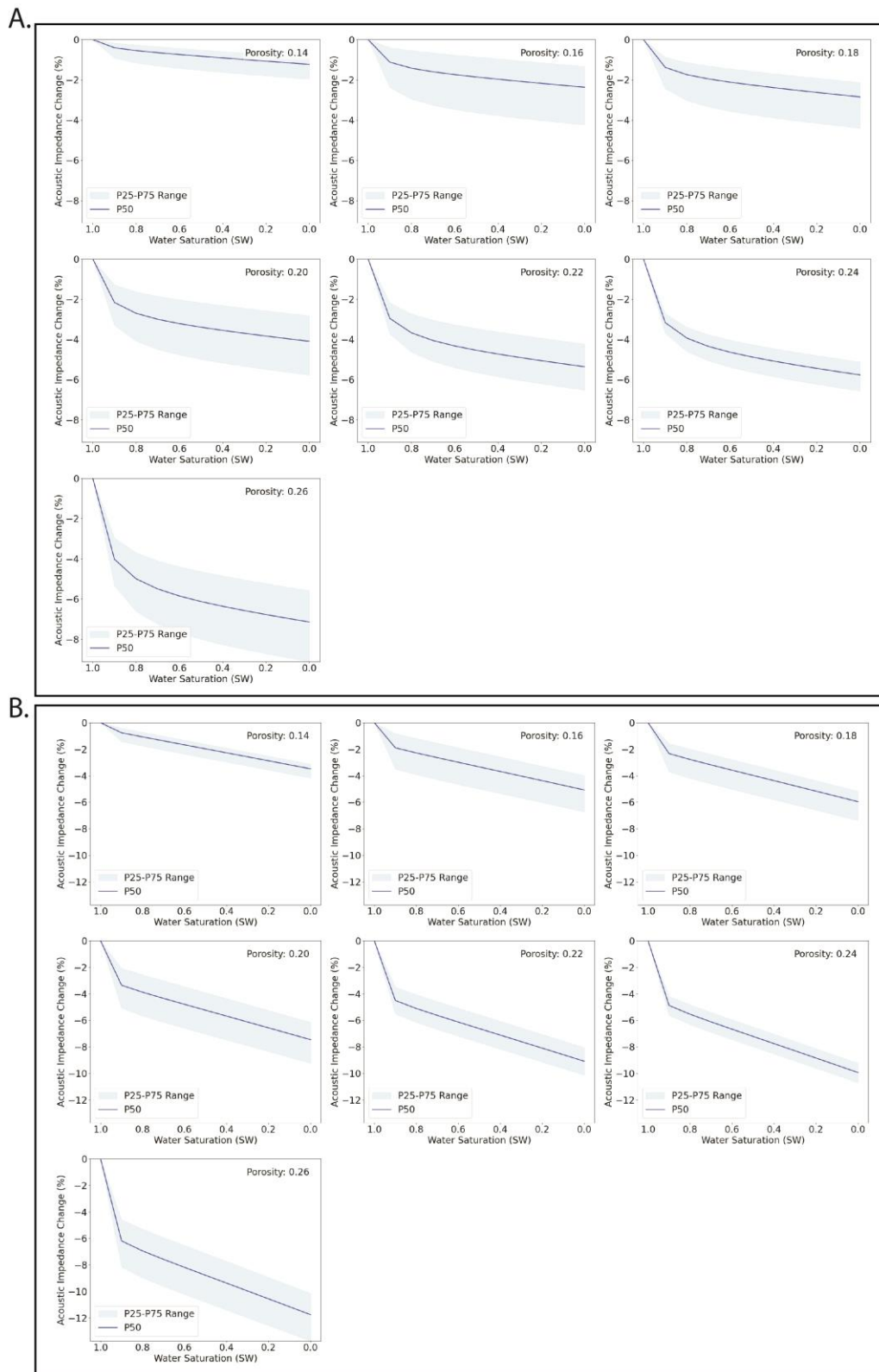
405

406 *FIGURE 6 BUNTER STOCHASTIC ACOUSTIC IMPEDANCE MODELS FOR VARYING POROSITY VALUES AFTER FLUID*

407 *SUBSTITUTION FOR FLUIDS. A) CARBON DIOXIDE, B) HYDROGEN*

408

409



410

411 FIGURE 7 HELSBY STOCHASTIC ACOUSTIC IMPEDANCE MODELS FOR VARYING POROSITY VALUES AFTER FLUID

412 SUBSTITUTION FOR FLUIDS. A) CARBON DIOXIDE, B) HYDROGEN

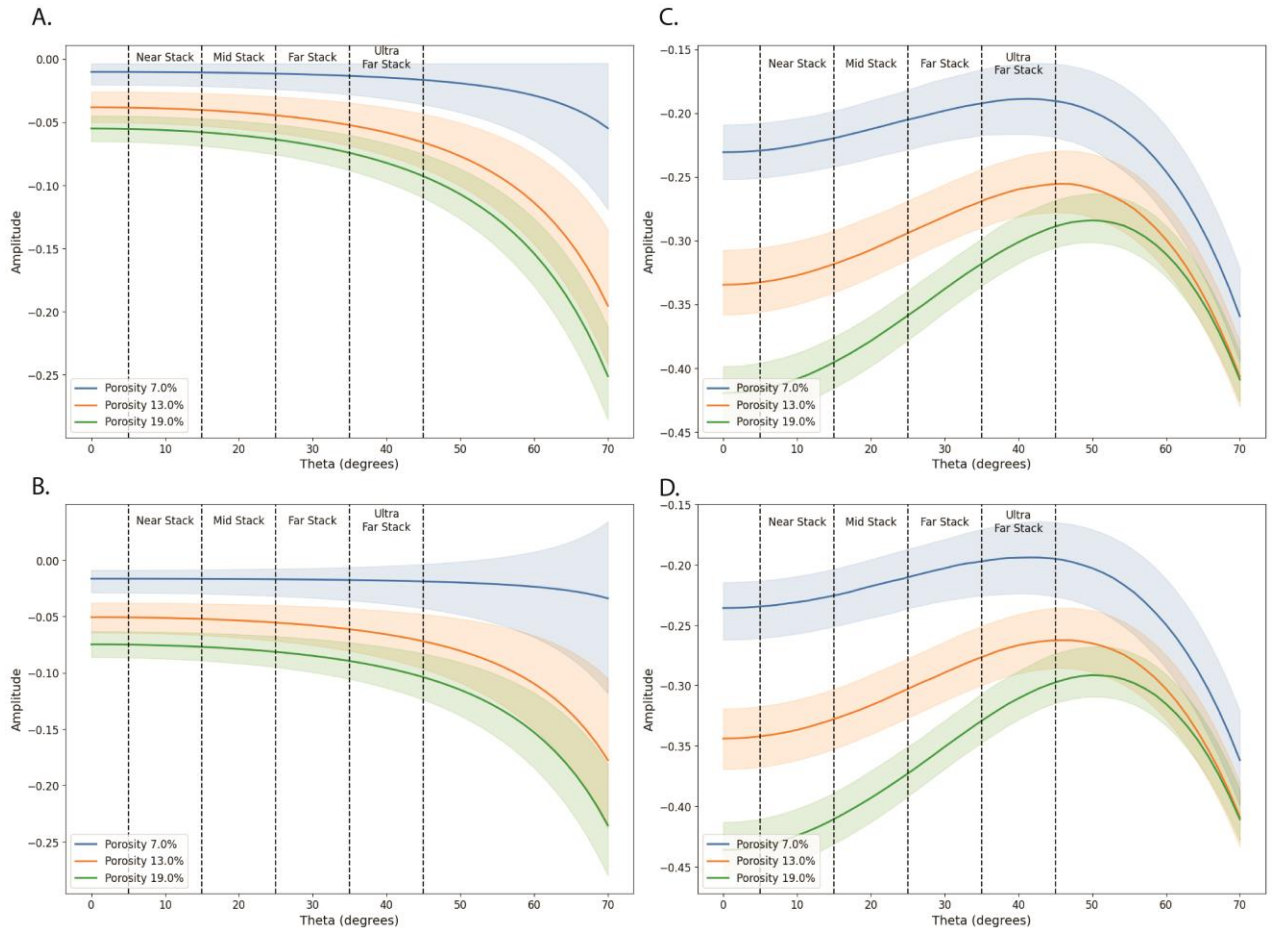
413 1.6.2 AVO responses

414 Figure 8 shows the modelled AVO responses for the reservoir–reservoir and reservoir–seal
415 interface for the Leman Sandstone at 7%, 13% and 19% (other values in Appendix 12 - 17).
416 The reservoir-reservoir interface shows small decreases in the amplitude for typical changes
417 in the recorded reflection offsets from seismic data, however these small decreases do result
418 in large percentage changes, for example at 19% porosity, the amplitude at 5° is -0.072 and
419 at 45° the amplitude is -0.097, a change of -35.6%. More notable differences in amplitude
420 occur at offset angles which are greater than that which would typically be recorded with a
421 conventional seismic survey (45°+), and this is common for all porosities. However, for the
422 reservoir–seal interface there are noticeable differences to the amplitude at typical survey
423 offsets for all porosities. The largest change as offset increased was for the 19% porosity seal-
424 reservoir interface, where from 5° (near stack) to 45° (ultra far stack) there was a relative
425 amplitude change of +0.14.

426 As the Bunter Sandstone has two possible seals within the Southern North Sea, halite and
427 claystone, both interface lithologies were modelled for their AVO response (Figure 9). For the
428 reservoir-reservoir interface AVO analysis, both carbon dioxide and hydrogen results show
429 moderate to minor differences in amplitude with an increase in offset from the near stack to
430 the ultra-far stack with a difference of 17.0 - 18.7% and 5.9 – 4.7% (7 – 19% porosities)
431 respectively. The amplitude difference for the carbon dioxide filled reservoir is smaller with
432 an increasing offset, with the most noticeable change occurring at offsets of +50° where
433 amplitudes decrease rapidly. The inverse is true for hydrogen, where there is a minor increase
434 in amplitude for all porosities throughout increasing offset, with the most notable changes
435 being large increases again after +50°. The evaporite seal–reservoir interface shows very
436 similar results for both hydrogen and carbon dioxide (Figure 6). Minor amplitude differences
437 are apparent; however these do not impact the trend of the amplitude differences. The
438 claystone seal model again has similar results for both carbon dioxide and hydrogen, with only
439 minor amplitude differences up until reaching the ultra-far offset values. At the ultra-far offset

440 values, the lower porosities amplitude falls, whereas the higher porosity values increase
 441 slightly.

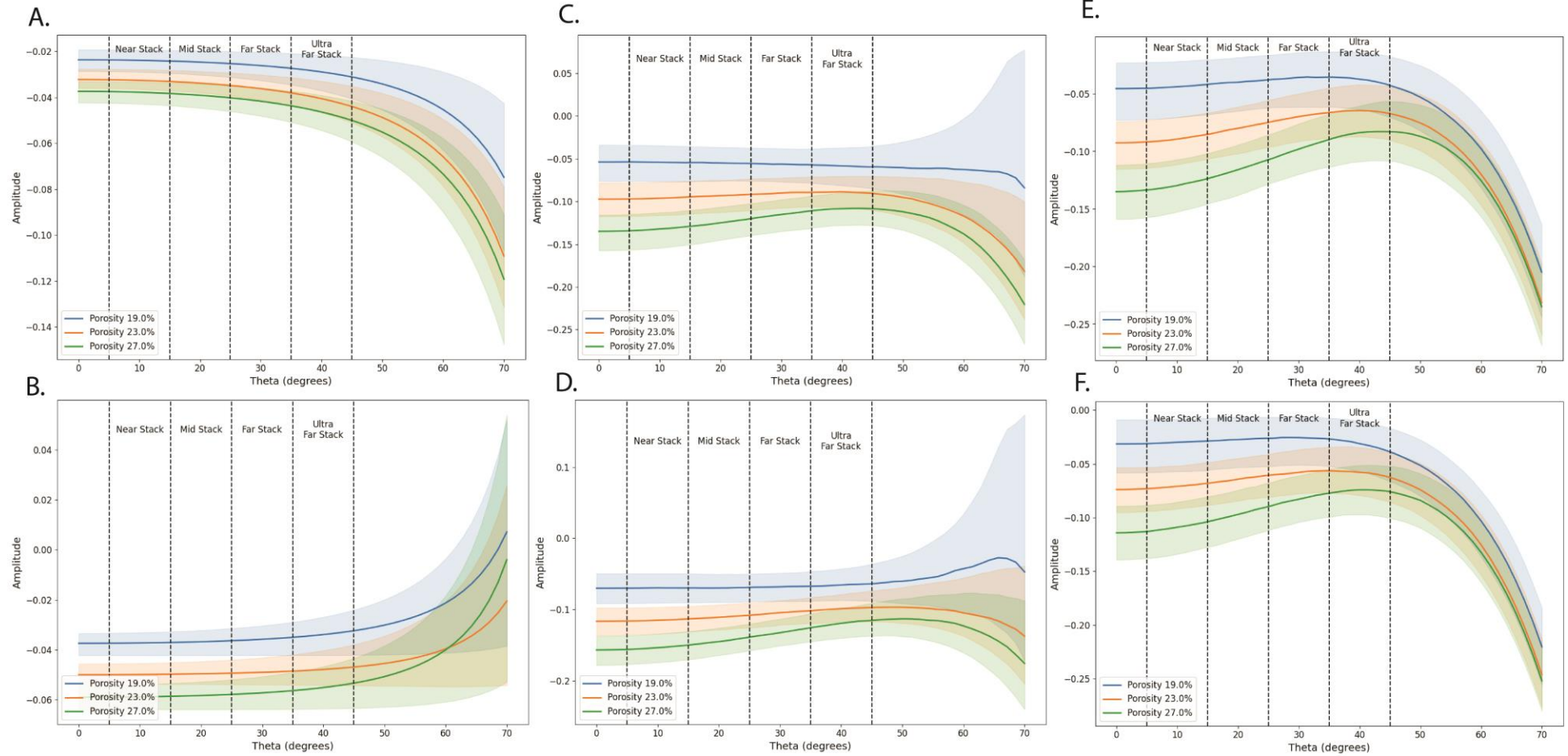
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443

444 *FIGURE 8 LEMAN AMPLITUDE VERSUS OFFSET FOR RESERVOIR-RESERVOIR INTERFACE FOR (A) CARBON DIOXIDE AND (B)*

445 *HYDROGEN. SEAL-RESERVOIR INTERFACE FOR (C) CARBON DIOXIDE AND (D) HYDROGEN*



446

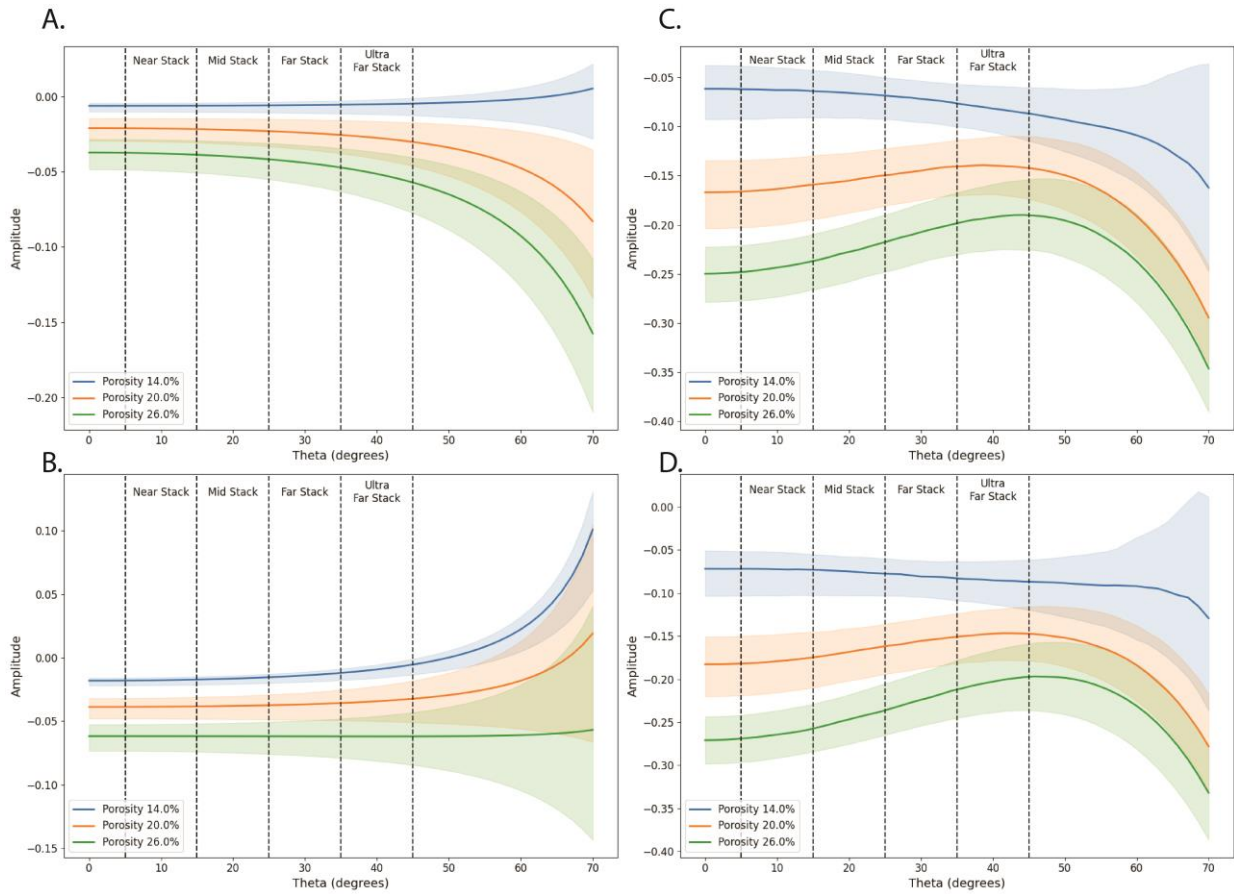
447 FIGURE 9 BUNTER AMPLITUDE VERSUS OFFSET FOR RESERVOIR-RESERVOIR INTERFACE FOR (A) CARBON DIOXIDE AND (B) HYDROGEN. SEAL-RESERVOIR (EVAPORITE) INTERFACE FOR (C)

448 CARBON DIOXIDE AND (D) HYDROGEN. SEAL-RESERVOIR - (CLAYSTONE) INTERFACE FOR (E) CARBON DIOXIDE AND (F) HYDROGEN.

449 The results for the Helsby Sandstone show a minor difference of decreased amplitude for the
450 reservoir–reservoir interface for carbon dioxide and a minor increase for hydrogen in the
451 typically recorded offset ranges (Figure 10). At large offsets (+45°), the carbon dioxide
452 reservoir – reservoir interface shows a decreased value for amplitude for every porosity
453 except for the 14% porosity values, which increase. Hydrogen results show all amplitudes
454 increase at these offsets at greater than 45°, with the lowest porosity, 14%, showing the
455 greatest increase. For the carbon dioxide seal-reservoir interface, an increase in amplitude
456 from low to high offsets is observed for all porosities. This increase in relative amplitude peaks
457 in the range of 50°- 60°, after which it falls rapidly. For hydrogen the results for higher
458 porosities are like that of the carbon dioxide, however, for the lower porosities, notably 14%,
459 a gradual decrease in relative amplitude occurs, with a greater drop off offsets of 65°+ (Figure.
460 8).

461 1.6.3 Interface modelling

462 Reservoir-seal and reservoir-reservoir interfaces were modelled for the Bunter Sandstone for
463 hydrogen and carbon dioxide (Figure 11). All models show initial constructive interference at
464 wedge thicknesses <10 ms. All models show the onset tuning to occur at a wedge thickness
465 of 14 ms, after which constructive interference occurs. The reservoir-seal interfaces both have
466 onset tuning thickness of 28 ms, while the reservoir-reservoir interfaces onset tuning
467 thickness is 29 ms. The interface wedges for hydrogen (Figure 11 E,F) show higher amplitude
468 values than those for carbon dioxide (Figure 11 C,D).

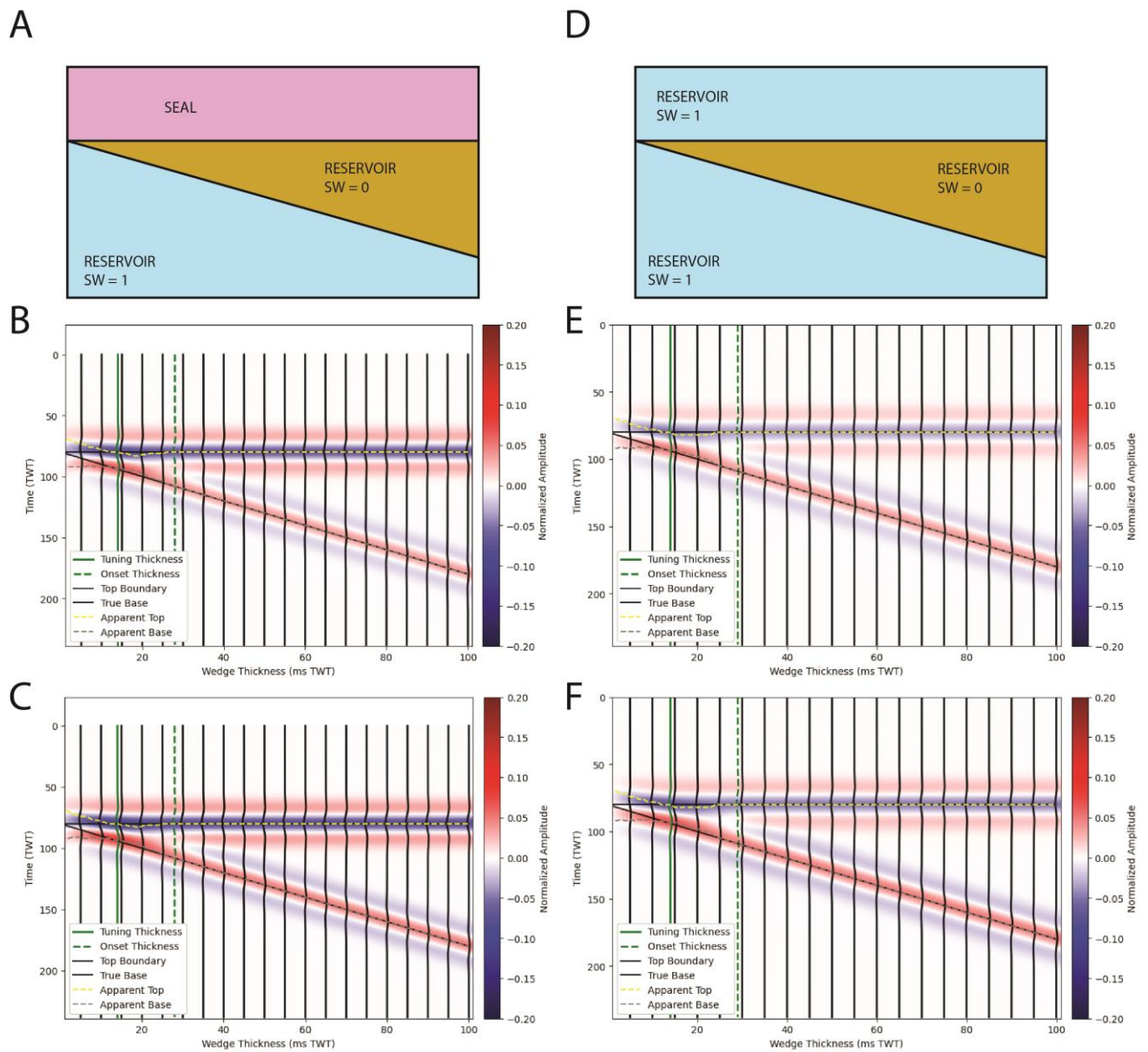


469

470 *FIGURE 10 HELSBY AMPLITUDE VERSUS OFFSET FOR INTERFACE FOR (A) CARBON DIOXIDE AND (B) HYDROGEN. SEAL-*

471 *RESERVOIR INTERFACE FOR (C) CARBON DIOXIDE AND (D) HYDROGEN*

472



473

474 *FIGURE 11 INTERFACE SEISMIC WEDGE MODELS. A) 2D BLOCK DIAGRAM OF GEOLOGY SIMULATED FOR B AND C. B)*

475 *RESERVOIR SATURATED WITH CARBON DIOXIDE (C) HYDROGEN. D) BLOCK DIAGRAM OF SIMULATED GEOLOGY FOR E AND*

476 *F. E) RESERVOIR SATURATED WITH CARBON DIOXIDE, (F) HYDROGEN. FREQUENCY USED FOR WAVELET IS 35HZ*

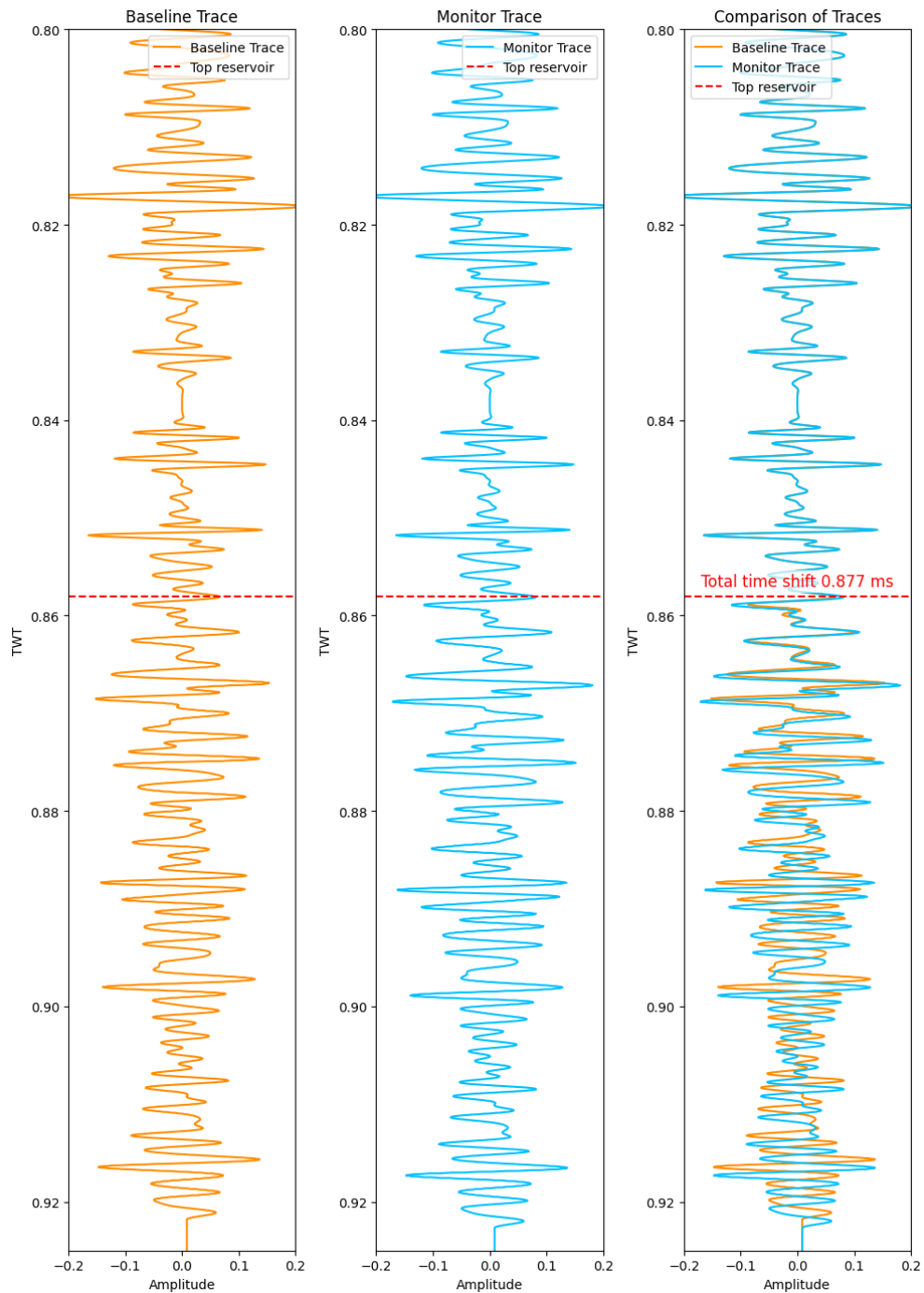
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479 1.6.4 Time Shift

480 Synthetic seismic traces were calculated for the Bunter Sandstone from well log data (well
481 42/25-d3, 130 m section of reservoir). Traces were made for pre and post-fluid-substitution
482 (20% water saturation) of carbon dioxide to act as baseline and monitor seismic traces. Figure
483 12 shows the monitor, baseline, and an overlay for the synthetic seismic well traces from the
484 Bunter Sandstone well for carbon dioxide. A positive timeshift for the monitor initiates at the
485 top of the reservoir when brine is replaced with carbon dioxide, with a shift in seismic traces
486 (Figure 12). The difference in TWT at the bottom of the reservoir is 0.877 ms over the reservoir
487 interval of 130 m. Time shifts for the Bunter Sandstone were calculated using the velocity
488 values generated from the gassmann equations during the stochastic fluid substitution
489 analysis in section 5.1.2 (equation 16).

490 Initial low water saturations (0.7,0.8) show the greatest timeshift over any set unit thickness,
491 with the p50 value at 0.7 having a timeshift of 2.46 ms for 250 m (Figure 12). This aligns with
492 the values seen in section 4.1.2 where large decreases in V_p are initially observed at relatively
493 high-water saturation values (Figure 3). Extrapolating values to match the reservoir thickness
494 in Figure 12, at 0% water saturation and a 130 m reservoir, the calculated timeshifts are 0.93
495 ms for the p50, 0.64 ms for the p25 and 1.11 ms for the p75. This locates the calculated value
496 from the log derived timeshift (0.72 ms) within the range of provided values.



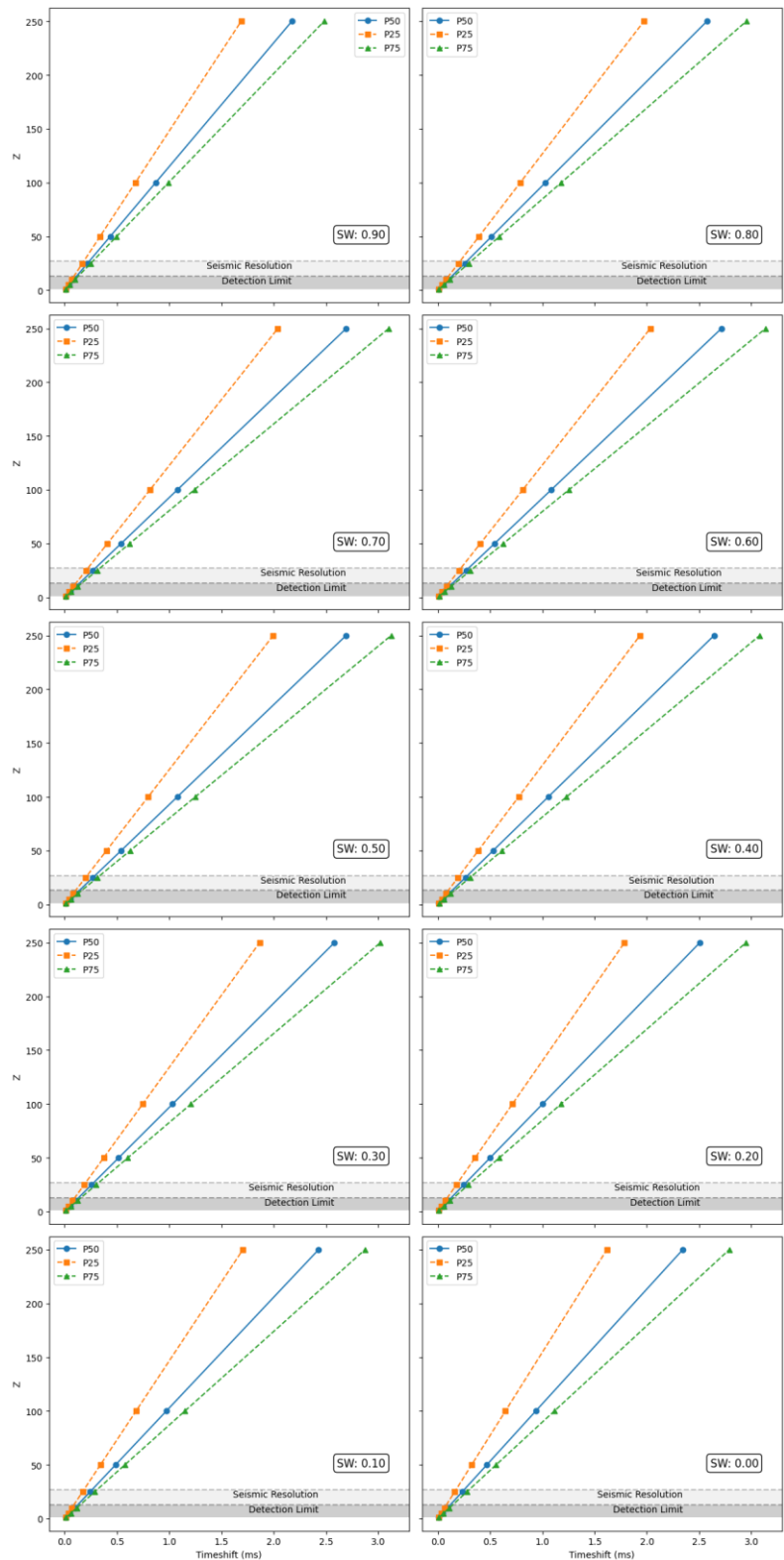
497

498 *FIGURE 12 BUNTER RESERVOIR INTERVAL FROM WELL 42/25-D3 (RED LINE = TOP OF RESERVOIR). (A) BASELINE*

499 *SYNTHETIC SEISMIC LOG, (B) MONITOR SYNTHETIC SEISMIC LOG AFTER GASSMANN FLUID SUBSTITUTION 100% CARBON*

500 *DIOXIDE SATURATION. (C) A + B OVERLAIN ONE ANOTHER FOR VISIBLE TIMESHIFT COMPARISON*

501



502

503 *FIGURE 13 SYNTHETIC TIMESHIFT MODELS FOR THE BUNTER SANDSTONE. 90% – 0% WATER SATURATION IS MODELLED*

504 *FOR A THICKNESS OF 0 – 250. P25, P50 AND P75 VALUES ARE INCLUDED. THE RESOLUTION (27 M) AND DETECTION LIMIT*

505 *(13 M) OF THE SEISMIC FOR THIS WELL AND DEPTH ARE INCLUDED.*

506 1.7 Discussion

507 1.7.1 Results

508 The results from the stochastic modelling of the storage reservoirs are expected to exhibit a
509 decrease in acoustic impedance when brine is replaced by either carbon dioxide or hydrogen
510 (Figure 5,7). For all reservoir intervals, higher porosities result in a greater change to acoustic
511 impedance. Between the reservoir formations, for the same porosity, for example 19%
512 porosity for the Leman and Bunter Formations, there are large differences to the change in
513 acoustic impedance values, for the Leman, a p50 of 9.2% and for the Bunter a p50 of 4.2% at
514 20% water saturation (Figure 5,6).

515 The acoustic impedance results for the Bunter Sandstone have a narrower range for the p25
516 and p75 results compared with both the Leman and Helsby examples (Figure 6-8). The
517 difference in ranges for outputs is likely the result of two factors. Firstly, the input data for
518 both the Leman and Helsby multivariate distributions shows a much larger range of values,
519 and a higher quantity of outliers present than compared with the Bunter values (Figure 14).
520 The wider ranges of generated values from the multivariate distributions coincide with
521 formation and porosity intervals with large p25 – 75 ranges for acoustic impedance results,
522 for example the Leman 13% porosity and Helsby 22% porosity interval (Figure 5,6,14).
523 Secondly, the increase in pore-fluid being substituted led to large ranges within the output
524 results. Every output result for change in acoustic impedance shows a significantly lower
525 range in output values for the initial 100% – 70 % water saturation, with saturations from 70%
526 – 0% showing increased ranges for the p25 – p75 values. It is likely the increased variation in
527 ranges for results shown for acoustic impedance is from a combination of these effects.

528 1.7.2 Comparison with published results

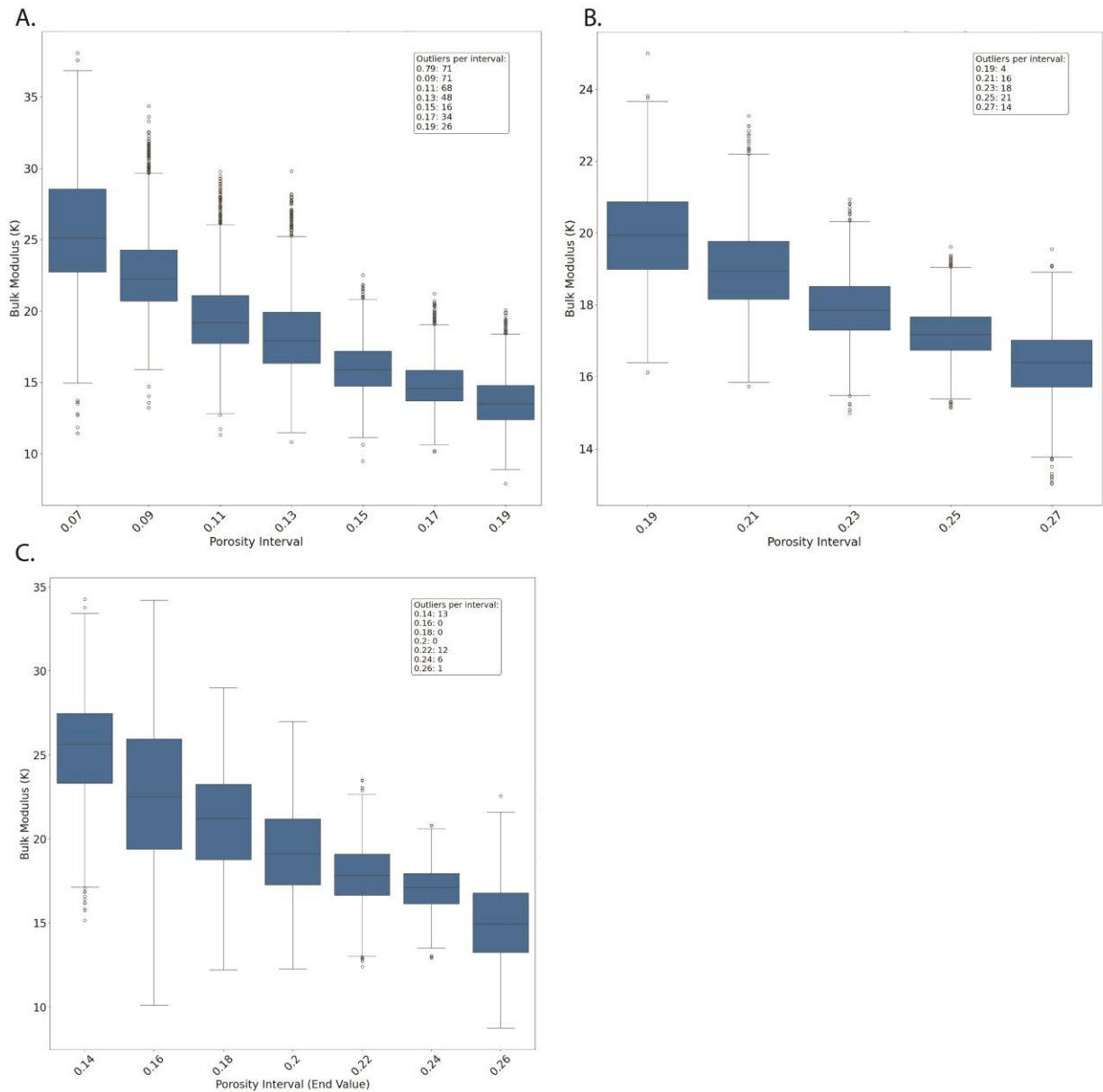
529 We discuss the results of our modelling with other published results for the same reservoir
530 storage formations. Our results (Table 4) show different values to those given in reports on
531 monitoring of the stratigraphy we investigated, notably to James et al. (2016b) for the Leman,
532 to Green and Grammer (2016) for the Helsby and to BEIS (2021) for the Bunter Sandstone.
533 Seismic monitoring is a valid technique to monitor migration pathways for carbon dioxide
534 using change of acoustic impedance. However, the properties unique to the rock being
535 monitored may mean that the change in elastic properties is below that of the detection limit
536 of the seismic data. As a rule of thumb, an acoustic impedance contrast of 4% is required for

537 a 4D seismic survey to detect the change in a feature (Lumley and Behrens, 1998). Table 4
538 shows that the predicted acoustic response from the Leman is well above this 4% boundary,
539 however the Bunter is only just above this boundary and the Helsby is < 4% boundary. As the
540 cited sources did not provide the parameters used within their workflow or the output
541 models, direct comparisons with the results presented in this study are difficult. Had such
542 data been given in a readily accessible data base more in-depth comparisons could have been
543 concluded.

544 While changes in acoustic impedance values in seismic data can aid in the monitoring of
545 subsurface fluid migration, utilising the changes to seismic amplitude with different seismic
546 reflection offsets, utilising different qualities within the same dataset, may aid in further
547 detecting the change in acoustic impedance and provide more informative results for carbon
548 dioxide plume monitoring. For example, both the Leman and the Bunter Sandstone (Table
549 3, Figure 8,9) show larger % changes for the reflection coefficient and hence amplitude at the
550 interface of reservoir – reservoir and seal – reservoir than the % increase when calculating
551 just acoustic impedance change (Table 3).

552 The results of timeshift analysis also indicate notable variations in reflection two-way-time
553 because of changes in fluid saturations (Figure 13). The plotted detection limit (13 m) and
554 seismic resolution (27 m) show that at the detection limit, the resolvable timeshift values
555 range from 0.09 ms to 0.11 ms, and for the seismic resolution, the timeshift values vary from
556 0.22 ms to 0.27 ms. Typical detection limits for timeshift values reported from separate
557 monitor seismic surveys range from 0.1 ms – 2 ms in literature (MacBeth and Izadian, 2023).
558 The calculated timeshift of 0.8 Sw is 0.77 ms for the Bunter Sandstone from well 42/25d-2
559 (Figure 12), and is therefore likely detectable on a monitor seismic survey. However, this
560 timeshift occurs from a 130 m reservoir thickness interval, as such reservoir thickness below
561 the suggested timeshift detection limit (13 m) may not be detectable in a monitor survey.

562 The relatively positive findings from our study, however, do not excuse the literature sources
563 for failing to give quantifiable inputs and results for their fluid substitution modelling and
564 analysis. If the cited sources are supportive of seismic monitoring and such methods are
565 proposed for large-scale infrastructure projects, there should be stringent evidence supplied
566 in a repeatable and reliable manner, as shown in this study.



567

568 *FIGURE 14 BOX PLOTS BULK MODULUS FOR POROSITY INTERVALS FROM MULTIVARIATE DISTRIBUTIONS FOR A) LEMAN,*

569 *B) BUNTER, C) HELSBY*

570

571 The reproducibility and reliability of methods for subsurface monitoring is important for
 572 subsurface infrastructure projects, as it allows for evaluation of results to be more efficient
 573 and undertaken reliably, strengthening evidence for proposed projects (Steventon et al.,
 574 2022). However, a common theme regarding site specific subsurface storage, is the lack of
 575 data supplied to allow for results to be seen as both reproducible (same data same
 576 methodology), or reliable (same data different methodology). While best efforts were made

577 to replicate the results of those published in literature (Table 4), this was not possible (Green
578 and Grammer, 2016; James et al., 2016a, 2016b; BEIS, 2021). While we cannot comment on
579 which results are more accurate, we can provide all data and the methodologies we use so
580 that the results shown are reproducible and method replicable.

581 1.7.3 Stochastic simulations

582 The stochastic approach enabled the capture of variation in reservoir properties that is
583 common across storage sites (Gibson-Poole et al., 2024). While this approach was taken for
584 reasons of practicality and data availability, the two types of data set used have differing
585 implications for the results from one another. For a dataset that contains more than one well,
586 the results will be more representative of the target stratigraphy throughout the whole area.
587 As the multi-variate distributions are derived from several wells within the same area, the
588 variance in elastic properties of the target stratigraphy, and different logging tools are
589 accounted for and incorporated within the model. For single-well datasets, while the results
590 are not as applicable to a regional area, the stochastic approach taken does provide valuable
591 insights into the uncertainty prediction for a highly localised area in and around the wellbore.
592 Value is also gained when comparing the two datasets, using a wider range of data from which
593 to generate distributions from allows for an indication of how reservoir heterogeneity may
594 impact fluid substitution and hence seismic response.

595 1.7.4 Implications for hydrogen exploration and storage

596 While proposed native hydrogen source rock settings typically involve basement rocks and
597 non-sedimentary basin-based processes, these generation pathways do not exclude the
598 possibility of a sedimentary reservoir overlaying potential generation processes, and hence
599 acting as a reservoir for the migration of native hydrogen into them (Jackson et al., 2024).
600 Understanding the potential seismic response of hydrogen in porous materials can have
601 applications in exploration in sedimentary sequences.

602 Our work shows that through forward modelling hydrogen, the elastic properties of a rock
603 saturated with hydrogen are affected similarly to methane (natural gas) (Figure 3). Thus,
604 geophysical exploration workflows used for predicting the likelihood of gas may be applicable
605 to native hydrogen exploration.

606 Hydrogen in pore space gives a larger acoustic impedance change than carbon dioxide (Figure
607 5). This has implications for storage and management of hydrogen within the subsurface, as
608 is proposed for areas of the UKCS or in salt caverns (Jahanbakhsh et al., 2024). Time-lapse
609 (4D) seismic data can afford a valuable method for the monitoring of storage complexes
610 (Morgan et al., 2020). Our work agrees with other more computationally intensive methods
611 (e.g. Gao et al. (2024)) that ideally should be modelled and chosen, such that hydrogen within
612 the pore space enables the 4% change in acoustic impedance required for 4D seismic
613 detection. Hydrogen also shows greater change in AVO than carbon dioxide emphasising the
614 need for careful survey design when consider time-lapse (4D) seismic for monitoring potential
615 storage sites or detecting natural accumulations. We did not examine possible time shifts
616 from hydrogen substituted into a sandstone reservoir. However, as hydrogen causes
617 compressional velocity increases at relatively high water saturations (+80%) (Figure 3), we
618 would expect a similar timeshift to that shown in Figure 12 and 13.

619 1.7.5 Future work and limitations

620 While the injection phase of carbon capture sites is typically expected to last decades, the
621 migration and chemical reactions of carbon dioxide in the subsurface will continue for far
622 longer (Metz et al., 2005). Most modelling scenarios consider carbon dioxide in the super
623 critical phase just after injection, over longer time scale (>50 years) considerations need to be
624 given to carbon dioxide dissolved within brine and any mineral precipitation. While these
625 chemical reactions will take significant time, >10 years to dissolve into water, and >100 for
626 the precipitation of carbonate minerals, an understanding of whether seismic methods could
627 offer effective monitoring of these subsurface changes is essential. The modelling approach
628 here could be extended to investigate different scenarios and the resulting elastic properties.
629 Such models would investigate the elastic properties of brine with significant carbon dioxide
630 dissolved within, and the host reservoir with carbonates precipitated within the pore space,
631 both of which are likely to modify the elastic properties.

632 The most common seismic monitoring methods for oil and gas production (Djuraev et al.,
633 2017) and for CCS projects (Ma et al., 2016) utilise active source reflection surveying, requiring
634 baseline and monitor seismic surveys to map plume migration. Acquisition of monitor seismic
635 surveys is a large expenditure for carbon capture sites, with typical individual survey costs
636 being in the 10's of millions (Waal and Calvert, 2003). Other seismic monitoring methods that

637 do not rely on follow up surveys may prove more cost-effective than these traditional
638 techniques. Recent advances in both land and ocean bottom seismic receiver technology have
639 allowed for the application of passive seismic techniques for monitoring purposes. Seismic
640 arrays are typically deployed for an extended period of time, and as such the continuous
641 records of ambient seismic noise can be used to develop subsurface imagery through
642 interferometry (e.g. Cao and Askari (2019)), as well as for seismic event detection, location
643 and characterisation (Verdon et al., 2010). Seismic event detection and characterisation is
644 particularly important before, during and post-injection. It is possible to both distinguish
645 whether detected seismic events are natural or induced and track the impact of injection on
646 reservoir integrity (Payre et al., 2014). Passive seismic monitoring is regularly employed
647 onshore, however applying these techniques offshore can be difficult due to the logistical
648 challenges in dense instrument deployment and levels of ambient seismic noise offshore. To
649 account for this, recent studies utilising passive seismic techniques for offshore monitoring
650 have incorporated array processing techniques on a combination of both onshore broadband
651 seismometers and offshore geophones, allowing for previously uncatalogued events to be
652 detected (Zarifi et al., 2022; Jerkins et al., 2023). The modelled results here demonstrate
653 changes in elastic properties that are equally as important when considering the application
654 of passive seismic methods (Eisner et al., 2009). Further work could extend the modelling to
655 consider whether the modelled changes in compressional velocity could be detected in
656 different array configurations and noise environments (e.g, Stork et al. (2018)).

657 Our work on timeshifts does not account for the affects that heterogeneities such as thin beds
658 may have. Thin beds and low frequencies can both cause tuning effects to occur within 4D
659 seismic data sets (MacBeth et al., 2020), and if a thin bed is < tuning thickness can be assumed
660 that the timeshift signal drops to 0 (MacBeth and Izadian, 2023). Characterisation of the
661 heterogeneities within a storage complex and inclusion within the forward modelling
662 workflow would allow for more accurate timeshift results.

663 The Q factor is the measure of attenuation observed within seismic waves (Jyothi et al., 2017).
664 Changes in reservoir fluids have been shown to modify the value of Q (Joel et al., 2003).
665 Measuring the Q factor within a 4D seismic dataset could provide viable ways to monitor
666 change in carbon dioxide saturation within reservoirs.

667 1.7.6 *Conclusions*

668 We have used a stochastic Gassmann fluid substitution model to investigate the potential
669 seismic response of potential storage reservoirs on the UKCS. We parametrise the models'
670 using data from multiple wells to evaluate the implications of varying reservoir porosity of
671 carbon dioxide and hydrogen on the elastic properties and hence geophysical responses.

672 Our results show that while seismic methods are valid for monitoring carbon dioxide plume
673 migration, in key reservoir intervals on the UKCS likely changes in elastic properties, and
674 acoustic impedance, may be lower than that reported and close to detection limits. Extra to
675 relying on 4D seismic and amplitude comparison, AVO and timeshift analysis may also be
676 required to understand plume migration for geology where its acoustic impedance responses
677 are calculated to be low (<4%).

678 We also calculate the results for hydrogen in the subsurface to understand responses of
679 possible native hydrogen reservoirs or for hydrogen storage sites. Results for hydrogen show
680 that it affects the elastic properties in a similar way to natural gas (from 100 to 0 % water
681 saturation), and thus we can expect typical industry quantitative seismic techniques to be
682 applicable for both the exploration of native hydrogen reserves and for the monitoring of
683 hydrogen in storage.

684 We also discuss the difference in our results from published literature for the UKCS. While we
685 cannot comment on the rightness of our results compared with those in published reports for
686 target CCS sites, we can be open and transparent with our scientific practices, making all our
687 code and input data available at the time of publication. We suggest that this should be the
688 case for subsurface infrastructure of national importance, especially when CCS sites are
689 government-funded and not-for-profit activities, as it allows for proper scrutiny and scientific
690 process to be undertaken.

691

692

693

694 1.8 Tables

Reservoir	Assumed depth (m)	Pressure (MPa)	Temperature (c)	Density (Kg/m ³)	Bulk modulus (Gpa)
Leman	2447	30.4	72.5	173.6 (Methane)	0.068 (Methane)
				18.3 (Hydrogen)	0.050 (Hydrogen)
				781 (Carbon dioxide)	0.199 (Carbon dioxide)
Bunter	1406	15.2	57	100 (Methane)	.024 (Methane)
				10.3 (Hydrogen)	.023 (Hydrogen)
				641 (Carbon dioxide)	.068 (Carbon dioxide)
Helsby	792	9.68	30	71.2 (Methane)	.014 (Methane)
				7.3 (Hydrogen)	.014 (Hydrogen)
				763 (Carbon dioxide)	.105 (Carbon dioxide)

695 TABLE 1 – FLUID ELASTIC PROPERTIES AT RESERVOIR CONDITIONS FOR LEMAN, BUNTER AND HELSBY FORMATIONS

696

697

Cut off parameter	Minimum Value	Maximum Value
Volume Shale (Vshale)	0%	30%
Porosity (Φ)	5%	NaN
Bulk density (ρ_{bulk})	2.00 g/cm ³	2.67 g/cm ³

698 TABLE 2 – RESERVOIR CUTOFF VALUES FROM DIFFERENT ROCK PROPERTIES

699

700

701

702

Formation	Stochastic Porosity Groups (Φ %)
Leman	7, 9, 11, 13, 15, 17, 19
Helsby	14, 16, 18, 20, 22, 24, 26
Bunter	19, 21, 23, 25, 27

703 TABLE 3 – POROSITY GROUPS OF CHOSEN STRATIGRAPHY FOR STOCHASTIC ANALYSIS

704

705

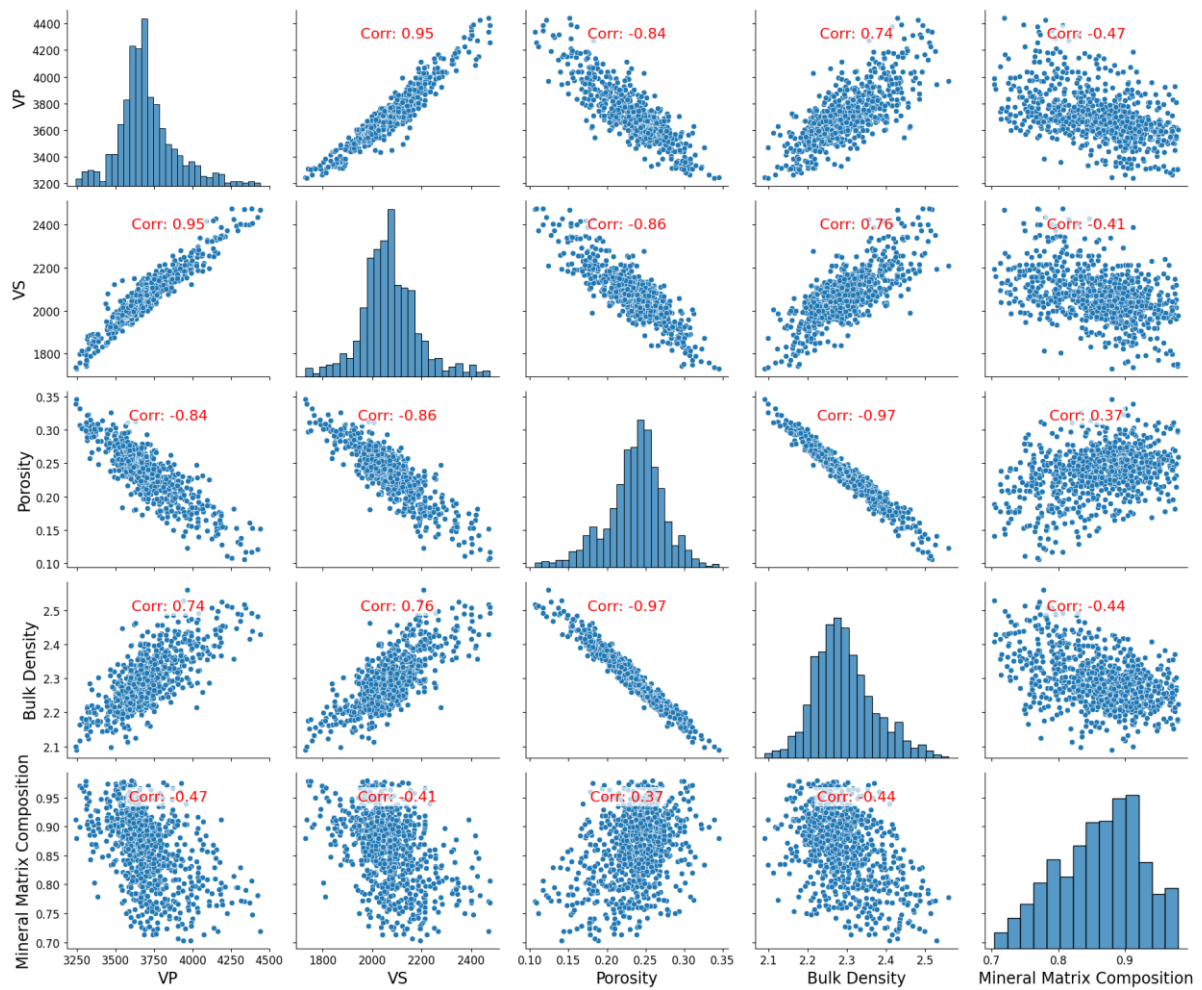
706

Stratigraphy	Calculated AI Change p50 (Water saturation 20%)	Literature Ai change	Calculated AVO (Rc) % Change Difference between Near stack – Far stack offsets	Timeshift	Notes
Leman (Φ 15)	-8 (Figure 5)	Not quantified but 'Very poor' (James et al., 2016b)	Res – Res: 38.2 Seal – Res: 22.2	Nan	Seal (Zechstein) may cause an issue
Bunter (Φ 23)	-6 (Figure 6)	12 – 20% (BEIS, 2021)	Res – Res: 25.4 Seal – Res (Claystone): 4.48 Seal – Res (Evaporite):-23.5	0.877ms (Figure 12)	No data given by (BEIS, 2021) on how value calculated,
Helsby (Φ 16)	-2 (Figure 7)	Not quantified, but 'Maybe detectable' at 60% carbon dioxide saturation (Green and Grammer, 2016)	Res – Res: -3.32 Seal – Res:0.91	Nan	

707 TABLE 4 INVESTIGATED STRATIGRAPHY WITH RESULTS FOR SELECT POROSITY. RESULTS FROM THE LITERATURE ARE ALSO

708 PRESENT

709 1.9 Appendix



710

711 APPENDIX 1 CROSS PLOT OF WELL ELASTIC AND MINERALOGICAL PROPERTIES OF THE BUNTER SANDSTONE RESERVOIR

712 SECTION FROM WELL 42/25-D3

713

Well	Formation	Depth
42/25d-3	Bunter SST	1406 - 1538 m
110/13b-21	Helsby SST	2600 - 2680 m
43/28a-3	Leman SST	
44/23b-11	Leman SST	
44/27-1	Leman SST	
47/10-8	Leman SST	
48/12a-7Z	Leman SST	
48/2b-3	Leman SST	
49/20a-7	Leman SST	
49/28-18	Leman SST	

714 APPENDIX 2 WELL DATA UTILISED WITHIN STUDY

715 1.10 Acknowledgements

716 1.10.1 Author contributions

717 Barnett (conceptualization, data curation, formal analysis, investigation methodology, project
718 administration, visualisation, writing – original draft, writing – review and editing), Ireland
719 (conceptualization, funding acquisition, supervision, writing – review and editing), Van der
720 Land (supervision, writing – review and editing), Dunham (writing – review and editing)

721 1.10.2 Funding information

722 Hector Barnett's PhD is funded through the Centre for Doctoral Training (CDT) in Geoscience
723 and the Low Carbon Energy Transition.

724

725 1.10.3 Data availability

726 All data generated and code used within this manuscript is available at
727 <https://figshare.com/s/01c10efe1839c03c28ff>

728 Well data were provided by the North Sea Transition Authority under an Open Government
729 Licence. Data were interpreted using SLB's Petrel and Techlog software which was provided
730 under an academic licence.

731

732 1.11 Bibliography

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